

**An Experimental and Modeling Study of the Combustion of Aromatic Surrogate Jet Fuel
Components**

BY

SOUMYA GUDIYELLA

B.Tech, Osmania University, Hyderabad, India, 2006

THESIS

Submitted as partial fulfillment of the requirements for the degree of Doctor of Philosophy in
Chemical Engineering in the Graduate College of the
University of Illinois at Chicago, 2012

Chicago, Illinois

Defense Committee:

Kenneth Brezinsky, Chair and Advisor, Mechanical and Industrial Engineering
Randall J. Meyer, Chemical Engineering
Christos G. Takoudis, Chemical Engineering and Bioengineering
Suresh K. Aggarwal, Mechanical and Industrial Engineering
Robert S. Tranter, Argonne National Laboratory

This thesis is dedicated to my parents, Dr. Shivarani Siddula Gudiyella and Dr. Sukumar Gudiyella and my advisor, Prof. Kenneth Brezinsky; without their support and guidance this thesis would never have been possible.

ACKNOWLEDGEMENT

First and foremost I want to thank my advisor Prof. Kenneth Brezinsky for his continuous support and guidance, for the past five years. I thank him for teaching me the basics of conducting research, for providing me the freedom to experiment with different hypotheses, and for guiding me in bringing these hypotheses to fruition. The ideas presented in most of the sections of this thesis are elaborated views of the key points of our discussions.

I thank the committee members, Dr. Robert S. Tranter (Argonne National Laboratory), Prof. Christos G. Takoudis, Prof. Suresh K. Aggarwal and Prof. Randall Meyer for their time and guidance and for providing advice which helped in improving this thesis. I would also like to thank Dr. Tranter for the discussions that helped in improving the experimental measurements.

I want to thank Prof. Hai Wang from University of Southern California for the interesting discussions that provided me an extended perspective on modeling and led to the improvement of m-xylene oxidation model.

I want to thank my colleague, Tom Malewicki for his help in conducting the m-xylene experiments. I want to thank Alex Fridlyand for his help in building an accompanying experimental set-up for faster completion of 1,3,5-trimethylbenzene experiments.

I want to thank the former students of this lab, Dr. Andrea Comandini, Dr. Raghu Sivaramakrishnan, Dr. Ashwin Raman, Dr. Brad Culbertson and Dr. Stephen Garner. I thank Dr. Andrea Comandini for providing several valuable insights into modeling of polycyclic aromatic hydrocarbons and for building an experimental set-up for measuring the polycyclic aromatic hydrocarbons. I thank Dr. Raghu Sivaramakrishnan for teaching me the basics of modeling and Dr. Ashwin Raman for teaching me the usage of chemical kinetic modeling software. I thank Dr. Brad Culbertson for teaching me how to plan and conduct the experiments. I thank Dr. Stephen Garner

for helping me with the temperature calibration experiments and also for helping me in repairing the malfunctioned equipment over the course of my experiments.

I want to extend my thanks to my family and friends for their continuous support during these five and half years. Specifically, I would like to thank my parents, Dr. Shivarani Siddula Gudiyaella and Dr. Sukumar Gudiyaella for their encouragement and support and also for providing favorable circumstances for successful completion of my Ph.D. They have been great sources of inspiration for me and will remain so. I would also like to thank my uncle, Mr. Pavan K. Gudiyaella and my aunt, Mrs. Jessica D'Amico who have been my family here in Chicago. They taught me how to adapt to the American culture and provided me a sense of family away from my home. Among my friends, I would specifically like to thank Mrs. Mythili Kottalanka and Mrs. Sumithra Ramanujam for their patience and their timely and friendly advice.

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SUMMARY

Jet fuels comprise a major share of liquid transportation fuels and are used to power both civilian and military aircraft. Rapid growth of the aviation sector has led to increased consumption of jet fuels, caused increased emissions of carbon, nitrogen, sulfur species and a number of volatile organic compounds and a wide range of particulate matter. These emissions cause significant environmental damage and the inhalation of particulate matter is hazardous to human health.

A direct experimental and numerical study of jet fuels is not feasible because jet fuels consist of several hundreds of chemical components belonging to different chemical classes. For example, a speciation experimental study would require the quantification of the decay of each of these chemical species present in jet fuels which would make the experiments impossible. The numerical study would require development of the chemical kinetic pathways for the decay of each of these species which would make these models for jet fuels voluminous and the size of these models will be too large for the current computational resources. In addition to this, thermochemical data of most of the jet fuel components needs to be developed or improved so that it can be used in chemical kinetic models.

Hence, a simplified approach was followed in conducting the experiments and developing a chemical kinetic model for the combustion of jet fuels. Experiments and models were developed for surrogates of jet fuels. These surrogates consisted of three or four component chemical mixtures of a particular composition such that they mimic the physical and chemical nature of the jet fuel. Two surrogate fuels were chosen for this project and these are called the 1st and 2nd generation surrogates. The 1st generation surrogate is comprised of iso-octane, n-decane and toluene. The 2nd generation surrogate is comprised of iso-octane, n-dodecane, n-propylbenzene and 1,3,5-trimethylbenzene. In the present work, the combustion chemistry of the aromatic surrogate fuel

components, n-propylbenzene, 1,3,5-trimethylbenzene and m-xylene was studied. The combustion chemistry of n-alkane and iso-alkane components of the jet fuels is being studied by another researcher from this laboratory. The species, m-xylene was also studied so that it could be integrated into the 1,3,5-trimethylbenzene oxidation model. The species, toluene, has been previously studied in this laboratory and hence the chemistry of this species has been adapted from the prior work. This project was executed in three correlated approaches

- 1) **Development of an experimental database:** Experiments were conducted in the High Pressure Single Pulse Shock Tube on aromatic surrogate fuel components of jet fuels which are m-xylene, 1,3,5-trimethylbenzene and n-propylbenzene for pressures of 20 – 60 atm, for temperatures ranging from 900 – 1800 K and for different equivalence ratios $\phi = 0.5, 1, 2$ and ∞ . Hence, an experimental database for the combustion of these three aromatic surrogate fuel components is now available for different temperatures and pressures.
- 2) **Development of a thermochemical database:** The products formed from the oxidation of these aromatic fuels were analyzed both qualitatively and quantitatively by using GC and GC/MS. Several volatile organic compounds (VOC's) and polycyclic aromatic hydrocarbons (PAHs) were also measured in the products. Since, the compounds formed from the fuel breakdown are now known, the thermochemical database for these species was developed either from the sources available in literature or by using group additivity based estimates or density functional theory.
- 3) **Development of a chemical kinetic validation database:** A detailed chemical kinetic model was developed for each chemical species so as to include the chemical kinetic pathways responsible for the formation of these VOCs and PAHs from the fuel (step 2). This model was not only validated against our experimental data but also for other experimental data available in literature, so as to develop a comprehensive validation database.

In addition to steps 1, 2 and 3, oxidation experiments of jet fuel, Jet-A POSF 4658 and 1st and 2nd generation surrogate were conducted in the laboratory by another researcher and excellent agreement was observed when the chemical reactivity of surrogate fuels and the jet fuels were compared. The results imply that the chosen surrogate fuel is successful in replicating the combustion behavior of jet fuels. Hence, in the present work, an experimental, thermochemical and chemical kinetic database was developed for combustion of aromatic surrogate fuel components of jet fuels which can later be integrated with models for n-decane and iso-octane so as to provide a comprehensive model for the combustion of jet fuels and surrogate fuels.

1. INTRODUCTION

1.1. Scope and Outline

Energy is one of the most important needs of the humanity and it is used to operate devices which help in improving our standard of living. For example, energy is required in various sectors of modern life like transportation, food production, communications, lighting and other basic amenities.¹ However, energy is available in nature in a very crude form and it has to undergo conversion processes that impart the characteristics necessary for using energy in practical devices. The need for energy sources rises as the standards of living are improved. In addition to this, the rapid industrialization and growth in the developing countries, has further increased the usage of energy.¹

One of the most abundant and readily convertible forms of energy is fossil fuels. The usage of fossil fuels has increased tremendously in the past few years, which has led to the depletion of fossil fuels at faster rates. The world energy consumption (in millions tonnes of oil equivalent) is shown in Fig 1, for the year 1970 and the projections are drawn until 2030^{1,2}. From the graph we can observe that the trends of energy consumption continue to increase. There are also some environmental issues caused by the extensive use of fossil fuels. For example, one of the greenhouse gases, CO₂, which is emitted during the combustion of fossil fuels, results in global warming. Another example is the formation of soot, which is a byproduct of incomplete combustion. Inhalation of soot particles causes adverse health effects which are both carcinogenic and mutagenic. Hence, the combined effects of the increased depletion of the fossil fuels and environmental pollution have encouraged the scientific community worldwide to provide viable solutions to these problems.

Few of the solutions are

- 1) Discovering alternative sources of energy and developing the technologies to assist the efficient conversion of energy from these resources to usable form.
- 2) Reducing the formation of the pollutants during the combustion of fossil fuels not only reduces environmental pollution but also helps in achieving higher efficiency of conversion of energy to a usable form.

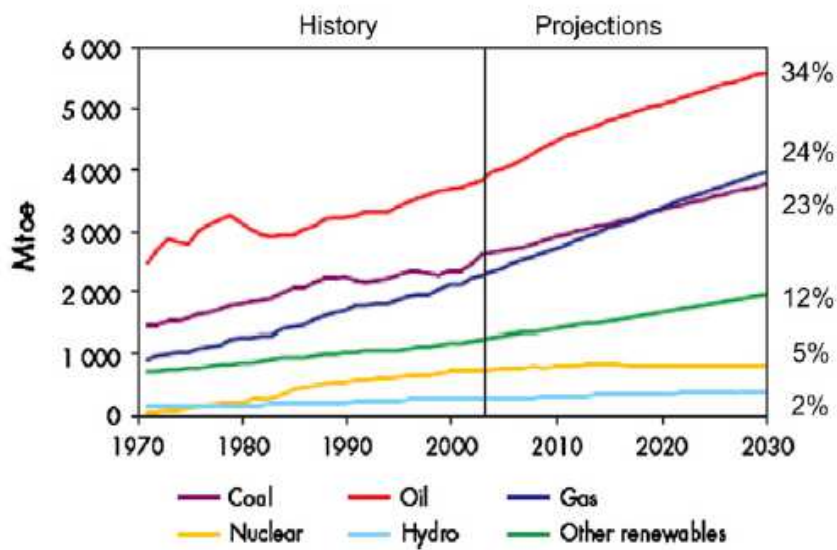


Fig 1. World energy consumption since the year 1970 and projections towards the year 2030¹.

1.1.1. Alternative Sources of Energy

Alternative sources of energy include nuclear power and renewable means such as hydro, geothermal, wind, solar power and biomass¹. Despite the availability of such a wide range of renewable resources, the production of energy through these resources is significantly minor³. The total primary energy supply by fuel is shown in Fig 2. From the figure, it can be observed that the major contribution to energy production is from fossil fuels (such as coal, oil and natural gas). The percentage contribution of each of these sources to the production of energy is shown for the years 1973 and 2009 in Fig 3. From comparison of the two pie diagrams shown in Fig 3, it can be observed that the total production of energy from fossil fuels has increased from about 5292 Mtoe (million tonnes of oil equivalent) in 1973 to 9829 Mtoe in 2009 (calculated by multiplying the total Mtoe of that particular year with combined percentage contribution of coal, oil and natural gas to the total energy supply). There is also a significant increase in utilizing nuclear power for energy from 55 Mtoe in 1973 to 705 Mtoe in 2009. The use of biofuels has almost doubled from the year 1973 to 2010, from 623 Mtoe to 1239 Mtoe, but it still contributes to a very minor share of the energy production. The percentage contribution of the hydropower, geothermal, solar and wind energy to the total energy production is minute when compared to the contribution of fossil fuels to the total energy supply. All these statistics indicate that fossil fuels will continue to be major contributors to energy production at least for a significant amount of time, until efficient conversion technologies could be built for the large scale utilization of the renewable sources for the production of energy.

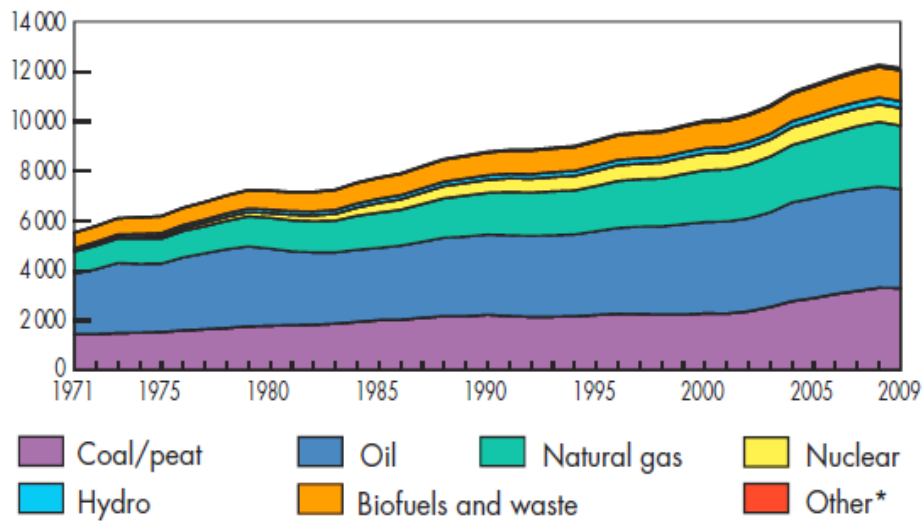


Fig 2. Total primary energy supply (TPES) from 1971 to 2010 by fuel (in Mtoe) ³.

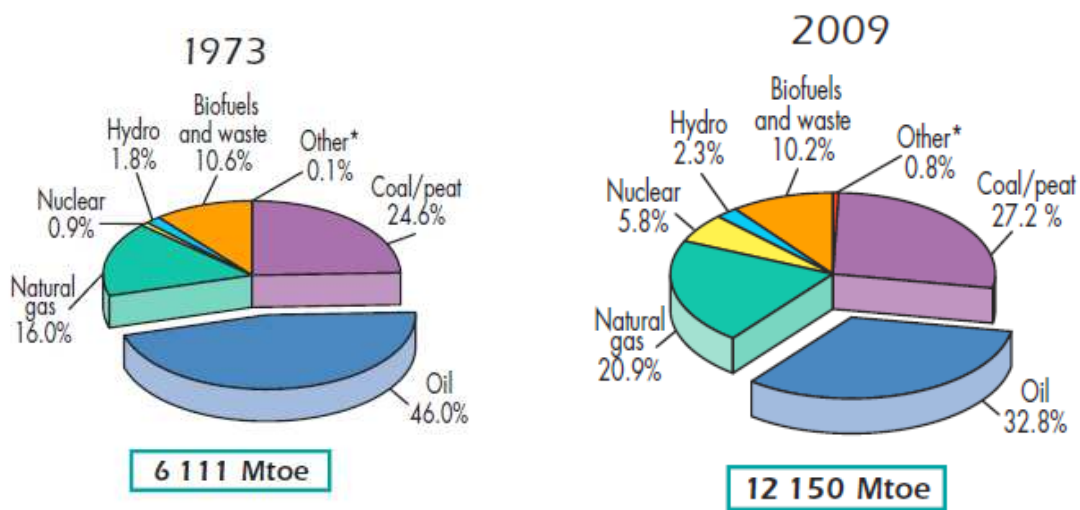


Fig 3. Fuel shares of TPES ³.

1.1.2. Achieving Higher Efficiency from the Fossil Fuels

Since fossil fuels will remain the significant contributors to the production of energy for the next few decades, efforts have been made to reduce the CO₂ emissions. For example, power plants are now using increasingly more natural gas instead of coal to generate electricity. The advantage of using natural gas is that it leads to an increase in efficiency and also produces lower CO₂ per unit chemical energy due to higher hydrogen content. It also produces lower NO, CO, SO_x and particulate matter. In recent years, significant improvements have been made in the carbon dioxide capture and sequestration technologies that decarbonizes power generation plants burning heavy hydrocarbons. Low carbon fuels can also be produced from the captured CO₂¹.

Another area where fossil fuels are widely used other than electricity generation is the transportation sector. Liquid transportation fuels such as jet fuels, gasoline and diesel fuels are produced from petroleum. Currently about 96% of the energy needs of the transportation sector are met by fossil fuels, which contribute to a great fraction of CO₂ and soot emissions. Unlike for power plants, decarbonization technologies cannot be used in transportation vehicles. Hence a different strategy has to be employed in reducing the emissions.

Among the liquid transportation fuels, aviation fuels constitute a major share. Rapid globalization has led to increase in air traffic over the past few decades. Projections by the aviation industry predict a future growth of about 5 % per year⁴. Increase in air traffic has also contributed to increase in emissions such as carbon, nitrogen, sulfur species and a number of volatile organic compounds and a wide range of particulate matter⁵. These emissions cause significant environmental damage and the inhalation of particulate matter is hazardous to human health. The key element in reducing the emissions is knowledge of the combustion chemistry of these fuels. The coupling of computational fluid dynamics with detailed chemical kinetics will provide insight into

the effect of the fuel composition on pollutant formation and thereby allows the chemical processes to serve as an optimization parameter for increasing the fuel efficiency and reducing the emissions. Apart from this, if we can quantify the combustion behavior of jet fuels in terms of the species composition of the fuel and the pollutants that could be emitted as a result of this fuel composition, the data thus obtained will serve as a benchmark in comparing the combustion behavior of other liquid fuels to jet fuels and help in interpreting the relationship between the change in fuel composition to the pollutants emitted.

1.1.3. Surrogate Fuels that Emulate the Jet Fuels

Quantification of the combustion behavior of jet fuels requires the development of an experimental and chemical kinetic validation database. The experimental database will provide information about the combustion characteristics of jet fuels such as the chemical reactivity, autoignition behavior and flame extinction limits. The kinetic database will also provide the chemical pathways for the formation of various products. The development of such an extensive validation database is a challenging task because of the complex chemical nature of jet fuels. Jet fuels are gasoline and kerosene based fuels and they consist of several hundreds of chemical components.

The jet fuel sample was analyzed using the two dimensional GC x GC system at UIC. Using the two dimensional gas chromatographic (GC x GC) technique the components of the jet fuel sample were separated using two columns of different selectivity (RTX-5 and RTX-17), which were connected in series via a thermal modulator. The sample was injected into the first chromatographic column, which is also called the primary column (RTX-5). Molecules eluted from the primary column were trapped or periodically sampled by a modulator. The modulator injected these trapped

components onto a second column (RTX-17) at regular intervals. These fractions were separated in the second column and eluted into the detector⁶. The chromatograph of the jet fuel sample analyzed using the 2-D GC x GC system is shown below, in Fig 4. Each peak represents single species that was quantified.

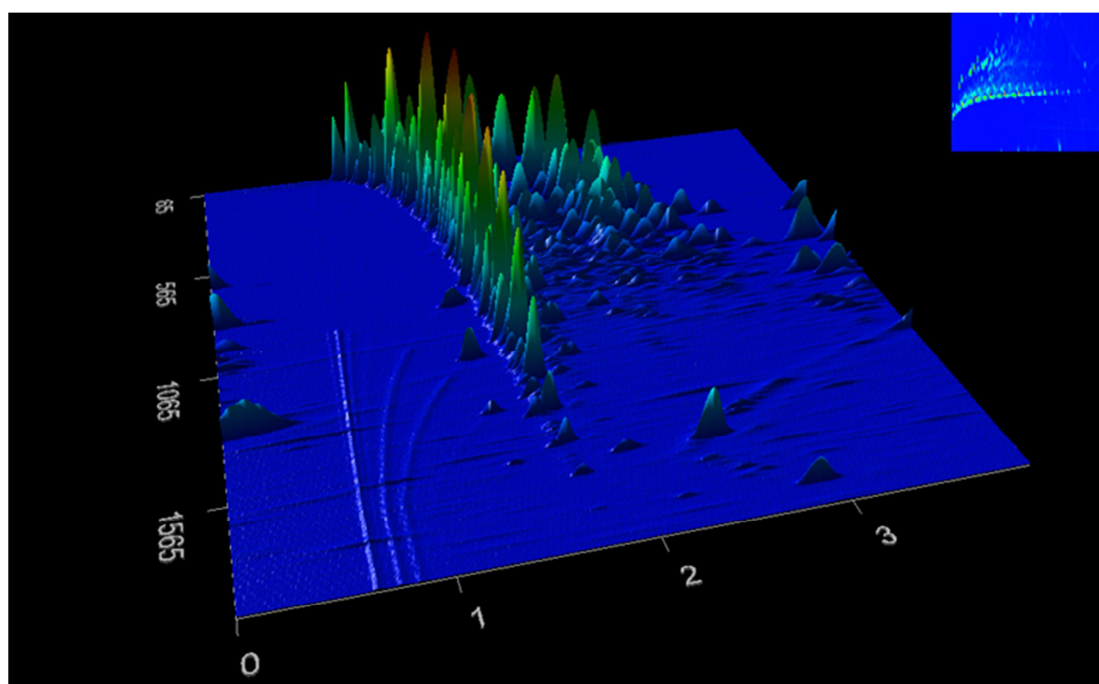


Fig 4. 2-D GC x GC chromatogram of JP-8 obtained at UIC.

Development of a composite fuel model based on a combination of each of these species is prohibitive because the size of the model would be too large for the current computational resources. In addition, the composition of the individual components of jet fuels vary in each geographic location because the composition of the refinery streams and the feed stocks vary with

time even though the overall chemical class composition of the jet fuel remains almost the same. The typical composition of the jet fuels is shown in Fig 5.

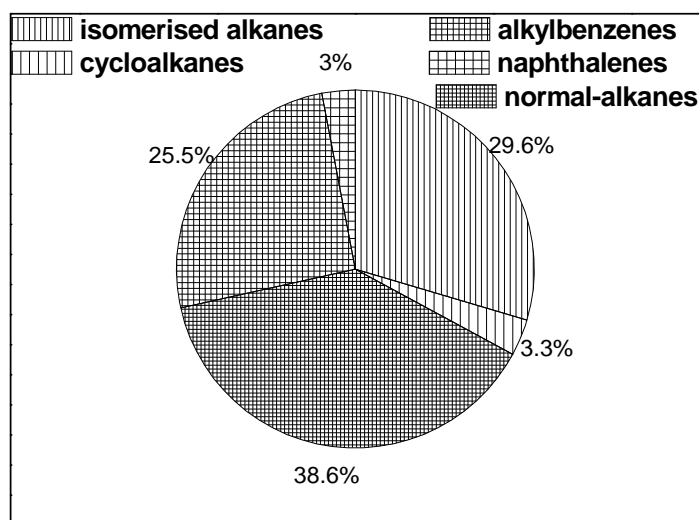


Fig 5. Molecular class composition of Jet-A POSF 4658⁷

The complex and variable chemical composition of jet fuels poses a problem in developing a detailed chemical kinetic model of the complete jet fuel. Hence, simplified “surrogate fuels” are chosen. A surrogate fuel is composed of a mixture of a few pure components such that it emulates the physical and chemical characteristics of the parent fuel. Hence, the main focus has been on developing the appropriate surrogate fuels for the aviation fuels and developing an experimental, thermochemical and chemical kinetic database for the combustion of individual surrogate fuel components, the surrogate fuels and representative jet fuels for the temperature and pressure conditions of practical combustion devices.

This project is a collaborative effort among different universities, which includes Princeton University, Pennsylvania State University, the University of Connecticut and the University of Illinois at Chicago. The project is sponsored by Air Force Office of Scientific Research (AFOSR), through the grant number FA9550-07-1-0515. This grant was awarded in 2007 Multi-disciplinary University Research Initiative (MURI) competition in the category of “Science-Based Design of Fuel Flexible Chemical Propulsion/Energy Conversion Systems”. The project title is, “Generation of Comprehensive Surrogate Kinetic Models and Valid Databases for Simulating Large Molecular Weight Hydrocarbon Fuels”⁸ and the principal investigator is Prof. Frederick L. Dryer from the Princeton University.

The selection of the surrogate fuel components and the composition of the surrogate fuels were determined predominantly by Prof. Dryer’s group at Princeton University. The surrogate fuel was chosen such that its molecular fragment groupings can adequately emulate the autoignition, heat release rate, adiabatic flame temperature, local mixing limited stoichiometric constraint, extinction and sooting behavior of jet fuels⁹. The components comprising the surrogate fuel were chosen to represent a few of the generic classes of molecular structure found in existing jet fuels. The structures of the selected surrogate components are shown in Fig 6 and Fig 7. The percent composition of each individual surrogate fuel component in the surrogate fuel was determined by matching against targets such as the sooting propensity, H/C ratio, average molecular mass and the derived cetane number (DCN)⁹. The derived cetane number measurements of the ‘prototype jet fuel’, Jet A POSF 4658, surrogate fuels and surrogate fuel component mixtures were performed using an ignition quality testing (IQT) apparatus. The name POSF 4658 refers to the specific batch of jet fuel and is named as such only for logistical purposes¹⁰. The empirical formula of POSF 4658 was determined experimentally using the Perkin Elmer 2400 Series II CHN Analyzer. The Threshold Sooting Index (TSI) is a direct measure of the sooting propensity and the TSI was

determined by using the smoke point technique¹¹. Over the course of this project two different surrogate fuels were chosen by the Princeton group for further examination. The agreement in the degree of emulation was closer for the second fuel than the first fuel. The first surrogate fuel matched only the DCN and the H/C ratio, whereas the second surrogate matched the DCN, H/C ratio, and molecular weight and TSI measurements when compared to that of POSF 4658. These surrogate fuels are called the 1st and 2nd Generation Surrogate. The composition of these surrogate fuels and the comparison with the combustion targets of each surrogate fuel and of Jet A POSF 4658 are shown in Table 1.

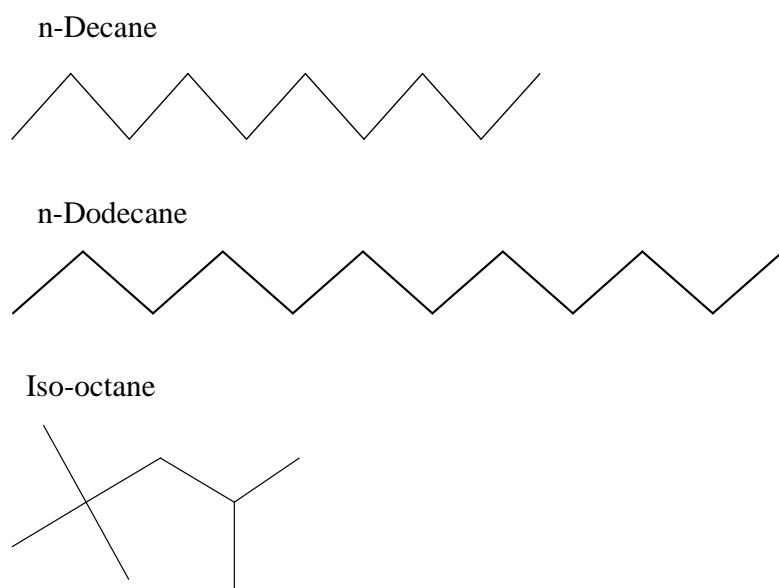


Fig 6. Aliphatic surrogate fuel components of jet fuels

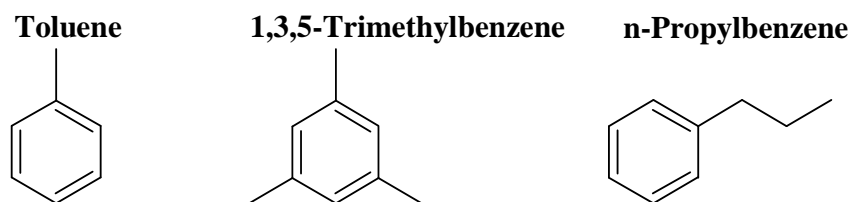


Fig 7. Aromatic surrogate fuel components of jet fuels

Table 1. 1st Generation and 2nd Generation Surrogate formulation and comparison of DCN, H/C, MW, TSI of surrogate fuels with that of Jet-A POSF 4658

Mole Fraction					MW			
					DCN	H/C	/gmol-1	TSI
Jet-A POSF 4658					47.1	1.957	142.01	21.4
1st Generation	n-decane	iso-octane	toluene					
Surrogate	0.427	0.33	0.243		47.1	20.1	120.7	14.1
2nd Generation	n-dodecane	iso-octane	1,3,5-trimethylbenzene	n-propylbenzene				
Surrogate	0.4	0.24	0.07	0.23	48.5	1.95	138.7	20.4

The degree of agreement in the combustion properties of the proposed surrogate fuels (1st and 2nd generation surrogate) and POSF 4658 was evaluated by experimental measurements in different devices, by research groups at the universities mentioned in the preceding paragraph. The high temperature and high pressure speciation measurements and chemical reactivity of these fuels were studied in the High Pressure Single Pulse Shock Tube (HPST) by Tom Malewicki from Prof.

Kenneth Brezinsky's group at University of Illinois at Chicago. The low temperature speciation measurements and chemical reactivity of these fuels was studied in a Variable Pressure Flow Reactor (VPFR) by Prof. Dryer's group at Princeton University. The chemical kinetic molecular diffusion coupling of POSF 4658 and POSF 4658 surrogate were evaluated by measurement of strained extinction limit of diffusion flames, by Prof. Yiguang Ju's group at Princeton University. The shock tube ignition delay experiments of these fuels were conducted by Prof. Oehlschlaeger's group at Rensselaer Polytechnic Institute, at high temperatures. The ignition delay experiments in the negative temperature coefficient (NTC) regime were conducted in a rapid compression machine (RCM) by Prof. Jackie Sung's group at University of Connecticut. The TSI measurement of these fuels was determined by Prof. Santoro's group at Pennsylvania State University.

The experimental measurements and the degree of emulation of the combustion behavior of Jet-A POSF 4658 by 1st and 2nd Generation surrogates are discussed in publications by Dooley et al.^{7,9} and Malewicki and Brezinsky¹². The 1st Generation surrogate matched the diffusion flame extinction limits and the chemical reactivity of jet fuel (in a variable pressure flow reactor) adequately well. The 1st generation surrogate (n-decane/iso-octane and toluene mixture) failed to emulate the two stage autoignition behavior exhibited by POSF 4658 in the Rapid Compression Machine study. Based on these experimental results it was proposed that including larger molecular weight alkanes and alkyl aromatics could lead to improvement in the surrogate performance.⁹ This observation has led to the development of the 2nd generation surrogate in which the species decane in the first generation surrogate was replaced by a larger molecular weight alkane, n-dodecane and two alkylbenzenes, n-propylbenzene and 1,3,5-trimethylbenzene were introduced. The composition of the 2nd generation surrogate is provided in Table 1. Experimental measurements of the improved surrogate fuel and POSF 4658 in different devices showed that both the fuels exhibit the same global combustion behavior. The only exception being that the 2nd generation surrogate also could

not emulate the two stage autoignition behavior in the Rapid Compression Machine (RCM) and the authors mentioned that this disparity requires additional elucidation of the experimental techniques used in obtaining the ignition delay data⁷. From the various studies conducted on the two surrogates, Dooley et al.⁷ proposed that the chemical reactivity of the jet fuel primarily depends on the composition of the fuel fragments (methyl, methylene and benzyl type groups) formed during the combustion of the jet fuel.⁷ Hence the only criterion needed for successful emulation of jet fuel combustion behavior by a surrogate fuel is that the chosen surrogate fuel should be able to produce the same composition of fuel fragments as the real jet fuel.

Now that the validation database of the experimental measurements of the combustion behavior of the surrogate fuels and the jet fuel is documented, the next step is to develop the chemical kinetic models for simulating shock tube oxidation experimental data for the 1st, 2nd generation surrogate. These models will also be used to model the results of oxidation experiments examining Jet-A POSF 4658.

The surrogate fuel and jet fuel models are developed by including the kinetics of the individual surrogate fuel components. The individual surrogate fuel components are n-decane, n-dodecane, iso-octane, toluene, n-propylbenzene and 1,3,5-trimethylbenzene. Several experimental measurements exist in literature for the combustion of aliphatic components like n-decane, n-dodecane and iso-octane^{13,14}. However, very limited experimental or kinetic data is available for the combustion of the aromatic surrogate fuel components like n-propylbenzene and 1,3,5-trimethylbenzene. Hence experiments were also conducted on the individual surrogate fuel components, n-propylbenzene, 1,3,5-trimethylbenzene, n-decane, n-dodecane and iso-octane in order to develop and also to extend the existing databases for the combustion of these fuel components, for varied experimental conditions. The experiments on n-decane, n-dodecane and iso-octane were conducted by another researcher in the laboratory as a parallel program. Chemical

kinetic models for the oxidation of these species were developed^{15,16} to simulate the shock tube experimental results. My contribution to this project was to conduct experiments on the aromatic surrogate fuel components, n-propylbenzene and 1,3,5-trimethylbenzene and to develop chemical kinetic models for the oxidation and pyrolysis of these species. Development of chemical kinetic models for these species is important because jet fuels are comprised of aromatics (15 %) and the presence of aromatic species leads to the undesirable formation of polycyclic aromatic hydrocarbons due to the presence of the phenyl ring in the chemical structure. Hence, another important reason for studying the combustion of the aromatic surrogate fuel components is that the pathways to the formation of PAH species could be analyzed and linked to the particulate matter emissions from the jet fuels.

In general, the side chains of the alkylbenzenes (in this case n-propylbenzene and 1,3,5-trimethylbenzene) are oxidized or pyrolyzed initially to shorter side chain length alkylated aromatics or non-alkylated intermediates. For example it is well known, that toluene is initially oxidized to form benzene, by losing the methyl group. Therefore, we can safely assume that a few of the major products from the combustion of 1,3,5-trimethylbenzene will be m-xylene and toluene. The structure of 1,3,5-trimethylbenzene and lower alkylated intermediates, m-xylene and toluene and the non-alkylated aromatic, benzene, is provided in Fig 8. We previously investigated the oxidation and pyrolysis of toluene in our laboratory and developed a detailed chemical kinetic model¹⁷⁻¹⁹. Hence, this model can be integrated into the 1,3,5-trimethylbenzene oxidation model. However, limited experimental or kinetic data is available for the oxidation of m-xylene at our experimental conditions. Hence we conducted oxidation and pyrolysis experiments on m-xylene, and also developed a kinetic model in order to integrate it into the 1,3,5-trimethylbenzene oxidation model. Oxidation and pyrolysis experiments of n-propylbenzene, 1,3,5-trimethylbenzene and m-

xylene have been conducted in the High Pressure Single Pulse Shock Tube at University of Illinois at Chicago.

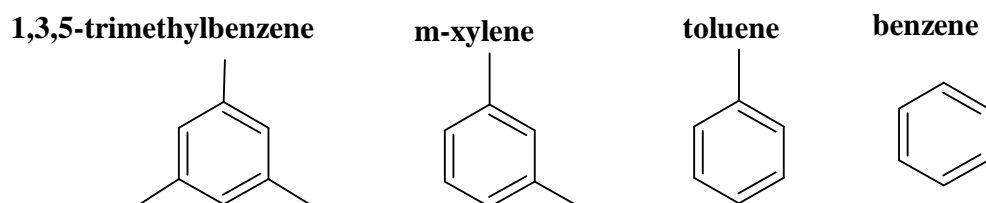


Fig 8. Structures of 1,3,5-trimethylbenzene, m-xylene, toluene and benzene

This introduction section provides only the overview of the project. The literature review for the species 1,3,5-trimethylbenzene, n-propylbenzene and m-xylene will be included in separate chapters wherein not only the experimental and modeling results but also the literature reports for each of these species will be discussed in detail. Therefore the topics that will be encountered in the subsequent chapters are fashioned in a specific way to be most relevant to the experimental and modeling results of the species being discussed.

A detailed discussion about the operating principles of the single pulse shock tube and the protocol followed in conducting the experiments is described in Chapter 2. The modeling software used and the basic principles of modeling are discussed in Chapter 3. The major findings in the experiments and the modeling studies of each of these species, n-propylbenzene (Chapters 4 and 5), m-xylene (Chapter 6 and 8) and 1,3,5-trimethylbenzene (Chapter 7 and 8) are then discussed.

2. EXPERIMENTAL APPARATUS

2.1. Introduction to Shock Tubes

The pioneering work in shock tubes was done by Vielle²⁰. Vielle made measurements of the speed of a pressure pulse in a 6-m cylindrical tube using a series of mechanical pistons along the tube and a rotating drum. He later on improved the experimental technique by dividing the tube into two sections with a thin diaphragm. Following the work of Vielle, later scientific advances in the development of shock tube were widely spread in time and rather disconnected. However, the shock tube was rapidly developed in the later 1940s and early 1950s and was mostly used for a variety of aerodynamic studies^{21–25}. During this period of time, the shock tube was not only used for qualitative measurements but also for quantitative measurements. For example, shock tube experimental studies were also conducted on measuring the rates of thermal dissociation of several simple diatomic molecules such as bromine (Br_2)²⁶ and oxygen (O_2)²⁷ and polyatomic molecules such as N_2O_4 ²⁸, NO_2 ²⁹, C_2N_2 ³⁰, N_2O ³¹ and NOCl ³² and various simple hydrocarbons. Since, then the shock tube has evolved into a useful tool to study physical and chemical processes at high temperature. There are several advantages in using the shock tube for studying chemistry

- 1) It instantaneously brings the test gas to a known steady high initial temperature and pressure which persists at this condition for a few hundred microseconds
- 2) Very high temperatures of the order of a few thousand K could be attained.
- 3) The gases are heated homogeneously in finite time without wall effects
- 4) The gases could be subjected to various pressures ranging from sub-atmospheric to a 1000 atm or higher
- 5) It could be conveniently used to study the chemistry of a variety of gases
- 6) It offers the flexibility to study both pyrolytic and oxidative chemistry

- 7) The progress of chemical reactions or physical processes, such as the relaxation of vibrational energy can be studied by including an optical device or some other means at some point along the tube

Even though the most of the kinetic research in shock tubes was primarily devoted to gas phase homogeneous systems, shock tubes were also used for heterogeneous kinetic studies. For example, Culbertson and Brezinsky investigated the heterogeneous kinetics of graphite particles with carbon dioxide and steam under high pressure conditions³³. The shock tube also provides an excellent environment for the study of nucleation and growth of particles from the vapor phase at high temperature. For example, Frenklach et al.³⁴ studied silicon particle nucleation and growth during gas phase pyrolysis of silane and soot particle formation behind shock waves from different hydrocarbon sources was investigated by Woiki et al.³⁵. Several important reviews of shock tube kinetics, have appeared earlier in the literature³⁶⁻⁴¹ and these studies provide a comprehensive and detailed view about the applications of shock tubes in chemical kinetics.

Even though the main thrust was focused on applying the shock tube for aerodynamic and high temperature kinetic studies, shock waves also find applications in several other fields such as geoscience, astrophysics, material synthesis and medicine^{42,43}.

2.2. Basics of a Shock Tube

The shock tube is a device in which a planar shock wave is produced. The shock tube consists of three sections, the driver, driven and the diaphragm sections. The driver section is filled with high pressure gas and the driven section is filled with low pressure test gas. The diaphragm separates the driver and the driven sections. After bursting of the diaphragm a series of event takes place which are described below and also shown in Fig 9.

- 1) A series of compression waves are formed in the driven section which rapidly coalesces to form the shock front. Simultaneously an expansion or rarefaction waves moves back into the driver section.
- 2) In the driven section, the experimental and the driver gas make contact at the 'contact surface' which rapidly moves behind the shock front.
- 3) The shock wave gets reflected from the end wall of the driven section and further heats the test gas to higher temperatures.
- 4) The rarefaction waves reflects from the end wall section of the driver section and the reflected rare fraction wave reaches the end wall section of the driven section and quenches the reflected shock wave.

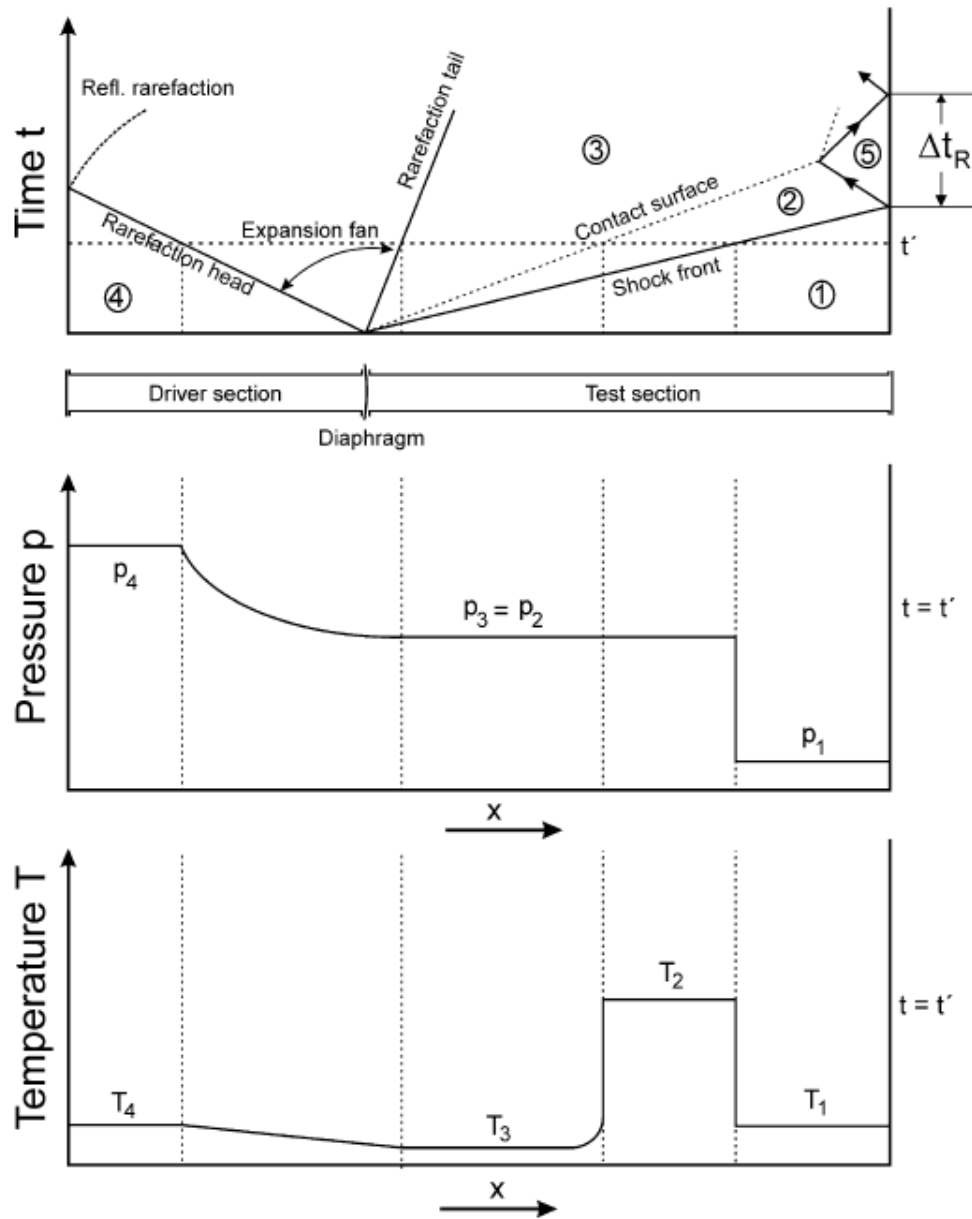


Fig 9. x - t Diagram of a simple shock tube. (1) Initial test gas, (2) shocked gas, (3) driver gas behind contact surface, (4) initial driver gas, (5) test gas subjected to reflected shock⁴².

The schematic of the shock tube, the pressure profile and the temperature profile along the shock tube, at a specific time, during the above mentioned sequence of events is shown in Fig 9.

The temperature and pressure are denoted by P and T , with the subscripts giving information about

the specific location within the shock tube. For example, P_1 and T_1 denote the temperature and pressure of the undisturbed test gas (region 1). P_2 and T_2 denote the temperature and pressure in the region between the shock front and the contact surface (region 2). P_3 and T_3 denote the temperature and pressure in the region between the contact surface and the rarefaction fan (region 3). P_4 and T_4 denote the temperature and pressure in the high pressure driven gas. P_5 and T_5 denote the conditions in the reflected shock region (region 5).

In most of the cases $T_4 = T_1$, since both the driven and driver section gases are at room temperature. The ratio in pressures, P_4 to P_1 determines the strength of the shock wave. The test gas temperature is initially raised from T_1 to T_2 after passing of the incident shockwave. After the incident shock wave is reflected from the endwall, the temperature of the test gas is further raised to T_5 (not shown in the temperature profile). In simple cases T_5 is about twice of T_2 .

2.3. The Single Pulse Shock Tube

The single pulse shock tube or the chemical shock tube was first developed by Glick et al.⁴⁴ to study the bond scission reactions of hydrocarbons. The modification in the single pulse shock tube when compared to the basic shock tube is the presence of a dump tank, in addition to the driver, driven and the diaphragm sections. The dump tank prevents multiple reflections of the shock wave and operates the shock tube in a single pulse fashion.

The advantage of using the single pulse shock tube over the basic shock tube is that conditions of instantaneous heating followed by rapid quenching of the reactive mixture after a short well defined reaction time by the cooling wave could be achieved. The pressure signal from one of the side-wall pressure transducers is shown in Fig 10 and it shows the instantaneous rise in pressure as a result of the arrival of the reflected shock wave and the drop in pressure after arrival of

the cooling wave after a short residence time. The shocked product samples can be withdrawn from a port located at the endwall section of the shock tube (region 5) and can be used for subsequent chemical analysis using Gas Chromatography and Mass Spectrometry. Hence, the shock tube has evolved into a scientific tool to study the chemical kinetics of various species over wide range of temperature and pressure conditions.

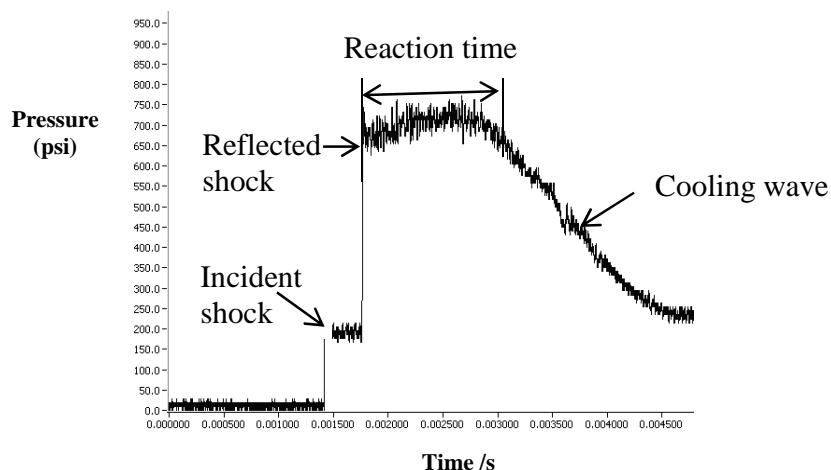


Fig 10. Pressure trace from a typical Single Pulse Shock Tube

2.4. The UIC High Pressure Single Pulse Shock Tube

The UIC High Pressure Single Pulse Shock Tube (HPST) has a similar construction as that proposed by Glick et al.⁴⁴. It also has a driver, driven, diaphragm and a dump tank section. One major difference in the construction of these two tubes is with regard to position of the dump tank. The shock tube design by Glick et al. had the dump tank positioned behind the high pressure driver

section whereas the UIC HPST has the dump tank situated adjacent to the diaphragm section and connected the driven section of the shock tube. A schematic of the UIC HPST is shown in Fig 11.

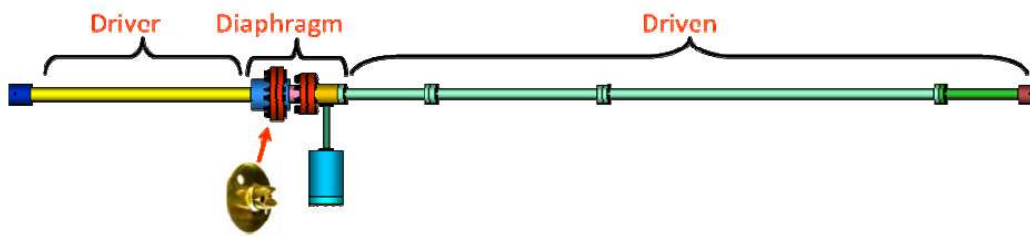


Fig 11. Schematic of the High Pressure Single Pulse Shock Tube (source Fiona Tranter, shock tube archive)

2.4.1. Outline

The essential features of a single pulse shock tube discussed in previous sections are also applicable for the High Pressure Single Pulse Shock Tube at UIC. A very detailed description of the design, construction and operation of the shock tube is presented in an earlier publication^{45,46}, hence only a brief outline will be provided here.

The driver section of the shock tube is a 60 in. long tube with a bore of 2 in. and a wall thickness of 1 in. The driven section is constructed in a modular fashion and consists of three pieces of interchangeable and variable lengths of 20, 40 and 80 in., all of which have a bore of 1 in. and a wall thickness of 1 in. These sections of variable lengths are connected to a transducer section,

which consists of eight transducer ports and a capped end wall section with a gas sampling port and a ninth transducer port. The current driven section set-up of the shock tube consists of the 80 in. long section connected to the 21 in. transducer section, which leads to nominal reaction times on the order of 1.5 ms. The shock tube is a convergent area tube and increased shock strengths can be achieved due to the reduction of bore from 2 in. to 1 in. from the driver to the driven section. The dump tank placed just ahead of the diaphragm section on the driven side rapidly quenches the reflected shock wave, thereby permitting the shock tube to be operated in a single pulse fashion. The driver section and the various parts of the driven section were machined from a solid bar of 17-4 PH stainless steel. The following sections will discuss in detail, how various experimental parameters such as reaction pressure, temperature, reaction times and species concentrations were determined.

2.4.2. Shock Velocities, Reaction Times and Reaction Pressures

The shock velocities are calculated from the response of six piezoelectric pressure transducers (PCB model nos. 113A23 [0-10000 psi] and 113A22 [0-5000 psi]) located in the side wall of the transducer section. The first transducer that is placed farthest from the endwall section is used as a trigger channel and signals are subsequently collected once the incident shock wave triggers this transducer. The output from the transducers is fed to an in-house data acquisition system (DAQ) for subsequent operations performed by the DAQ. The in-house data acquisition software written in Labview by Dr. R. S. Tranter, is used to extract the time intervals and the reaction time.

The shock velocities can be calculated from the known time intervals and the distances between the pressure transducers. The shock velocities are shown as a function of the transducer

spacing in Fig 12. The uncertainty in the measurement of the shock velocities is $\leq 1\%$. To get the best measure of the reflected shock wave velocities, the shock velocities obtained using the six sidewall transducers are extrapolated to the endwall. The extrapolated endwall velocities are then used to determine the temperature of the reflected shock using the chemical thermometer technique, which will be discussed shortly. The extrapolated endwall velocities thus give a best estimate of the temperature conditions that persist in the endwall section, right where the samples are drawn for subsequent analysis.

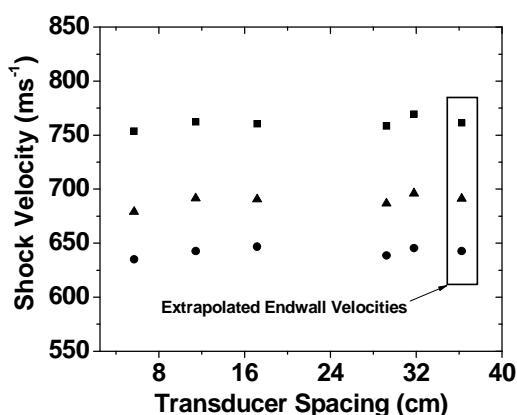


Fig 12. Shock velocities shown at different locations of the transducer section, for three shocks.

The pressure trace from the endwall pressure transducer (P9) is shown in Fig 13 and it is a plot of pressure (psi) vs. time (s). The reaction time is the time interval between arrival of the reflected shock wave at the end wall pressure transducer and the time at which reaction pressure reaches 80% of the maximum pressure due to quenching by the rarefaction wave. This is shown by the ‘RxnTime’ line in the figure and the reaction time is 1.54863 ms. The reaction pressure is the

average maximum pressure that is attained by the reflected shock wave during the reaction time and is denoted by P_{\max} . The times at which the shock wave arrives at the pressure transducers is also recorded by the DAQ and can be seen in the time /s section of the figure.

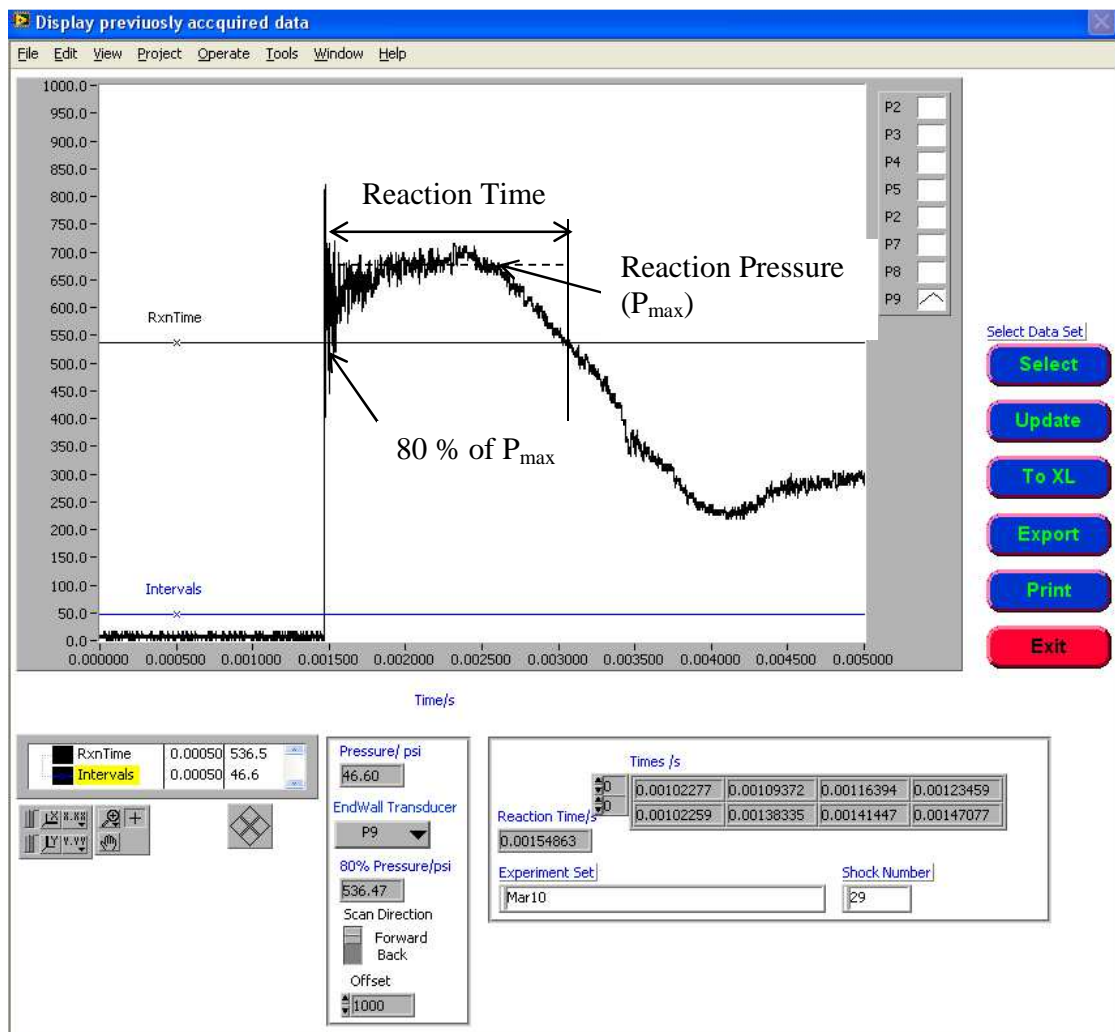


Fig 13. A typical pressure profile recorded by the endwall pressure transducer P9.

2.4.3. Reaction Temperature

2.4.3.1. Temperature from Ideal Shock Tube Theory

Apart from shock velocities and reaction time another important experimental parameter is the reaction temperature. The temperature in the reaction zone must be accurately known to evaluate the experimental data and to simulate the experimental results. The reaction temperature could be calculated from standard shock tube equations. These equations require the experimental parameters such as shock wave velocity and initial temperature and pressure conditions to compute the temperature in region 5.

Ideal Shock Tube Theory is usually used to describe the gas flow and the conditions of temperature, pressure and density in a shock tube after bursting of the diaphragm. This theory is based on the assumptions that gas flow is inviscid and adiabatic. It also assumes that the sequence of events that take place after bursting of the diaphragm is instantaneous and the gases inside the shock tube can be described by ideal gas equation of state. The theory also assumes that there are negligible heat losses by conduction, radiation and convection, due to the short residence time, low emissivity and inviscid nature of the gases. If the initial conditions in the driven section of the shock tube, such as T_1 , P_1 , and ρ_1 are known, then the conditions in the reflected shock region, T_5 , P_5 and ρ_5 can be determined by using the equations derived from Ideal Shock Tube Theory^{42,43}. Only the equation used to calculate the temperature in the reflected shock region will is provided below. More detailed information about the derivation can be obtained from Gaydon and Hurle⁴².

$$\frac{T_5}{T_1} = \frac{\{2(\gamma-1)M_1^2 + (3-\gamma)\}\{(3\gamma-1)M_1^2 - 2(\gamma-1)\}}{(\gamma+1)^2 M_1^2}$$

where γ = specific heat of the test gas

$$M_1 = \frac{W_s}{a_1}$$

$$a_1 = \sqrt{\frac{\gamma P_1}{\rho_1}}$$

Mach number, M_1 is the ratio of velocity of shock wave in the region (W_s) to the speed of sound in the same region (a_1) and T_1 , P_1 , and ρ_1 denote the temperature, pressure and density, respectively.

2.4.3.2. Chemical Thermometers

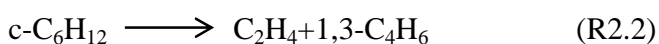
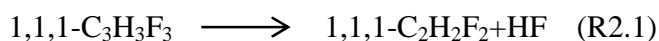
However, these equations are valid up to relatively modest pressures and temperatures and for our experimental conditions, which are at high pressures and high temperatures; the temperature computed using these ideal equations may not give a precise value due to non-ideal gas dynamic effects during propagation of the shock wave. In such cases when the temperature in the reaction zone cannot be computed accurately from the ideal shock tube equations, the temperature in the reflected shock region is determined using the chemical thermometer technique, wherein the reflected shock velocities are correlated to the temperature determined from chemical reactions in the test section. The temperature determined using the chemical thermometer is referred to as the ‘chemical’ temperature. The temperature determined using the ideal shock tube relations is referred to as the ‘ideal’ temperature.

Three chemical thermometers, cyclohexene, 1,1,1-trifluoroethane (TFE) and carbon disulfide were used for a combined ideal temperature range of 1100 to 2388 K. The use of three chemical thermometers enabled us to make measurements over a wide ‘ideal’ temperature range of 1100 – 2388 K. Cyclohexene decomposes unimolecularly in the ideal temperature range of 1100 to

1176 K TFE decomposes unimolecularly in the ideal temperature range of 1253 to 1446 K. CS₂ decomposes in the ideal temperature range of 2109 to 2388 K. The decomposition of carbon disulfide is not unimolecular and a different procedure was adopted to determine T₅ when CS₂ is used as a thermometer. The procedure for determining the temperature behind the reflected shock region (T₅) using each of these chemical thermometers is described in the sections below.

2.4.3.2.1. TFE and Cyclohexene

The rate coefficient parameters for the decomposition of TFE and cyclohexene are critical in determining the temperature. HF elimination from TFE and retro-diels-alder decyclization of cyclohexene have well characterized high pressure limit rate constants and occur in a unimolecular fashion, as shown in reactions, R2.1 and R2.2.



The rate constant for (R2.1) is taken from Tsang and Lifshitz, who studied the unimolecular decomposition of TFE in a single pulse shock tube at 2.5 bars and a temperature range of 1050 – 1200 K⁴⁷. They also performed an RRKM calculation and obtained k_∞ for two ΔE_{down} values of 500 and 1000 cm⁻¹. The difference in the calculated temperature when either of these rate constants is used is no more than 10 K. Since the authors recommended the use of the rate constant that was determined using the energy transfer parameter of 500 cm⁻¹, this rate constant was used to determine the temperature in the reflected shock region. The rate constant for (R2.2) is considered

from Kiefer and Shah.⁴⁸ The authors developed an RRKM model for R2.2 and from this model an expression for the high pressure limit rate coefficient has been obtained. The rate constants for reactions (2.1) and (2.2), which were taken from Tsang and Lifshitz⁴⁷ and Kiefer and Shah⁴⁸ are shown in equation (2.3) and (2.4).

$$k_{\infty(2.1)} = 4 \times 10^{15} \exp(-39000/T) \text{ s}^{-1} \quad (2.3)$$

$$k_{\infty(2.2)} = 4 \times 10^{15} T^{-0.005} \exp(-33467/T) \text{ s}^{-1} \quad (2.4)$$

(unit of k_{∞} : cc, mol, s⁻¹)

Dilute mixtures of TFE and cyclohexene (about 100 ppm) were prepared in bath gas Argon. Experiments were conducted in the High Pressure Single Pulse Shock Tube for reflected shock pressures of 25 and 50 atm. For each of the experiments the temperature behind the reflected shock wave was calculated from equation (2.5) based on the decomposition of the parent molecule.

$$T5 = \frac{\left(-\frac{E_a}{R}\right)}{\ln\left\{\left[\frac{\ln(1-x)}{At}\right]\right\}} \quad (2.5)$$

$$\text{Where } x = \frac{([TFE]_0 - [TFE]_f)}{[TFE]_0} \quad (2.6)$$

E_a and A are the activation energy and the pre-exponential factor for the decomposition of TFE. For the experiments using TFE and cyclohexene, E_a and A are taken from equations (2.3) and

(2.4). t is the reaction time obtained from the endwall pressure transducer, x is the extent of reaction and $[TFE]_0$ and $[TFE]_f$ are obtained from the analysis of the preshock and postshock samples respectively.

2.4.3.2.2. Carbon Disulfide (CS_2)

The chemical thermometers, TFE and cyclohexene span a ‘chemical’ temperature range from 1071 – 1359 K. At temperatures above 1359 K, using TFE as a chemical thermometer gives inaccurate estimate of the conversion of TFE to difluoroethene. At temperature above 1359 K carbon disulfide is used as a chemical thermometer.

The rate constants for the decomposition of CS_2 are obtained from the publication of Saito et al.⁴⁹, who measured the unimolecular decomposition rate constant of CS_2 behind reflected shock waves.



CS_2 decomposes unimolecularly at the lower temperatures when CS_2 starts to decay to CS and S (R2.7). At higher temperatures, the S atom produced in the unimolecular decay reacts with CS_2 and forms CS and S_2 (R2.8). To minimize the secondary reaction (R2.8), a very low concentration of CS_2 in argon (about 30 ppm) was used to conduct the temperature calibration experiments. However, to get an accurate estimate of the temperature both the reactions R2.7 and

R2.8 were used to calculate the ‘chemical’ temperature behind the reflected shock waves. The rate constants of these two reactions are shown in Table 2.

Table 2. *CS₂ Model Rate Constants*

Reaction	A (mol/cm³s)	E_a (cal/mol)
R 2.7 ⁴⁹	2.51E+14	74000
R 2.8 ⁴⁹	1.00E+14	4070

The rate constants for these two reactions, R2.7 and R2.8 were included in the chemical kinetic model and the CS₂ decomposition was simulated for a particular, temperature, pressure and the reaction time. The initial temperature was guessed and the simulations were performed until the temperature at which the experimental CS₂ conversion matched the simulated CS₂ conversion. This temperature was taken to be the ‘chemical’ temperature of the reflected shock.

2.4.3.2.3. Temperature Calibration using the Chemical Thermometers

Two different approaches are used for this technique.

- 1) Internal chemical thermometer technique
- 2) External chemical thermometer technique

In the internal chemical thermometer technique, both the chemical thermometer and the reagent of interest are subjected to the same temperature and pressure conditions. The chemical

thermometer is “internal” to the reagent mixture which implies that the reagent mixture consists of the chemical thermometer and decomposition of the chemical thermometer is followed to determine the temperature in the reaction zone. One of the important criteria of using this technique is that the species formed from the decomposition of the chemical thermometer should not interact with the species formed due to decomposition of the reagent mixture. Internal chemical thermometer technique is used in the shock tube community to determine the reaction temperature as long as there are no cross-reactions between the reagent and the chemical thermometer^{50,51}.

Since many of the experiments involved in this study, consist of complex mixtures of stable species and radicals, we used the external chemical thermometer technique⁵². In this technique, the chemical thermometer is “external” to the reagent mixture and hence the reagent mixture does not consist of the chemical thermometer. Experiments are conducted on both the reagent and the chemical thermometer for similar temperature and pressure conditions. Since the mixtures consist of very dilute concentrations of the chemical thermometer in Argon, the experiments are essentially conducted in pure bath gas Argon. Hence, the post-shock temperature for pure Argon bath gas using a chemical thermometer could be correlated against some experimentally measured parameter such as shock velocity and a temperature calibration curve can be developed that can be applied to Argon containing very small amounts of reagent.

A typical temperature calibration plot is shown in Fig 14. The plot shows the temperature on the y-axis and the extrapolated end wall velocities on the x-axis. To get the best measure of the reflected shock wave velocity the shock velocities obtained using the side wall transducers are extrapolated to the end wall. The extrapolated end wall velocity provides the best estimate of the reflected shock velocities at the end wall where the gas samples are withdrawn. For each shock, based on the pre-shock and post-shock concentrations of the chemical thermometers, cyclohexene TFE and CS₂ and the reaction time, t , the temperature T_5 was determined using the procedure described in Sections

2.4.3.2.1 and 2.4.3.2.2. Hence a correlation could be drawn between the range of temperature measurement and the range of the extrapolated end wall velocities. Based on our hypothesis, that for such dilute concentrations, the experiments could be essentially assumed to be carried out in pure bath gas argon, we can then determine the temperature of any shock consisting of a different reagent based on the extrapolated endwall velocity, for that particular shock. The temperature calibration plot using CS_2 as the chemical thermometer is shown in Fig 15.

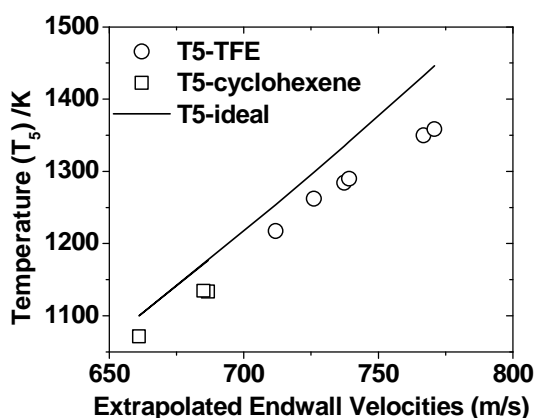


Fig 14. T5 for nominal post shock pressure of 50 atm, [-]-T5 calculated from ideal shock tube relations; [□]-T5 calculated from cyclohexene decomposition; [o]-T5 calculated from DFE decomposition

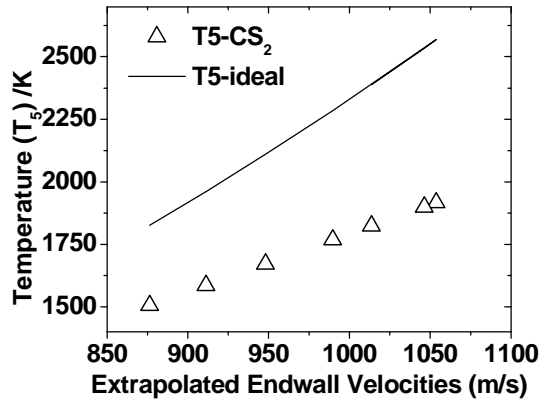


Fig 15. T_5 for nominal post shock pressure of 50 atm, [-]- T_5 calculated from ideal shock tube relations; [Δ]- T_5 calculated from CS_2 decomposition

The temperature calibration plot including all the three chemical thermometers is shown in Fig 16. Cyclohexene, 1,1,1-trifluoroethane and carbon disulfide were used for a ‘chemical’ temperature range of 1071-1134 K, 1217-1359 K and 1619-2033 K respectively, for nominal reflected shock pressures of 25 and 50 atm. For temperatures between 1134 and 1217 K and 1359 K and 1619 K, an interpolated calibration curve was used. The diaphragm opening process causes minor variations ($\pm 20\%$) in the final pressure; consequently the experiments are referred to as being performed at “nominal” pressures of 25 and 50 atm.

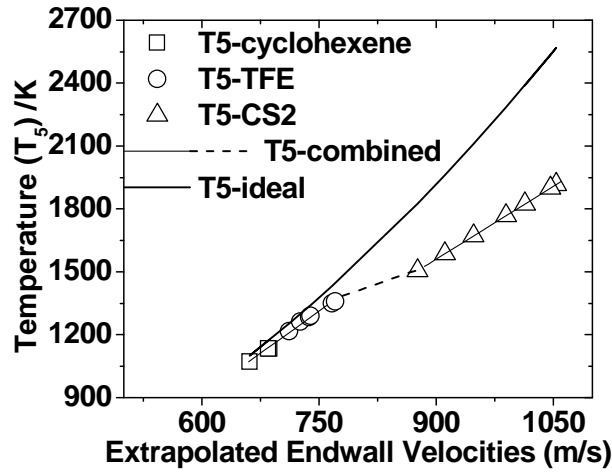


Fig 16. Temperature calibration plot using all the three chemical thermometers. T5 for nominal post shock pressure of 50 atm, [-]-T5 calculated from ideal shock tube relations; [□]-T5 calculated from cyclohexene decomposition; [o]-T5 calculated from DFE decomposition; [Δ]-T5 calculated from CS₂ decomposition, [---]-interpolated calibration line

2.4.4. Reagent Mixtures and Ancillary Equipment

Shock waves are produced by means of bursting of a diaphragm which is placed between the driver and the driven section of the shock tube. For the present work, aluminum diaphragms were used. These diaphragms are circular in shape with mutually perpendicular scores in the center, which facilitates clean opening of the diaphragm and the generation of a shock wave with minimal disturbances. Diaphragms with two different score depths were used to generate shock waves of different average reflected shock pressures of 25 and 50 atm. The types of the diaphragms used and their score depths are provided in the table below.

Table 3. Diaphragm Specifications

Average Reflected Shock Pressure (bars)	Material	Thickness (0.001")	Score Depth (0.001")
25	Aluminum	25	10
50	Aluminum	25	5

Reagent mixtures consisting of the reactant, ~100 ppm (99+%, Acros Organics) and krypton (99.999%, Specialty Gases of America) diluted in bath gas, argon (99.999%, Airgas) were prepared manometrically in heated tanks and allowed to stand overnight before use. A freeze-thaw procedure was used before admitting the reactants into the mixture vessel to minimize the air content. Krypton was added as an internal standard in the experiments to account for any dilution of the post-shock gases by the driver gas, helium (99.998%, Airgas). Since krypton is an inert compound, the post-shock and pre-shock samples of the mixture should show same concentration of krypton. The ratio of concentration of krypton in the post-shock sample to the concentration of krypton in the pre-shock sample (r_k) should be close to 1. In case of dilution of post-shock gases by helium the concentration of krypton will be reduced and the ratio of concentrations of krypton in the post to the pre-shock samples (r_k) will be lower than 1. In order to obtain the actual concentrations, the concentrations of the species in the diluted mixture are divided by r_k . The concentrations of the species in the pre-shock and post-shock samples are determined using gas chromatography and mass spectrometric techniques which are explained in detail in the following section (Section 2.4.5).

Low initial concentrations of the fuel were used in the experiments in order to maintain isothermal conditions in the shock tube and to attain good carbon totals. These low mole fractions

minimize the temperature drop due to initial endothermic reactions and temperature rise due to later exothermic oxidation reactions, thereby maintaining isothermal conditions over the time range (1.5 – 2.0 ms) of the current experiments. The table of experimental conditions for the three different fuels, n-propylbenzene, m-xylene and 1,3,5-trimethylbenzene are provided in the subsequent chapters along with the modeling results.

Prior to each experiment, the driven section of the shock tube was evacuated to 1×10^{-3} torr by a rotary-pump (Edwards E2M-1.5) and a turbo-pump (Edwards EXT-250HI). A separate rotary pump (Edwards RV-8) was used to evacuate the driver section. The shock tube and all the lines to the shock tube were heated to 100 °C to minimize the fuel losses due to condensation. The gas samples were withdrawn from the center of the shock tube via a straight channel connected to the gas sampling port. The location of the gas sampling port minimizes the boundary layer effects; the sample is withdrawn from the center and close to the endwall section of the shock tube. The boundary layer effects become prominent for low pressures around 6-10 atm, where the concentration of the fuel is observed to reach a low non zero stable value even at very high temperatures, indicating incomplete conversion of the fuel. All the experiments in this paper were performed for nominal reflected shock pressures above 20 atm where boundary layer effects are minimized.

2.4.5. Analytical Technique

Gas chromatography and mass spectrometric techniques were used to identify and quantify the species present in the pre-shock and the post-shock samples. Gas chromatography is a separation method in which the components of a gas mixture are partitioned between the stationary and the mobile phases⁵³. The stationary phase is a layer of liquid or a polymer on an inert solid

phase which is present inside a glass or a metal column and the mobile phase is the carrier gas which carries the gas phase sample through the column. The gas phase components partition between the stationary and the mobile phases and are separated from one another based on their relative vapor pressures and their affinities towards the stationary phase. The device which operates on the principle of gas chromatography is the Gas Chromatograph (GC). While gas chromatography enables us to quantify the species, mass spectrometry is used to identify the species. In mass spectrometry the samples are ionized and the charged particles are repelled and attracted by charged lens into the mass analyzer. Here the ionic species are separated by their mass-to-charge ratio (m/z) by either magnetic or electrical fields. Hence, the coupling of gas chromatographic and mass spectrometric techniques enabled us to quantify and identify the stable intermediates from our experiments.

The sample from the shock tube is transferred to the analytical apparatus through a heated line (150 °C) and was analyzed by two GCs connected in series with the sample lines to and from the GC's were heated to 150 °C. The first GC (HP-6890) (closest to the end wall section of the shock tube) was used for the measurement of single ring and multi-ringed aromatic hydrocarbons, so as to minimize and prevent the loss of species due to condensation. The first GC system was equipped with a Flame Ionization detector (FID) connected to a DB-17MS column. The FID has a detection capability up to sub-ppm levels and the DB-17MS column has a good separation capability for the polycyclic aromatic hydrocarbons. The first GC oven was temperature programmed to 320 °C and this excludes the possibility of species being retained on the GC column. In addition to this, a post-run performed at 320 °C for prolonged periods of time showed a stable baseline, with no polycyclic aromatic hydrocarbons eluting from the column. The second GC (GC2) was used for the measurement of alkanes, alkenes, CO, CO₂, O₂ and inert gases. The separation and measurement of such gaseous species was attained with a HP-PLOT Q column connected to the

FID for the measurement of alkanes, alkenes, CO and CO₂. A nickel catalyst (Methanizer) was placed in between the HP-PLOTQ column and the flame ionization detector (FID) to convert CO and CO₂ eluting from the column to methane, thereby permitting CO and CO₂ to be detected on the FID. GC2 was equipped with a Thermal Conductivity Detector (TCD) connected to a MOLSIEVE 5A column, which enabled the detection of O₂ and krypton. Identification of reaction products was achieved with the aid of mass spectrometer. The three detectors were calibrated and the calibrations were periodically checked for consistency. More details about the experimental set up could be found in the publication of Comandini et al.⁵⁴

During the course of the experiments, the fuels (1,3,5-trimethylbenzene, n-propylbenzene and m-xylene) were calibrated numerous times and the calibration factors were periodically checked. The calibration factor of the species of interest was determined by injecting a sample containing known concentration of the species, diluted in helium. The calibration chart of 1,3,5-trimethylbenzene (135-tmb) is shown in Fig 17. The ordinate shows the concentration of the species in ppm. The abscissa shows the peak area obtained for each of the concentrations of the species divided by the injection pressure. From the chart, it can be observed that three separate mixtures of 135-tmb concentrations of approximately 17 ppm, 75 ppm and 211 ppm were prepared by diluting 135-tmb in helium. The peak area is obtained from the GC analysis and since the injection pressure of each sample is known, and the peak area and pressure are used together to obtain the peak area/psi numbers. The slope of the line is the calibration factor (shown in *Fig 17* as $y = 3.00601e-5x$). Using this calibration factor the concentration of 1,3,5-tmb can be determined in an unknown sample if the peak area/psi value is known for 135-tmb in the sample. Repetitive runs on the GCs with a single mixture composition and varied mixture composition were performed to attain an accurate calibration.

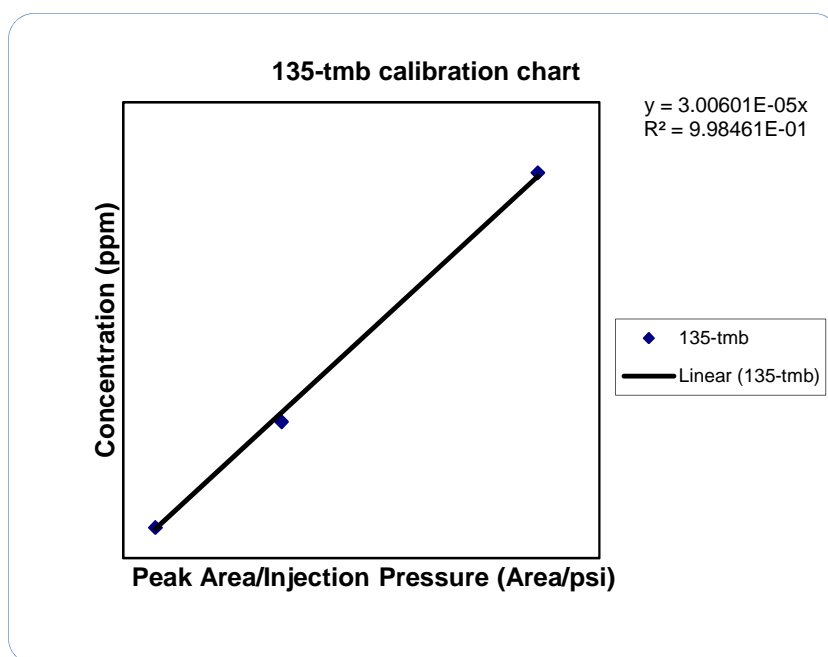


Fig 17. 1,3,5-Trimethylbenzene (135-tmb) calibration chart.

For a few of the species measured in the experiments like O₂, CO, CO₂, methane (CH₄), ethane (C₂H₆), ethene (C₂H₄), acetylene (C₂H₂), propane (C₃H₈), propene (C₃H₆), 1,2-propadiene (C₃H₄), propyne (C₃H₄), 1,3-butadiene (C₄H₆), toluene (C₆H₅CH₃), benzene (C₆H₆), ethylbenzene (C₆H₅C₂H₅), m-xylene (C₈H₁₀), p-xylene (C₈H₁₀) and o-xylene (C₈H₁₀), calibration mixtures were available from Sigma Aldrich and Airgas and a single point calibration was used to determine the calibration factor. The gas mixtures provided by Sigma Aldrich and Airgas were injected and the area/psi was noted for the concentration of each species present in the gas mixture, and this is referred to as the single point calibration. For example, if the concentration of methane in the Sigma Aldrich mixture is 15 ppm, the calibration factor of methane (concentration divided by area/psi) was

obtained for 15 ppm . For two ringed, three ringed and four ringed species, which have a low vapor pressure, based on the feasibility of obtaining the species, a different calibration procedure was adopted. For the species such as naphthalene, acenaphthylene, acenaphthene, fluorene, phenanthrene, anthracene, fluoranthene, pyrene, benzo(a)anthracene and chrysene, which are readily available in solution form, the calibration factors were determined using a procedure, which will be discussed shortly. For all the other polycyclic aromatic hydrocarbons, the calibration factors were estimated using flame ionization detector response factors.

For the polycyclic aromatic hydrocarbons which were available in solution, varying concentrations ($\mu\text{g/ml}$) of these species were prepared in dichloromethane. Unlike the calibrations for the single ringed aromatic and aliphatics, these calibrations were done in liquid phase, where about $1\mu\text{l}$ of the solution was injected onto the column using a syringe and the liquid calibrations were obtained. After obtaining the liquid phase calibrations, the gas phase calibration factors of these species were estimated using benzene as the reference or standard species. The gas phase calibration factors were computed using the formula shown below⁵⁵

$$\text{DRC}_{\text{GP-X}} = (\text{DRC}_{\text{L-X}}/\text{DRC}_{\text{L-S}}) \times \text{DRC}_{\text{GP-S}} \times (\text{M}_\text{X}/\text{M}_\text{S})$$

where $\text{DRC}_{\text{GP-X}}$ = gas phase calibration factor of the unknown species

$\text{DRC}_{\text{L-X}}$ = liquid phase calibration of the unknown species

$\text{DRC}_{\text{L-S}}$ = liquid phase calibration of standard (benzene)

$\text{DRC}_{\text{GP-S}}$ = gas phase calibration of the standard (benzene)

M_X = molecular weight of the unknown species

M_S = molecular weight of the standard (benzene)

The calibration factors of polycyclic aromatic hydrocarbons other than the ones mentioned above were estimated from the flame ionization detector response factors available in literature⁵⁶. Benzene was taken to be the standard and the gas phase calibration factors of the unknown species were calculated using the formula given below⁵³.

$$\text{Calibx} = (f_x/f_s) \times (\text{calibs}) \times (\text{MWs}/\text{MWx})$$

Where Calibx = calibration factor of the unknown compound

f_x = relative response factor of the unknown species

f_s = response factor of the standard species (benzene)

calibs = calibration factor of the standard species (benzene)

MWx = molecular weight of the unknown compound

MWs = molecular weight of benzene

2.4.6. Uncertainties in the Experimental Parameters

2.4.6.1. Uncertainties in Temperature

Two kinds of uncertainties are present in the temperature measurement. The first one is caused due to inconsistencies of the shock velocities, which results in a maximum error of 1% in the extrapolated endwall velocities. This deviation in temperature as a result of the error in the extrapolated velocities is minimized by the fact that for the same temperature and pressure conditions, the attenuation is similar for both the actual experiments and the temperature calibration

experiments. On the other hand there is an uncertainty in temperature due to the use of interpolated calibration fits among different chemical thermometers used for different temperature ranges. Maximum uncertainty in temperature as a result of the interpolated fits is less than ± 1 % for temperatures less than 1350 K and around ± 2 % for temperatures greater than 1350 K.

2.4.6.2. Uncertainties in Pressure

Reaction pressures and reaction times are obtained from a pressure trace recorded from a high frequency pressure transducer mounted in the end wall of the driven section parallel to the long axis of the shock tube. The uncertainty in the measured pressure by using the pressure transducers is $\pm 1\%$.

2.4.6.3. Uncertainties in Reaction Time

The present set up gave reaction times in the range of 1.2-2.0 ms with exact reaction times measured for each experiment. The reaction times vary by a maximum of 0.5 ms from the nominal reaction time of 1.5 ms. This variation is caused by the non-idealities in the quenching process as a result of usage of inserts of varying lengths as we step up in temperature to attain a flat plateau shock pressure profile. As the exact reaction time, pressure and temperature of each shock is used in the simulation, these changes in the reaction times do not vary the computed results significantly.

2.4.6.4. Uncertainties in Species Concentration

Uncertainties in species mole fractions are estimated to be no more than 5% for GC measurements of the fuels and some of the major aliphatic and mono-aromatic hydrocarbons. For multi-ring aromatic hydrocarbons the error in the species measurement could be between 15-20%.

3. MODELING

3.1. Modeling Software, CHEMKIN

The CHEMKIN 3.6⁵⁷ and CHEMKIN 4.1⁵⁸ suite of programs have been used to simulate our experimental data. The program solves first order differential equations for the rate of change of species molar concentrations, and the solution of these equations describes the species evolution for a particular temperature, pressure and reaction time. The differential equations are shown in equation (2.9) and (2.10) and are derived from mass and energy conservation equations, assuming an adiabatic constant pressure process. More details about how equations (2.9) and (2.10) are derived are provided in chapter 6 of ‘An Introduction to Combustion’ textbook by Turns⁵⁹. Each of the terms in the equation (2.9) and (2.10) are explained below.

$$\frac{d[X_i]}{dt} = \dot{\omega}_i - [X_i] \left[\frac{\sum \dot{\omega}_i}{\sum_j [X_j]} + \frac{1}{T} \frac{dT}{dt} \right] \quad (2.9)$$

Where

$$\frac{dT}{dt} = \frac{\left(\frac{\dot{Q}}{\dot{V}} \right) - \sum_i (\dot{\omega}_i \bar{h}_i)}{\sum_i ([X_i] \bar{h}_i)} \quad (2.10)$$

and the terms

$[X_i]$ = Molar concentration of species i

ω_i = molar production rate of the i^{th} species, which can be written as a summation of the rate of progress variables for all reactions involving the i^{th} species

Q = heat, T = temperature, t = time, \bar{h}_i = molar enthalpy of the species, V = volume

$$\dot{\omega}_i = \sum_{k=1}^K v_{ik} q_k \quad (2.11)$$

Where $v_{ik} = v_i'' - v_i'$ and v_i'' , v_i' are the stoichiometric coefficients in the chemical reaction expressed as $\sum_{i=1}^I v_{ik}' \chi_i \rightleftharpoons \sum_{i=1}^I v_{ik}'' \chi_i$ and χ_i is the symbol of the i^{th} species

Where q_k for the k^{th} reaction is the difference of the forward and reverse rates

$$q_k = k_{f_k} \prod_{i=1}^I [X_i]^{v_{ik}'} - k_{r_k} \prod_{i=1}^I [X_i]^{v_{ik}''} \quad (2.12)$$

k_{f_k} is the forward rate constant of the k^{th} reaction and k_{r_k} is the reverse rate constant of the k^{th} reaction

The forward rate constants have the following expression

$$k_{f_k} = A_k T^{\beta_k} \exp\left(\frac{-E_k}{R_c T}\right) \quad (2.13)$$

A_k is the pre-exponential factor, β_k is the temperature exponent and E_k is the activation energy of the reaction k.

T = temperature, t = time

V = volume, where $V = \frac{m}{\sum_i([X_i]MW_i)}$, m is the mass of the mixture and MW_i = molecular weight of the i^{th} species

The molar enthalpy of the species, \bar{h}_i in equation (2.10) is calculated using the calorific equation of state

$$\bar{h}_i = \bar{h}_{f,i}^0 + \int_{T_{ref}}^T \bar{c}_{p,i}^0 dT \quad (2.14)$$

The superscript o, ref, refers to the standard state of one atmosphere. The molar heat capacity of the species, at any temperature can be calculated from the equation provided below

$$\frac{\bar{c}_{p,i}^0}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \quad (2.15)$$

The coefficients, which are of the format a_i are called NASA polynomial coefficients. The molar enthalpy and entropy can also be calculated from the equations having 6 or 7 of these polynomials.

$$\frac{\overline{h^0}}{RT} = a_1 + \frac{a_2}{2}T + \frac{a_3}{3}T^2 + \frac{a_4}{4}T^3 + \frac{a_5}{5}T^4 + \frac{a_6}{T} \quad (2.16)$$

$$\frac{\overline{s^0}}{RT} = a_1 \ln T + a_2T + \frac{a_3}{2}T^2 + \frac{a_4}{3}T^3 + \frac{a_5}{5}T^4 + a_7 \quad (2.17)$$

Hence, the input files to CHEMKIN provide information about

- (1) The initial species concentration, the temperature, pressure and the reaction time.
- (2) The kinetic information consisting of several reactions which describe the reactant decay and the formation of other products.

<i>Reaction</i>	A_k	β_k	E_k
C3H8+H=NC3H7+H2	1.33E+06	2.54	6756

- (3) The NASA polynomials or the thermochemical information required to calculate the molar heat capacities, enthalpy and entropy are provided in the following format.

HE	L10/90HE	1	0	0	OG	200.000	6000.000	1000.	1
2.50000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			2
-7.45375000E+02	9.28723974E-01	2.50000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				3
0.00000000E+00	0.00000000E+00	-7.45375000E+02	9.28723974E-01	0.00000000E+00					4

The thermochemical information is also used to calculate the reverse rate constants, when the rate constants for the reverse reaction are not provided. The first set of 7 constants belong to the temperature range of 1000 to 6000 K and the second set of 7 constants belong to the temperature range of 200 to 1000 K

The output of the program provides information about the time evolution of all the species of the model as a function of temperature and pressure. The simulations are performed assuming an adiabatic constant pressure process. For shock tube experiments with less than 15% endwall pressure increase the adiabatic constant pressure process assumption leads to reasonable accuracy in predicting the stable species profiles.⁴⁶ All the pressure profiles considered for these simulations had less than 15% endwall pressure increase. The influence of reactions occurring in the quenching

period have insignificant effect on the concentration of the stable species; hence the quench was not simulated.⁴⁶

Reaction path analysis and Sensitivity analysis⁵⁷ were the two important tools (provided by CHEMKIN^{57,58}) that were used to refine the chemical kinetic models that were built in this project. Reaction path analysis gives information about the contribution of each reaction to the net rate of production or destruction of each species ($\dot{\omega}_i$). The sensitivity analysis provides quantitative information about how each rate coefficient affects the temperature and species fractions. In the simplest form, the sensitivity coefficient can be expressed as

$$S_{i,j} = \frac{\frac{d[A]_i}{[A]_i}}{\frac{dk_k}{k_k}}$$

The sensitivity coefficient represents the concentration sensitivity of species $[A]_i$ for a rate parameter k_k . A negative sensitivity coefficient indicates that increase in rate constant for reaction k , results in decrease in the yield of species i .

Using the reaction path analysis and sensitivity analysis tools, the important reactions in the model which directly influenced the decay of the fuel or the formation and destruction of the intermediates were identified and in some cases, these reactions were modified to improve the predictions of the model against the experimental data.

4. DISCUSSION OF N-PROPYLBENZENE OXIDATION EXPERIMENTS AND MODELING RESULTS

4.1. Introduction

Previous studies^{60,61} probed the kinetics of n-propylbenzene oxidation at atmospheric pressure and for temperatures below 1250 K. Won et al.⁶² measured the extinction strain rates of n-propylbenzene flames. Roubaud et al.⁶³ performed ignition delay experiments on a series of aromatics including n-propylbenzene around 17 atm and at a temperature of about 840 K. The present study further extends the temperature and pressure range of n-propylbenzene oxidation kinetics to high temperature and high pressure conditions which are pertinent to the operation of practical devices. The oxidation experiments of n-propylbenzene were performed in our High Pressure Single Pulse Shock Tube.

4.2. Experimental Results

The oxidation experiments of n-propylbenzene were performed for two different nominal reflected shock pressures of 25 and 50 atm, for fuel lean, stoichiometric and fuel rich conditions. The experimental conditions are listed in Table 4.

Table 4. *n*-Propylbenzene experimental conditions

Average Shock Pressure /atm	Fuel /ppm	Temperature Range /K	Φ	Reaction Time /ms
28	86	907-1550	0.54	1.40-2.05
51	90	959-1558	0.55	1.27-1.78
49	90	838-1635	1.0	1.21-1.95
24	89	905-1669	1.9	1.36-2.93
52	90	847-1640	1.9	1.26-1.95
54	83	1027-1678	∞	1.19-2.07

4.2.1. Effect of Pressure and Equivalence Ratio on *n*-Propylbenzene and Oxygen Decay

The fuel and oxidizer decay are shown as a function of temperature, pressure and equivalence ratio in Fig 18 (a - b). The concentration of the fuel is plotted against the reflected shock temperature for two different equivalence ratios of 0.5 and 1.9 and for two different nominal reflected shock pressures of 25 and 50 atm. The consumption of the fuel was observed to be independent of the pressure and is slightly dependent on the equivalence ratio. The consumption of the oxidizer was also seen to be independent of the pressure but it is slightly dependent on Φ for temperatures greater than 1200 K.

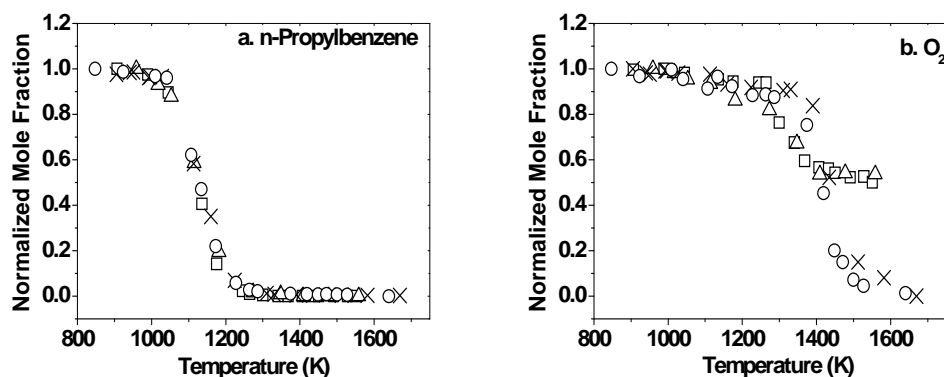


Fig 18. a) *n*-Propylbenzene and b) oxygen decay profiles from the shock tube oxidation experiments of *n*-propylbenzene, [Δ] - average $P5 = 51$ atm, $\Phi = 0.55$, [\square] - average $P5 = 28$ atm, $\Phi = 0.54$, [o] - average $P5 = 52$ atm, $\Phi = 1.9$, [X] - average $P5 = 24$ atm, $\Phi = 1.9$, nominal reaction time = 1.5 ms

4.2.2. Effect of Equivalence Ratio on the Formation of the Intermediates

Several stable intermediates were identified and quantified from the current sets of experiments. These included aliphatic hydrocarbons such as CO, CO₂, methane (CH₄), ethane (C₂H₆), ethene (C₂H₄), acetylene (C₂H₂), allene (C₃H₄), propyne (C₃H₄), 1,3-butadiene (C₄H₆), diacetylene (C₄H₂), vinylacetylene (C₄H₄) and aromatic hydrocarbons such as styrene (C₆H₅C₂H₃), toluene (C₆H₅CH₃), benzene (C₆H₆), benzaldehyde (C₆H₅CHO), bibenzyl (C₁₄H₁₄), phenol (C₆H₅OH), benzofuran (C₈H₆O), indene (C₉H₈), naphthalene (C₁₀H₈), fluorene (C₁₃H₁₀) and anthracene (C₁₄H₁₀).

Species such as benzaldehyde, phenol and benzofuran which are formed either by addition or addition-elimination reactions of benzyl and phenyl radicals with HO₂, OH and O₂ radicals are referred to as the oxygenated intermediates. Species such as toluene, styrene, benzene, ethylbenzene, ethene, ethane, methane and bibenzyl are referred to as the pyrolytic intermediates.

These species are formed from the fuel or fuel radicals either by homolysis or beta-scission yielding both stable intermediates and radicals, the latter of which recombine with H atom, methyl or benzyl radical yielding the above mentioned intermediates. The maximum attained concentrations of several of the oxygenated and pyrolytic intermediates depended on the equivalence ratio.

The maximum concentrations of several of the oxygenated intermediates decreased with an increase in the equivalence ratio. On the other hand, the maximum concentrations of several of the pyrolytic intermediates increased with an increase in equivalence ratio. For instance, the species profiles of two oxygenated intermediates, benzaldehyde and benzofuran are shown in Fig 19 (a – b), for a nominal reflected shock pressure of 50 atm and for three different equivalence ratios ($\Phi = 0.55, 1, 1.9$). As evident from these figures, the maximum concentration of benzaldehyde and benzofuran was obtained for the fuel lean oxidation experiments and was twice greater than that of the maximum concentration of these species obtained from the fuel rich dataset. On the contrary, for a few of the major pyrolytic intermediates like methane, ethene, toluene and ethylbenzene the greatest concentrations were attained for the fuel rich dataset. These species profiles for three different equivalence ratios are shown in Fig 20 (a - d). The only major pyrolytic intermediate that showed the opposite behavior is styrene. Slightly decreasing maximum concentration of styrene was obtained for increasing Φ and the profiles are presented in Fig 21.

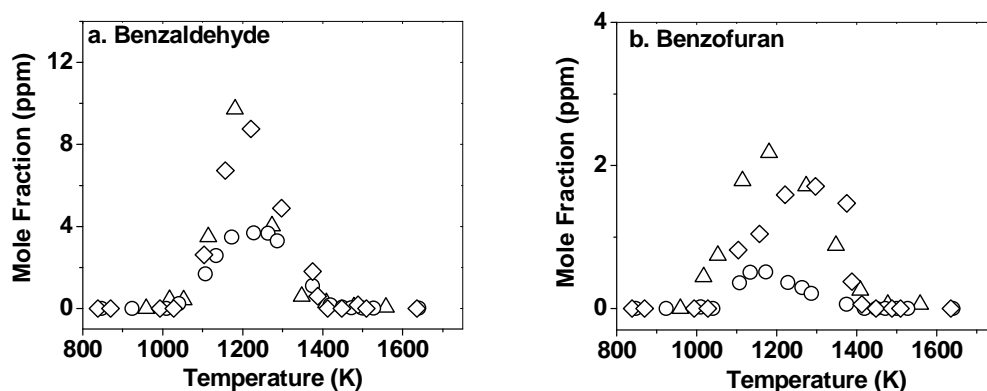


Fig 19. a) Benzaldehyde and b) benzofuran profiles as a function of equivalence ratio from the shock tube oxidation experiments of *n*-propylbenzene , [Δ] - average $P5 = 51$ atm, $\Phi = 0.55$, [\diamond] - average $P5 = 49$ atm, $\Phi = 1.0$, [\circ] - average $P5 = 52$ atm, $\Phi = 1.9$, nominal reaction time = 1.5 ms

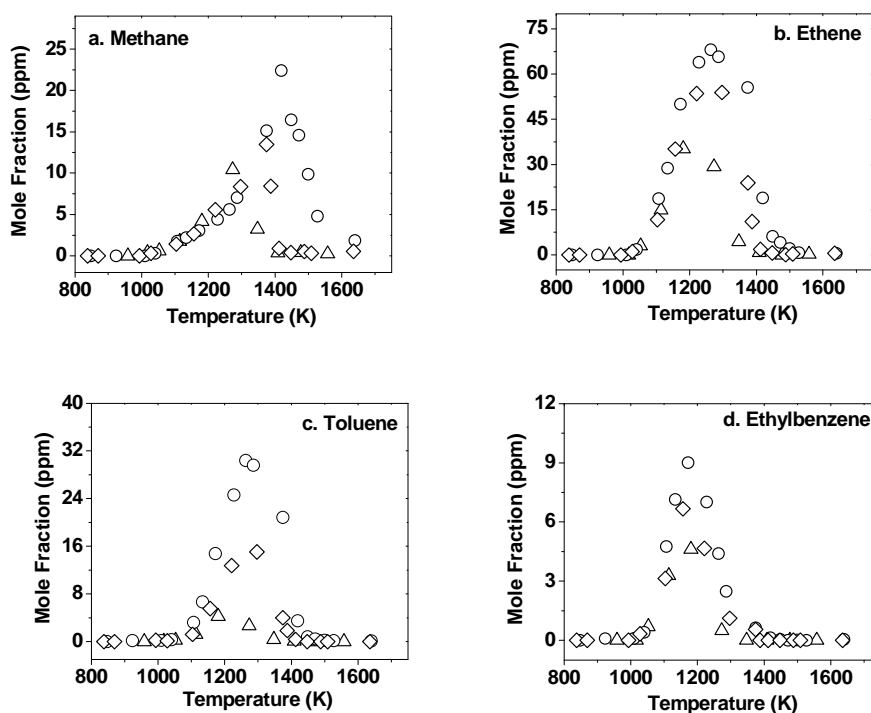


Fig 20. a) Methane, b) Ethene, c) Toluene and d) Ethylbenzene profiles as a function of equivalence ratio from the shock tube oxidation experiments of *n*-propylbenzene , [Δ] - average $P5 = 51$ atm, $\Phi = 0.55$, [\diamond] - average $P5 = 49$ atm, $\Phi = 1.0$, [\circ] - average $P5 = 52$ atm, $\Phi = 1.9$, nominal reaction time = 1.5 ms

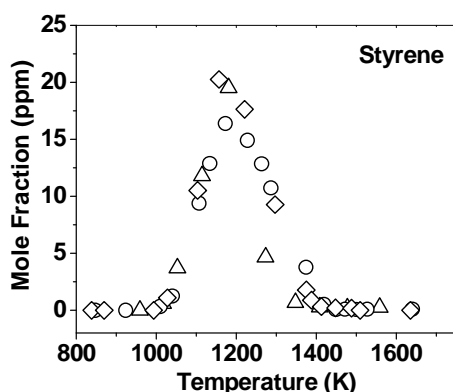


Fig 21. Styrene profiles as a function of equivalence ratio from the shock tube oxidation experiments of *n*-propylbenzene , [Δ] - average $P_5 = 51$ atm, $\Phi = 0.55$, [◇] - average $P_5 = 49$ atm, $\Phi = 1.0$, [○] - average $P_5 = 52$ atm, $\Phi = 1.9$, nominal reaction time = 1.5 ms

These variations in the product distribution as a function of Φ are indicative of a shift in the mechanistic pathways for the fuel decay. Knowledge of the major consumption routes of the fuel will assist us in interpreting the experimental data. Hence, a diversion is taken here and the major pathways of *n*-propylbenzene decay mentioned in literature are discussed. Litzinger et al.⁶⁰ proposed three different routes for *n*-propylbenzene consumption based on the species observed from their experiments. These pathways are illustrated in Fig 22.

(1) The abstraction of the benzylic, primary and secondary hydrogens by H, O, OH and HO₂ radicals produces 1-phenyl-1-propyl, 1-phenyl-2-propyl and 3-phenyl-1-propyl radicals respectively. The structures of these species are shown in Table 5. The 1-phenyl-1-propyl radical undergoes beta scission to form styrene and methyl radicals, (reaction I in Fig 22). The 1-phenyl-2-propyl radical isomerizes to form 2-phenyl-1-propyl radical which undergoes beta scission to form styrene and methyl radical (reactions II and III in Fig 22). The 3-phenyl-1-propyl radical undergoes beta scission to form benzyl and ethene (reaction IV in Fig 22).

(2) The homolysis of the side chain produces benzyl and ethyl radical (reaction V in Fig 22).

(3) The displacement of n-propylbenzene side chain by hydrogen atom produces benzene and n-propyl radical (reaction VI in Fig 22).

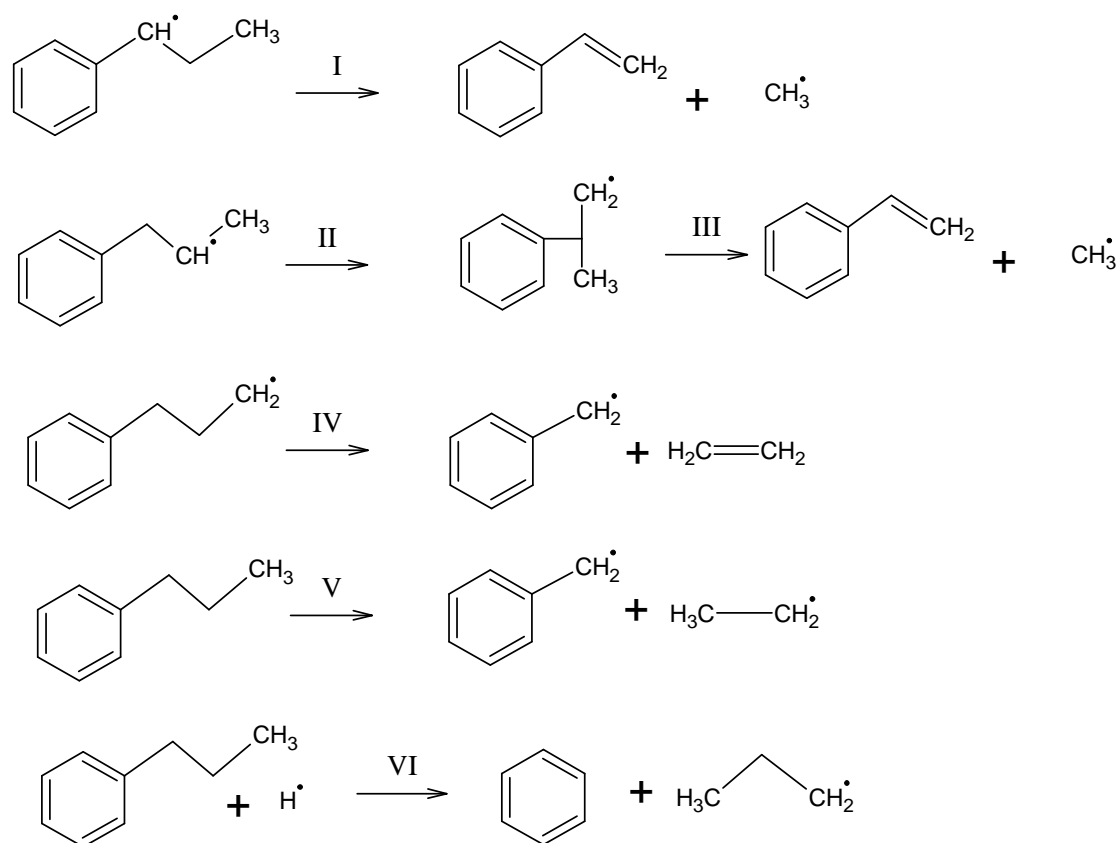


Fig 22. n-Propylbenzene decay pathways proposed by Litzinger et al.⁶⁰

Table 5. Structures of phenylpropyl radicals

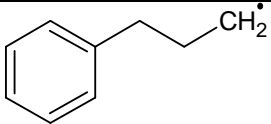
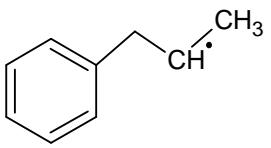
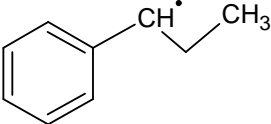
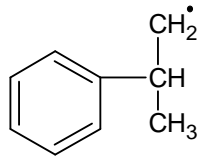
Species	Structure
3-phenyl-1-propyl radical (APHC3H6)	
1-phenyl-2-propyl radical (BPHC3H6)	
1-phenyl-1-propyl radical (CPHC3H6)	
2-phenyl-1-propyl radical (BPHROPY)	

Fig 23 shows the C-C and C-H bond energies of the n-propyl side chain of n-propylbenzene. Based on the lower benzylic and secondary C-H and benzylic C-C bond dissociation energies of the n-alkyl side chain we can infer that the hydrogen abstraction routes primarily produce styrene and methyl radical with minor amounts of benzyl and ethyl radical and the homolysis route primarily produces benzyl and ethyl radical. Now that we have a basic idea of how the fuel decays, we can now see how the observed species are qualitatively consistent with this information. For example, the increase in styrene with decreasing equivalence ratio is consistent with an increase in the radical pool capable of abstracting benzylic and secondary hydrogens from the n-propyl side chain. This qualitative observation will be confirmed by the reaction path analysis derived from the chemical kinetic model discussed shortly.

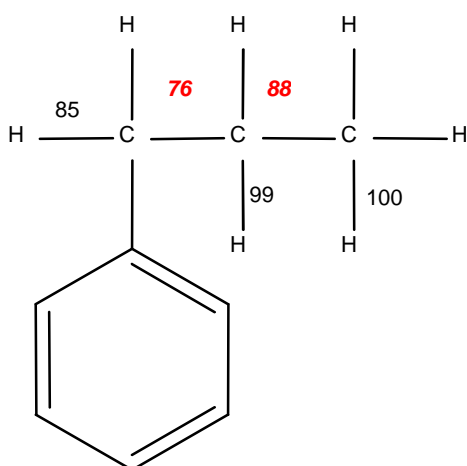


Fig 23. *C-H and C-C bond dissociation energies (kcal/mol) of the n-propyl side chain of n-propylbenzene. The C-H bond energies are computed using the thermochemistry from Dagaut et al.⁶⁴ and are denoted by plain numbers. The C-C bond energies are taken from Litzinger et al.⁶⁰ and are denoted by red bold italicized numbers.*

For another example, the maximum peak concentration of toluene and ethylene at fuel rich conditions highlights the increasing contribution of homolysis of the side chain when compared to the hydrogen abstraction pathways. Another indicator of dominance of the homolysis route is the increasing maximum concentrations of bibenzyl produced as a result of recombination of benzyl radicals and these plots are illustrated in Fig 24. The slightly decreasing concentration of styrene indicates the lower contribution of the hydrogen abstraction routes. Again these observations are confirmed by the reaction path analysis discussed later.

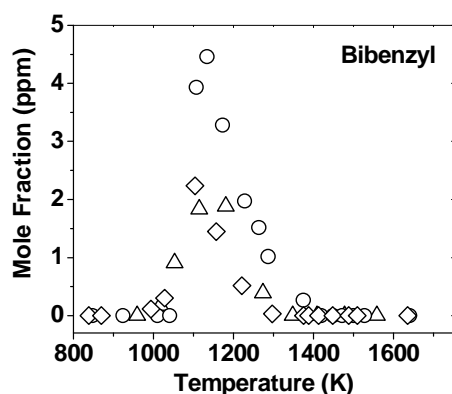


Fig 24. Bibenzyl profiles as a function of equivalence ratio from the shock tube oxidation experiments of *n*-propylbenzene , [Δ] - average $P_5 = 51$ atm, $\Phi = 0.55$, [◊] - average $P_5 = 49$ atm, $\Phi = 1.0$, [○] - average $P_5 = 52$ atm, $\Phi = 1.9$, nominal reaction time = 1.5 ms

In addition to bibenzyl, the concentration vs. temperature plots of other polycyclic aromatic hydrocarbons formed in these experiments are presented in Fig 25 (a - b), for nominal reflected shock pressure of 50 atm and at fuel rich conditions. A greater number of polycyclic aromatic hydrocarbons were identified and measured at the fuel rich and stoichiometric conditions when compared to fuel lean conditions. For the fuel lean dataset only two ringed compounds were at a high enough level to be quantified, whereas for the stoichiometric and fuel rich datasets, measurable concentrations of three ringed compounds like anthracene and fluorene were also detected.

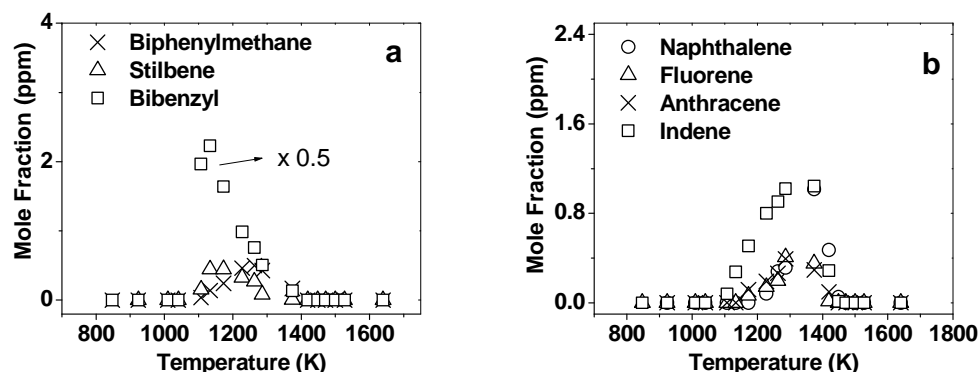


Fig 25. Polycyclic aromatic hydrocarbons formed from the shock tube oxidation experiments of *n*-propylbenzene, average $P_5 = 52 \text{ atm}$, $\Phi = 1.9$, a) [Δ] - Stilbene, [\square] - Bibenzyl, [\times] - Diphenylmethane, b) [Δ] - Fluorene, [\square] - Indene, [\times] - Anthracene, [\circ] - Naphthalene

4.3. Modeling

Chemical kinetic modeling provides the link between qualitative species rationalization and quantitative prediction. Predictive chemical kinetic modeling has special importance for *n*-propylbenzene since it is a suggested component of a surrogate jet fuel formulation that would be used to simulate the combustion behavior of an actual jet fuel.

The only existing detailed model for *n*-propylbenzene oxidation available in literature was developed by Dagaut et al.⁶¹. This model produces satisfactory predictions for *n*-propylbenzene consumption and formation of the major intermediates for their jet stirred reactor experimental data, at atmospheric pressure. The rate constants for most of the reactions were estimated from corresponding reactions of propane, toluene and other alkyl radicals or by using the rules provided in publications of Dean⁶⁵ and Walker⁶⁶.

The Dagaut et al.⁶¹ model has been used to simulate our experimental data. The simulations were performed for three different equivalence ratios, for a nominal reflected shock pressure of 50 atm and corresponding reaction times. The experimental and modeling profiles of the major species, fuel, oxygen, ethene, toluene, styrene, ethylbenzene and bibenzyl are plotted for each Φ and the results are shown in Fig 26 (a – i). The model shows fairly good predictions for the fuel decay. The model shows lower consumption of oxygen for all the experimental datasets. It also shows greater amounts than actually measured of toluene, ethylbenzene, ethene and bibenzyl for the fuel lean and stoichiometric datasets. It shows fairly good profiles for the formation and consumption of styrene. The peak modeling predictions at $\Phi = 0.5$, show the toluene and ethylbenzene concentrations increased by a factor of 6 and 2 respectively, when compared to the experimental data, in Fig 26 (b and c). As discussed in the previous section, toluene, ethylbenzene, ethene, bibenzyl, styrene and benzene are a few of the intermediates which are formed primarily from the fuel breakdown. The excellent agreement of the model with fuel and styrene profiles but poor agreement with the toluene profiles indicates that the relative contribution of the hydrogen abstraction, homolysis and the displacement pathways are probably different than those proposed by Dagaut et al. Hence, an independent n-propylbenzene oxidation model has been developed aiming to capture the fuel behavior and formation of the other intermediates with greater accuracy and relevance to surrogate fuel applications over the range of the current experimental conditions.

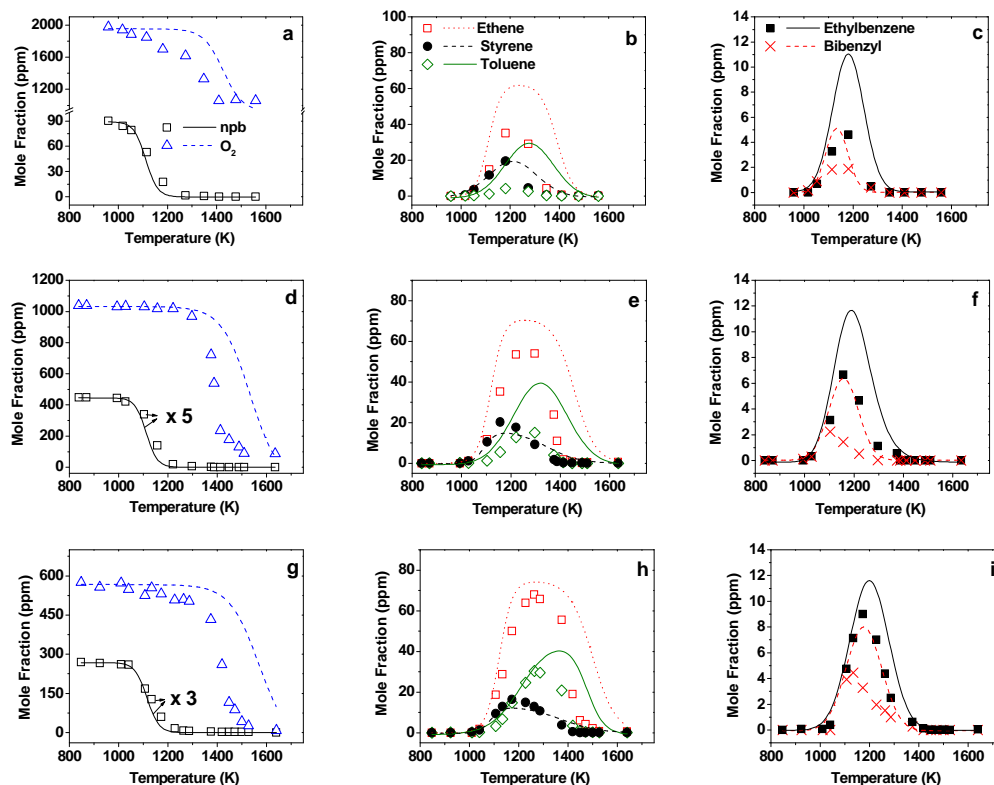


Fig 26. Experimental and modeling profiles of stable intermediates from the shock tube oxidation experiments of *n*-propylbenzene using the Dagaut et al. model⁶¹, [\square , -]- *n*-Propylbenzene, [Δ , ---]- O_2 , [\square ,]- Ethene, [\bullet , ---]-Styrene, [\diamond , -]- Toluene, [\blacksquare , -]- Ethylbenzene, [\times , ---]-Bibenzyl, [a – c] - average $P_5 = 51$ atm, $\Phi = 0.55$, [d – f] - average $P_5 = 49$ atm, $\Phi = 1.0$, [g – i] - average $P_5 = 52$ atm, $\Phi = 1.9$

4.3.1. UIC *n*-Propylbenzene Oxidation Model

A quantitative, predictive *n*-propylbenzene oxidation model has been developed to simulate our experimental data based in part on the qualitative pathways put forth by Litzinger and coworkers⁶⁰. The rate constant for homolysis of the *n*-propyl side chain to form benzyl and ethyl radical is taken from Roubaugh et al.⁶⁷. The rate constants for beta-scission of phenylpropyl radicals and recombination reactions of phenylpropyl radicals with hydrogen atom were estimated using the

rate constant rules proposed by Dean⁶⁵ and Allara and Shaw⁶⁸. A few reactions for the oxidation of phenylpropyl radicals were taken from Dagaut et al.⁶¹. This set of kinetics is shown in Table 6.

Table 6. Rate constants for the recombination, beta-scission and oxidation reactions of phenylpropyl radicals and homolysis of the n-propylbenzene side chain.

Reaction ^a number	Reaction ^b	A	n	E _a
983 ^{68,c}	CPHC3H6+H= C ₆ H ₅ C ₃ H ₇	1.00E+14	0	0
984 ^{68,c}	BPHC3H6+H= C ₆ H ₅ C ₃ H ₇	1.00E+14	0	0
985 ^{68,c}	APHC3H6+H= C ₆ H ₅ C ₃ H ₇	1.00E+14	0	0
986 ^{65,d}	CPHC3H6=C ₆ H ₅ C ₂ H ₃ +CH ₃	2.00E+13	0	42051
987 ^{65,d}	BPHC3H6=C ₆ H ₅ +C ₃ H ₆	2.00E+13	0	44167
988 ^{65,d}	APHC3H6=C ₆ H ₅ CH ₂ +C ₂ H ₄	2.00E+13	0	42051
989 ^{67,e}	C ₆ H ₅ C ₃ H ₇ =C ₆ H ₅ CH ₂ +C ₂ H ₅	3.00E+15	0	69600
990 ^{65,d}	C ₆ H ₅ C ₃ H ₇ =C ₆ H ₅ CH ₂ CH ₂ +CH ₃	8.00E+15	0	87862
991 ^{65,d}	C ₆ H ₅ C ₃ H ₇ =C ₆ H ₅ +NC ₃ H ₇	8.00E+15	0	102240
1010 ⁶¹	BPHC3H6 = BPHPROPY	2.00E+11	0	20000
1011 ⁶¹	BPHPROPY = C ₆ H ₅ C ₂ H ₃ +CH ₃	1.00E+14	0	49675
1013 ⁶⁰	BPHC3H6+H=C ₆ H ₆ +AC ₃ H ₅	1.00E+14	0	38000
1014 ⁶¹	BPHC3H6+O = C ₆ H ₅ CH ₂ +CH ₃ HCO	2.00E+13	0	4000
1015 ⁶¹	BPHC3H6+OH = C ₆ H ₅ CH ₃ +CH ₃ HCO	2.00E+13	0	4000
1016 ⁶¹	BPHC3H6+HO ₂ => C ₆ H ₅ CH ₂ +CH ₃ HCO+OH	2.00E+13	0	4000
1017 ⁶¹	CPHC3H6+O = C ₆ H ₅ CHO+C ₂ H ₅	1.60E+13	0	0
1018 ⁶¹	CPHC3H6+OH = C ₆ H ₅ CHO+C ₂ H ₆	1.60E+13	0	0
1019 ⁶¹	CPHC3H6+HO ₂ => C ₆ H ₅ CHO+C ₂ H ₅ +OH	5.00E+12	0	0

^aThe reaction number is the number of the reaction in the UIC n-Propylbenzene Oxidation Model

^bk = ATⁿ exp(−E_a/RT): rate constant (units: mol, s, cm³, cal).

^cEstimated based on rules proposed by Allara and Shaw⁶⁸

^dEstimated based on rules proposed by Dean⁶⁵

^eA-factor x 1.4

The rate constants for the abstraction of hydrogen atoms from the n-propyl side chain by R species (where R = H, OH, HO₂, CH₃ and O₂) were estimated from the rate constants of n-propane and toluene reactions. The procedure is described below and also shown in Table 7.

- 1) The rate constants for the abstraction of the primary hydrogens' by R species were estimated from rate constants for abstraction of the terminal hydrogens of n-propane by R species. Since there are half as many primary sites in n-propylbenzene as in n-propane, the pre-exponential factor is taken to be half of that of pre-exponential factor of the corresponding n-propane+R reaction and the same n and activation energy is considered
- 2) The rate constants for the abstraction of secondary hydrogens by R species are taken to be the same as that of the rate constants for abstraction of the secondary hydrogens in n-propane by corresponding R species
- 3) The rate constant of abstraction of benzylic hydrogens in the n-propylbenzene side chain by R species were estimated from the corresponding reactions for abstraction of the hydrogens from the methyl side chain in toluene. The estimated rate constants had the same n and activation energy but the pre-exponential factor was reduced by a factor of 2/3 to take into account the number of abstract-able hydrogens in the benzylic site of n-propylbenzene side chain when compared to the methyl side chain of toluene.

Table 7. Reactions of *n*-propylbenzene oxidation whose rate constant parameters were estimated based on the procedure described in Section 4.3.1

Reaction ^a Number	Reaction ^b	A	n	E _a	Modifications to the rate constant of reference reaction
Abstraction of the primary hydrogens					
992 ⁶⁹	$C_6H_5C_3H_7 + H = APHC3H6 + H_2$	6.63E+05	2.54	6756	A-factor x 0.5 of $C_3H_8 + H = NC_3H_7 + H_2$
993 ⁶⁹	$C_6H_5C_3H_7 + O = APHC3H6 + OH$	9.65E+04	2.68	3716	A-factor x 0.5 of $C_3H_8 + O = NC_3H_7 + OH$
994 ⁶⁹	$C_6H_5C_3H_7 + OH = APHC3H6 + H_2O$	2.97E+12	0.00	8219	A-factor x 0.5 of $C_3H_8 + OH = NC_3H_7 + H_2O$
995 ⁶⁹	$C_6H_5C_3H_7 + HO_2 = APHC3H6 + H_2O_2$	2.38E+04	2.55	16492	A-factor x 0.5 of $C_3H_8 + HO_2 = NC_3H_7 + H_2O_2$
996 ⁶⁹	$C_6H_5C_3H_7 + O_2 = APHC3H6 + HO_2$	1.99E+13	0.00	50933	A-factor x 0.5 of $C_3H_8 + O_2 = NC_3H_7 + HO_2$
997 ⁶⁹	$C_6H_5C_3H_7 + CH_3 = APHC3H6 + CH_4$	4.52E-01	3.65	7153	A-factor 0.5 of $C_3H_8 + CH_3 = NC_3H_7 + CH_4$
Abstraction of the secondary hydrogens					
998 ⁶⁹	$C_6H_5C_3H_7 + H = BPHC3H6 + H_2$	7.22E+05	2.40	4471	Same as $C_3H_8 + H = IC_3H_7 + H_2$
999 ⁶⁹	$C_6H_5C_3H_7 + O = BPHC3H6 + OH$	4.76E+04	2.71	2106	Same as $C_3H_8 + O =$ $IC_3H_7 + OH$
1000 ⁶⁹	$C_6H_5C_3H_7 + OH = BPHC3H6 + H_2O$	5.30E+12	0.00	5974	Same as $C_3H_8 + OH =$ $IC_3H_7 + H_2O$
1001 ⁶⁹	$C_6H_5C_3H_7 + HO_2 = BPHC3H6 + H_2O_2$	2.38E+04	2.55	16492	Same as $C_3H_8 + HO_2 =$ $IC_3H_7 + H_2O_2$
1002 ⁶⁹	$C_6H_5C_3H_7 + O_2 = BPHC3H6 + HO_2$	1.99E+13	0.00	50933	Same as $C_3H_8 + O_2 =$ $IC_3H_7 + HO_2$
1003 ⁶⁹	$C_6H_5C_3H_7 + CH_3 = BPHC3H6 + CH_4$	1.00E+00	3.46	5480	Same as $C_3H_8 + CH_3 =$ $IC_3H_7 + CH_4$
Abstraction of the benzylic hydrogens					
1004 ⁷⁰	$C_6H_5C_3H_7 + H = CPHC3H6 + H_2$	5.31E+02	3.4	3120	A-factor x (2/3) of $\Phi CH_3 + H = \Phi CH_2 + H_2$
1005 ⁷¹	$C_6H_5C_3H_7 + O = CPHC3H6 + OH$	1.97E+13	0.00	3522	A-factor x (2/3) of $\Phi CH_3 + O = \Phi CH_2 + OH$
1006 ⁷²	$C_6H_5C_3H_7 + OH = CPHC3H6 + H_2O$	1.63E+05	2.40	-602	A-factor x (2/3) of $\Phi CH_3 + OH = \Phi CH_2 + H_2O$
1007 ⁷⁰	$C_6H_5C_3H_7 + HO_2 = CPHC3H6 + H_2O_2$	6.23E+04	2.50	14683	A-factor x (2/3) of $\Phi CH_3 + HO_2 = \Phi CH_2 + H_2O_2$
1008 ⁷³	$C_6H_5C_3H_7 + O_2 = CPHC3H6 + HO_2$	1.74E+07	2.50	44946	A-factor x (2/3) of $\Phi CH_3 + O_2 = \Phi CH_2 + HO_2$

1009 ¹⁸	C ₆ H ₅ C ₃ H ₇ +CH ₃ =CPHC3H6+CH ₄	2.67E-05	5.60 9000	A-factor x (2/3) of ΦCH ₃ +CH ₃ =ΦCH ₂ +CH ₄
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^aThe reaction number is the number of the reaction in the UIC n-Propylbenzene Oxidation Model

^bk = ATⁿ exp(-Ea/RT): rate constant (units: mol, s, cm³, cal).

The estimated rate constants for abstraction of the n-propylbenzene side chain hydrogen atoms have been compared with other rate constants available in literature. Qi Chen and Froment⁷⁴ used bond dissociation energy, radical activity and thermochemistry as important guidelines to get an initial estimate of the rate constants. These rate constants were further constrained by minimization functions and thermodynamic analysis. Since the authors studied thermal, oxygen free cracking of the n-propylbenzene, only the rate constants for the pyrolytic steps of n-propylbenzene decay are provided. Dagaut et al.⁶¹ estimated the rate constants based on the rate rules given by Dean⁶⁵ and Walker⁶⁶ and from analogous n-propane, toluene and other alkyl radical reactions. Won et al.⁶² estimated the rate constants from analogous toluene reactions. The total rate constants for the abstraction of the n-propylbenzene side chain hydrogen atoms by H, O and OH radicals are compared in Fig 27. From the Fig 27 (a), it can be observed that all the estimated rate constants other than that of Qi Chen and Froment are within a factor a two. The reason for an order of magnitude difference between the rate constant provided by Qi Chen and Froment and the other three estimates is uncertain. A quick comparison of rate constants of other n-alkyl radical reactions in Qi Chen and Froment model with those currently available in literature also showed about an order of magnitude difference in rate constants. However, based on the agreement of our rate constants with those from Dagaut et al.⁶¹ and Won et al.⁶², the uncertainty in our estimated rate constants is probably no more than a factor of two.

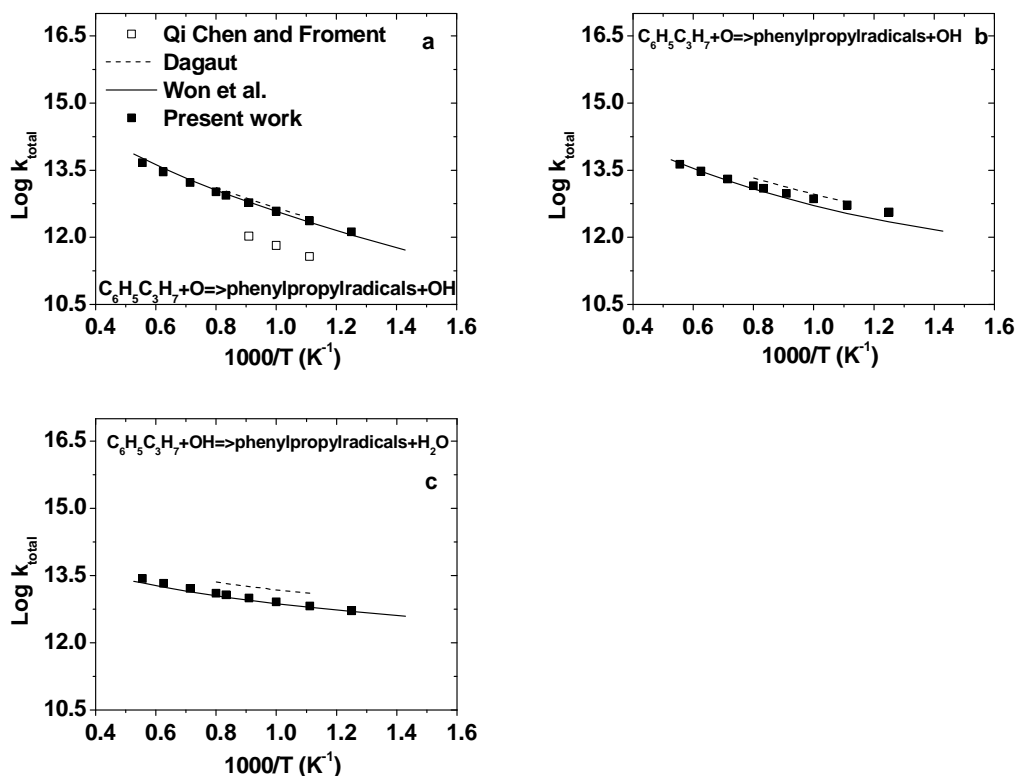


Fig 27. Comparison of total rate coefficients for the abstraction of side chain hydrogen atoms by H, O and OH radicals. [\square]-QiChen and Froment⁷⁴ (figure a), [-]-Won et. al.⁶² (figures a, b and c), [---] – Dagaut et. al.⁶¹ (figures a, b and c), [\blacksquare] – Present work (figures a, b, c), (a) $C_6H_5C_3H_7+H \Rightarrow$ phenylpropyl radicals + H_2 (b) $C_6H_5C_3H_7+O \Rightarrow$ phenylpropyl radicals + OH, (c) $C_6H_5C_3H_7+OH \Rightarrow$ phenylpropyl radicals + H_2O

The thermochemistry of n-propylbenzene and the phenylpropyl radicals were taken from Dagaut et al.⁶¹. Since this project is part of a collaborative effort with other universities⁸, the n-propylbenzene oxidation chemistry is coupled to a C₀-C₈ mechanism taken from Dooley et al.⁹, which includes the toluene, styrene, ethylbenzene, benzene chemistry and also the chemistry for the formation of lower carbon numbered intermediates from the above mentioned species up to CO and CO₂. The C₀-C₈ chemistry which is adopted from Dooley et al.⁹ also includes the H₂/O₂ chemistry.

The UIC n-Propylbenzene Oxidation Model has been validated against our high pressure experimental datasets (sections 4.3.2 and 4.3.3) and the flow reactor data of Litzinger et al.⁶⁰ and

jet stirred reactor data of Dagaut et al.⁶¹ (section 4.3.4). Unless specified, all the experimental profiles illustrated are denoted by symbols and all modeling results are denoted by lines.

4.3.2. Modeling of Aliphatic and Single Ring Aromatic Intermediates from the Shock Tube Experiments

The experimental and modeling profiles of n-propylbenzene and O₂, CO and CO₂ for all the experimental datasets are shown in Fig 28 and Fig 29 respectively. The model shows excellent agreement for the fuel decay for all the experimental datasets. The model also shows fairly good agreement with the oxygen decay and CO and CO₂ formation for all the experimental datasets. The excellent agreement of the experimental and modeling profiles for the fuel and oxygen decay for temperatures where the fuel is completely consumed (< 1300 K) during the observation time are suggestive that the oxidation kinetics of n-propylbenzene are accurate and sufficient. Other appropriate validation targets for the n-propylbenzene oxidation kinetics would be the concentration vs. temperature profiles of the stable intermediates like styrene, ethene, toluene, benzene, bibenzyl, ethane, methane and ethylbenzene.

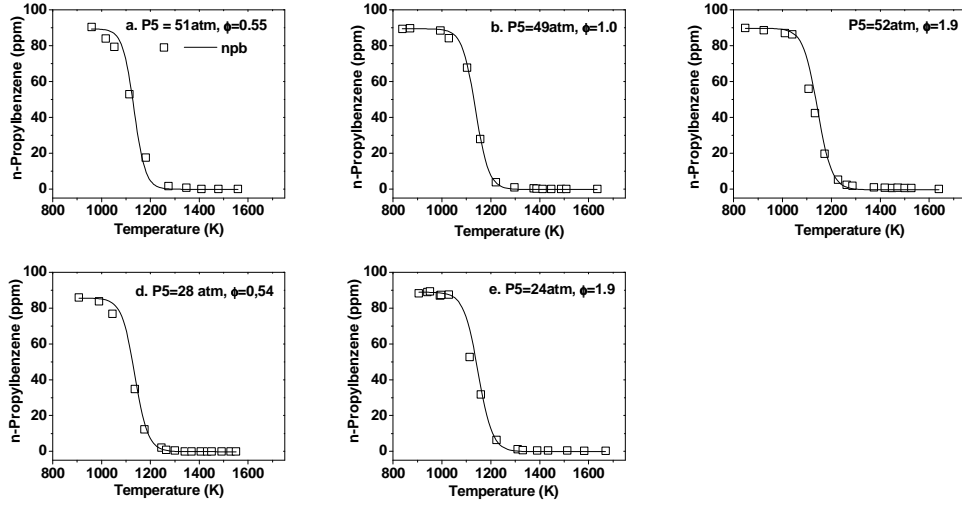


Fig 28. Experimental [□] and modeling profiles [-] of *n*-propylbenzene (npb) decay from the shock tube oxidation experiments of *n*-propylbenzene a) average $P_5 = 51$ atm, $\Phi = 0.55$ b) average $P_5 = 49$ atm, $\Phi = 1.0$, c) average $P_5 = 52$ atm, $\Phi = 1.9$, d) average $P_5 = 28$ atm, $\Phi = 0.54$ e) average $P_5 = 24$ atm, $\Phi = 1.9$

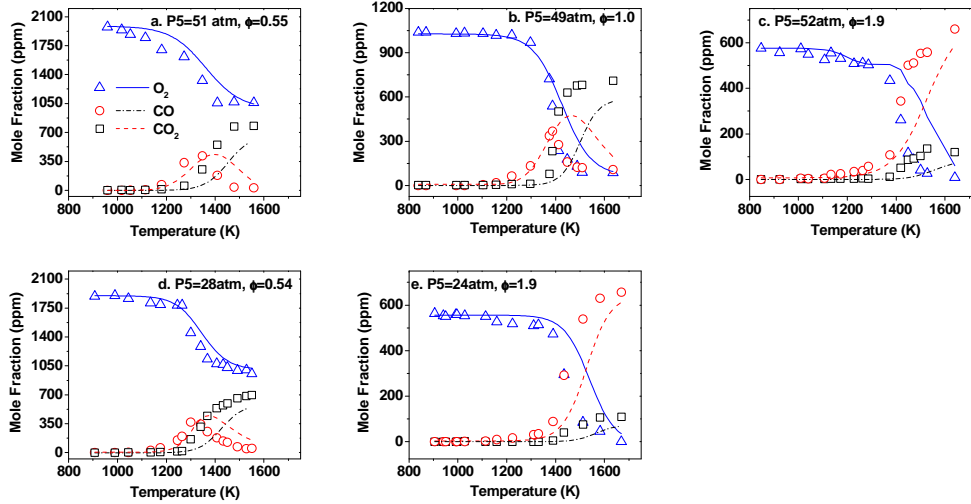
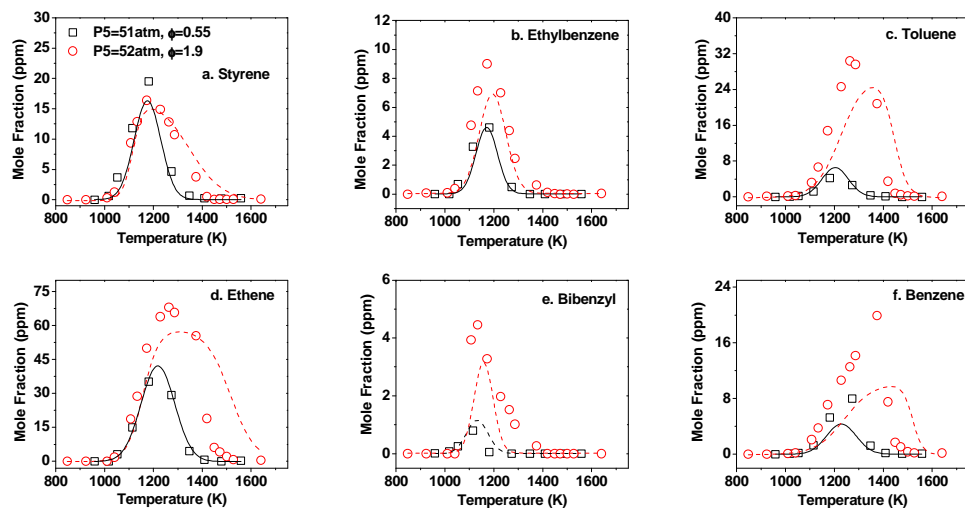


Fig 29. Experimental [□] and modeling profiles of O_2 [△, -] from the shock tube oxidation experiments of *n*-propylbenzene, CO [○, ---] and CO_2 [□, ...] a) average $P_5 = 51$ atm, $\Phi = 0.55$, b) average $P_5 = 49$ atm, $\Phi = 1.0$, c) average $P_5 = 52$ atm, $\Phi = 1.9$, d) average $P_5 = 28$ atm, $\Phi = 0.54$ e) average $P_5 = 24$ atm, $\Phi = 1.9$

The experimental and modeling profiles of the above mentioned intermediates are shown for a nominal reflected shock pressure of 50 atm and for two extremes of the equivalence ratio 0.5 and 1.9. The fuel lean and fuel rich datasets are chosen so that the differences in experimental and modeling species distribution could be distinctly observed. The experimental and modeling profiles for all the other experimental datasets can be found in the Appendix.

Among the single ring aromatics, fairly good agreement could be seen between the experimental and modeling profiles of styrene, ethylbenzene, toluene, ethene and bibenzyl for all the experimental conditions, shown in Fig 30 (a - e). Increased modeling peak concentrations of toluene, ethylbenzene, ethene, benzene and bibenzyl could be observed as we proceed from fuel lean to fuel rich experimental dataset, in Fig 30 (b – f) and this correlates with the results from the experiments.



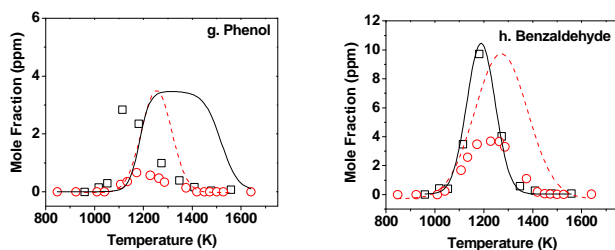


Fig 30. Experimental and modeling profiles of stable intermediates from the shock tube oxidation experiments of *n*-propylbenzene, [\square , -] - average $P5 = 51$ atm, $\Phi = 0.55$, [\circ , ---] - average $P5 = 52$ atm, $\Phi = 1.9$, a) Styrene, b) Ethylbenzene, c) Toluene, d) Ethene, e) Bibenzyl, f) Benzene, g) Phenol, h) Benzaldehyde

However, the modeling results for the fuel rich dataset show almost half the peak concentration of benzene than is found experimentally which could be attributed to the formation of increased amounts of phenol and benzaldehyde in the model. The dominance of the oxidation pathways of phenyl and benzyl radicals over the radical-radical recombination pathways leads to increased concentrations of phenol and benzaldehyde at fuel rich conditions and lower concentrations of benzene in the simulated profiles. The experimental and modeling profiles of phenol and benzaldehyde are shown in Fig 30 (g - h).

Among the aliphatics fairly good agreement is seen between the experimental and modeling profiles of methane ethane, acetylene, allene, propyne, 1,3-butadiene, vinylacetylene, and diacetylene and the profiles are shown in Fig 31 (a – i).

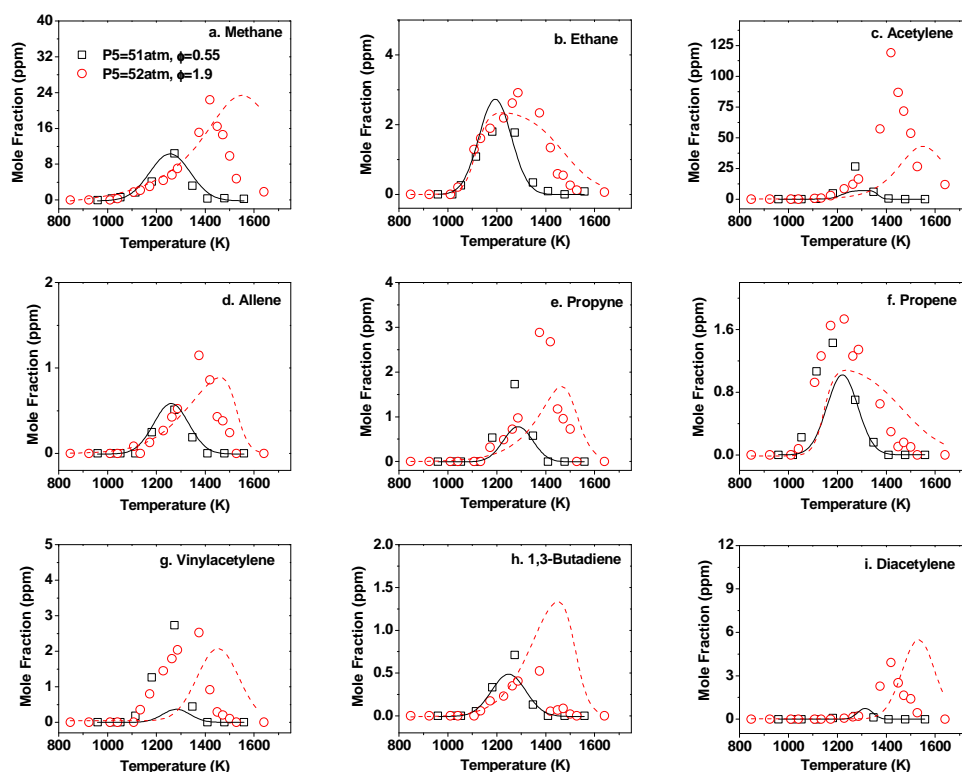


Fig 31. Comparison between experimental mole fraction profiles and model predictions [-] of stable intermediates formed from the shock tube oxidation experiments of *n*-propylbenzene. [□,-] - average $P5 = 51 \text{ atm}$, $\Phi = 0.55$, [○, ---] - average $P5 = 52 \text{ atm}$, $\Phi = 1.9$, a) Methane b) Ethane c) Acetylene d) Allene e) Propyne, f) Propene g) Vinylacetylene h) 1,3-Butadiene i) Diacetylene

For all the experimental datasets, the model shows fairly good results for the decay of the fuel and the formation of major intermediates like toluene, styrene, ethylbenzene, ethene and ethane, which are formed directly from the fuel and this assures us that the fuel decay part, C9 chemistry, is sufficiently accurate.

4.3.3. Modeling of Two Ringed and Three Ringed Aromatic Species from the Shock Tube experiments

Indene is the major polycyclic aromatic intermediate measured for all the datasets. The maximum concentration of indene attained for the stoichiometric and fuel lean data sets is about 6 ppm. The concentration of indene decreases to about 1 ppm for the fuel rich dataset. Minor amounts of naphthalene, benzofuran, ethynylnaphthalene, fluorene and anthracene were also measured.

Reactions for the formation of indene, naphthalene and anthracene were considered from the atmospheric pressure soot model of Slavinskaya and Frank⁷⁵. This model was developed for predicting the formation of polycyclic aromatic hydrocarbons and their growth up to five aromatic rings in methane and ethane fueled flames. It should be noted that the model of Slavinskaya and Frank has been developed for much lower pressures than those in our experiments; however their model could be used as an initial estimate of the important reactions in the formation of these polycyclic intermediates at our experimental conditions. Reactions for the formation of benzofuran, biphenylmethane and fluorene were included from High Temperature Mechanism of the Heavy Hydrocarbons from Ranzi's group⁷⁶.

The experimental and modeling profiles of indene are shown in Fig 32 and Fig 33. For our rich data about 1 ppm of indene is formed, whereas the modeling profiles show minor amounts, less than 0.3 ppm of indene being formed at higher temperatures, Fig 32 (a). Reaction path analysis of indene using the model that predicts indene in Fig 32 (a) at 1499 K for $\Phi = 1.9$, showed the contribution of cyclopentadienyl species in the formation of indene. Most of the indene at these conditions is formed from the recombination of cyclopentadienyl radical and vinylacetylene. Several recent studies⁷⁷⁻⁸⁰ have cited the importance of C5 species in the formation of indene and in the formation of other multi-ringed aromatic compounds. These pathways for the formation of indene by the recombination of C5 species seem to be relevant only for the fuel rich conditions and

at high temperatures. The modeling profiles (Fig 32 (b – c)) also show very low concentrations of indene being formed (< 0.02 ppm) at fuel lean and stoichiometric conditions, whereas the experiments show about 4 to 6 ppm of indene being formed at temperatures of around 1200 K, which is a significant amount for our low starting concentrations of n-propylbenzene. This severe under prediction of indene concentration in the modeling profiles indicates the possibility of having a different pathway for indene formation that is operative at lower temperatures ($T < 1400$ K) and for different equivalence ratios ($\Phi = 0.5 - 2.0$).

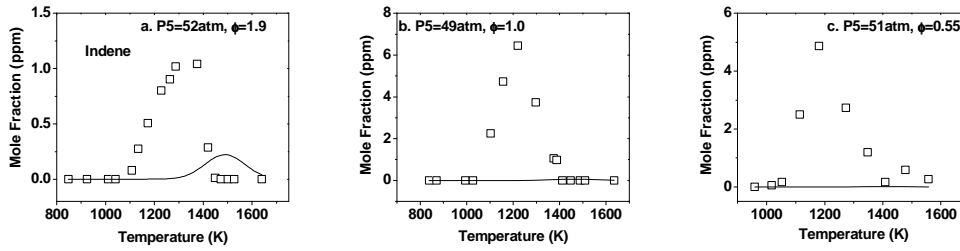


Fig 32. Comparison between experimental mole fraction profiles and model predictions [-] of indene from shock tube oxidation experiments of n-propylbenzene a) average $P5 = 52$ atm, $\Phi = 1.9$ b) average $P5 = 49$ atm, $\Phi = 1.0$ c) average $P5 = 51$ atm, $\Phi = 0.55$

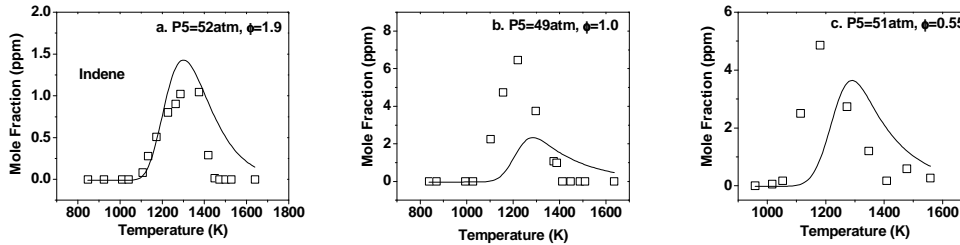


Fig 33. Comparison between experimental mole fraction profiles and model predictions [-] of indene from the shock tube oxidation experiments of n-propylbenzene a) average $P5 = 52$ atm, $\Phi = 1.9$ b) average $P5 = 49$ atm, $\Phi = 1.0$ c) average $P5 = 51$ atm, $\Phi = 0.55$

Lindstedt et al.⁸¹ and Vereecken and Peeters⁸² discuss in their paper the pathways for the formation of indene. The primary step is the formation of the C₉H₉ radical (1-phenyl-2-propenyl radical, referred to as RAD1 in Vereecken and Peeters⁸²) which subsequently cyclicizes and dissociates to form indene and a hydrogen atom. A detailed description of these pathways is provided in the references mentioned above and the kinetics for these pathways was adopted from Sivaramakrishnan et al.¹⁹ The C₉H₉ radical could be formed from the interactions of phenyl and allene, phenyl and propargyl radical and benzyl radical and acetylene. All these pathways were included in the sub-mechanism from Slavinskaya and Frank⁷⁵. Inclusion of these routes in the model had negligible effect on the production of indene for all the experimental conditions, which indicates the presence of another source for the formation of C₉H₉ radical. In addition to the pathways discussed previously, the C₉H₉ radical could also be formed from 1-phenyl-2-propyl radical by subsequent hydrogen abstraction reactions. The 1-phenyl-2-propyl radical dissociates to 1-propenylbenzene and H atom, and hydrogen abstraction reactions by H, OH, HO₂, CH₃ and O radicals produce 1-phenyl-2-propenyl radical (C₉H₉).

These pathways have been included in the model and are shown in Table 8. The modeling results with this set of kinetics are shown in Fig 33 (a – c) and considerable improvement in the prediction of indene concentrations could be observed. When Fig 32 (a - c) and Fig 33 (a – c) are compared, we can see that the peak modeling concentrations increased from 0.005 ppm to about 3.7 ppm, 0.016 ppm to 2.33 ppm and 0.2 to 1.4 ppm, for the fuel lean, stoichiometric and the fuel rich datasets respectively. Even though the modeling predictions are still lower than the experimental concentrations, the absence of these pathways severely under predicts the indene concentrations and hence the inclusion of these pathways was necessary. The sensitivity analyses of indene are shown in Fig 34. These analyses were performed for a pressure of 56 atm, temperature of 1250 K, a reaction time of 1.71 ms and for three different equivalence ratios. These conditions correspond to

the temperature at which peak concentrations of indene, about 4 ppm, are attained in the modeling profiles at fuel lean and stoichiometric conditions. The plot shows the normalized sensitivity coefficients of different reactions as a function of the equivalence ratio. From the graph it can be observed that the formation of indene is sensitive to the reactions producing 1-phenyl-2-propyl (BPHC3H6) and the C₉H₉ radical (reactions 998, 1000, 1027 and 1029).

Table 8. Reaction steps for the formation of C₉H₉ radical from 1-phenyl-2-propyl radical

Reaction ^a Number	Reaction ^b	A	n	E _a
1022 ^{65,c}	BPHC3H6=C ₆ H ₅ C ₃ H ₅ +H	3.00E+13	0	31586
1025 ^{65,c}	C ₆ H ₅ C ₃ H ₅ =C ₉ H ₉ +H	3.50E+15	0	107143
1026 ^{9,d}	C ₆ H ₅ C ₃ H ₅ +O=C ₉ H ₉ +OH	5.24E+11	0.7000	5884.0
1027 ^{9,d}	C ₆ H ₅ C ₃ H ₅ +OH=C ₉ H ₉ +H ₂ O	3.12E+06	2.0000	-298.0
1028 ^{9,d}	C ₆ H ₅ C ₃ H ₅ +HO ₂ =C ₉ H ₉ +H ₂ O	2.70E+04	2.5000	12340.0
1029 ^{9,d}	C ₆ H ₅ C ₃ H ₅ +H=C ₉ H ₉ +H ₂	1.73E+05	2.5000	2490.0
1030 ^{9,d}	C ₆ H ₅ C ₃ H ₅ +O ₂ =C ₉ H ₉ +HO ₂	4.00E+12	0.0000	39900.0
1031 ^{9,d}	C ₆ H ₅ C ₃ H ₅ +CH ₃ =C ₉ H ₉ +CH ₄	2.21E+00	3.5000	5675.0

^aThe reaction number is the number of the reaction in the UIC n-Propylbenzene Oxidation Model

^bk = ATⁿ exp(−E_a/RT): rate constant (units: mol, s, cm³, cal).

^cRate constant estimated based on rules proposed by Dean⁶⁵

^dRate constants same as analogous reactions of propene⁹

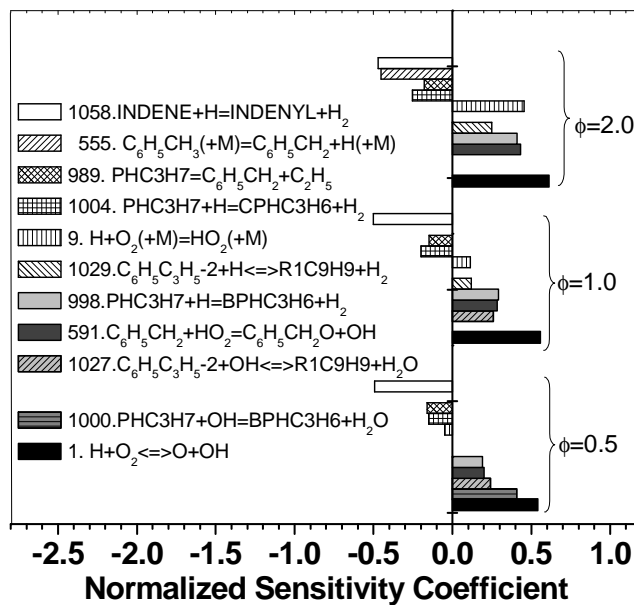


Fig 34. Sensitivity analysis of indene at different equivalence ratios for $P_5 = 55.9 \text{ atm}$, $T_5 = 1250 \text{ K}$ and reaction time = 1.71 ms

The experimental and modeling profiles of naphthalene at fuel lean conditions are shown in . The experimental and modeling profiles of naphthalene, fluorene and anthracene at stoichiometric and fuel rich conditions are shown in Fig 36 and Fig 37. The modeling profiles show less than 3 ppm, 0.5 and 2 ppm of naphthalene, fluorene and anthracene being formed for the experimental data set at fuel rich conditions (Fig 37). Unlike indene, naphthalene does not show a specific trend in its maximum peak concentration as a function of the equivalence ratio. The maximum peak concentrations of naphthalene in the experimental profiles are 0.3 ppm at $\Phi = 0.55$, 1.8 ppm at $\Phi = 1$ and 1.2 ppm at $\Phi = 1.9$. The maximum amount of naphthalene was formed at stoichiometric conditions. Since the experimental uncertainties in quantifying the polycyclic aromatic hydrocarbons is about 15-20 %, the maximum concentrations in naphthalene for the stoichiometric

and fuel rich conditions could be similar. The modeling profiles show that the maximum concentration of naphthalene increases as the Φ increases. The sensitivity analyses of naphthalene are included in Fig 38. These analyses were performed for a pressure of 56 atm, temperature of 1250 K, a reaction time of 1.71 ms and for three different equivalence ratios. From the graph it can be observed that the naphthalene formation is sensitive to the reactions involving phenylethynyl, cyclopentadienyl and benzyl radicals (reactions 1077, 1071 and 1076). The concentration of these species increases with increasing Φ , which results in increased formation of naphthalene in the modeling profiles. The displaced peaks for the other three ringed compounds like anthracene and fluorene could be due to unaccounted formation and consumption reactions.

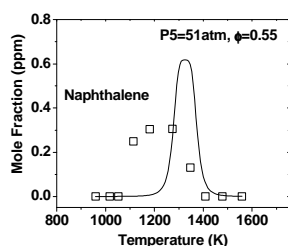


Fig 35. Comparison between experimental mole fraction profiles and model predictions [-] of naphthalene from shock tube oxidation experiments of *n*-propylbenzene, [□] – average $P5 = 51$ atm, $\Phi = 0.55$

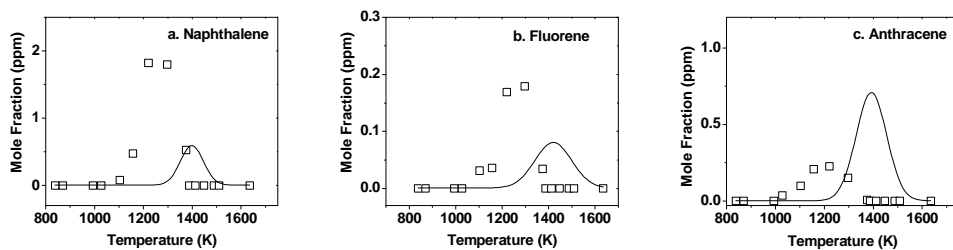


Fig 36. Comparison between experimental mole fraction profiles and model predictions of stable intermediates formed from the shock tube oxidation experiments of *n*-propylbenzene, [□] – average $P_5 = 49$ atm, $\Phi = 1.0$, a) Naphthalene b) Fluorene c) Anthracene

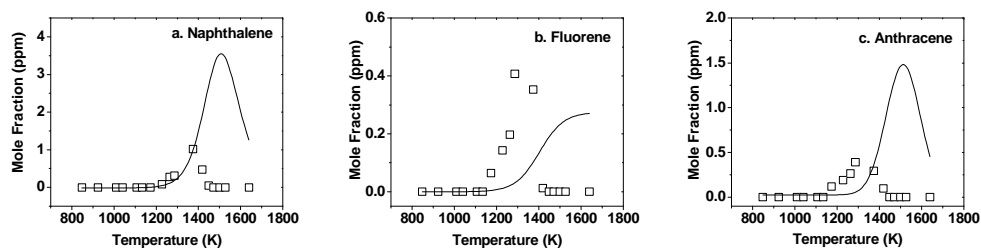


Fig 37. Comparison between experimental mole fraction profiles and model predictions [-] of stable intermediates formed from the shock tube oxidation experiments of *n*-propylbenzene, [□] – average $P_5 = 52$ atm, $\Phi = 1.9$ a) Naphthalene b) Fluorene c) Anthracene

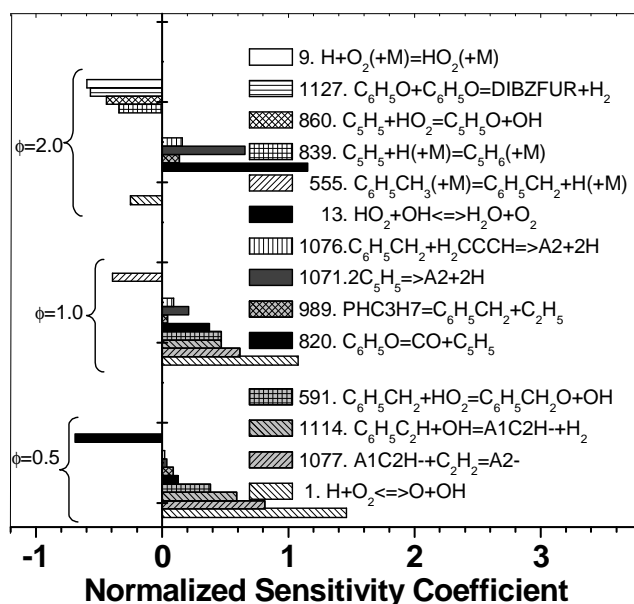


Fig 38. Sensitivity analysis of the naphthalene at different equivalence ratios for $P_5 = 55.9 \text{ atm}$, $T_5 = 1250 \text{ K}$ and reaction time = 1.71 ms

The modeling profiles for the other two intermediate benzofuran are shown in Fig 39. These graphs show benzofuran formation at higher temperatures only for the fuel rich dataset. The model includes the steps for formation of benzofuran by recombination and elimination reactions of phenoxy radicals with acetylene, styryl radicals with O and OH, benzyl radicals with CO and HCO and phenyl radicals with CH_3O ⁷⁶. Another route for the formation of benzofuran is from dibenzofuran. Including the pathway for the formation of dibenzofuran by recombination of phenoxy radicals and elimination of H_2O ⁸³ showed considerable amounts i.e., about 8 - 15 ppm of dibenzofuran in the modeling profiles, denoted by triangles in Fig 39. The reaction network for the formation of benzofuran from dibenzofuran is shown in Fig 40 as proposed in literature^{84,85} but detailed kinetics has not been provided as a result of which only a qualitative mechanistic

description is shown. In general, the model shows satisfactory predictions for the formation of two ringed and three ringed compounds.

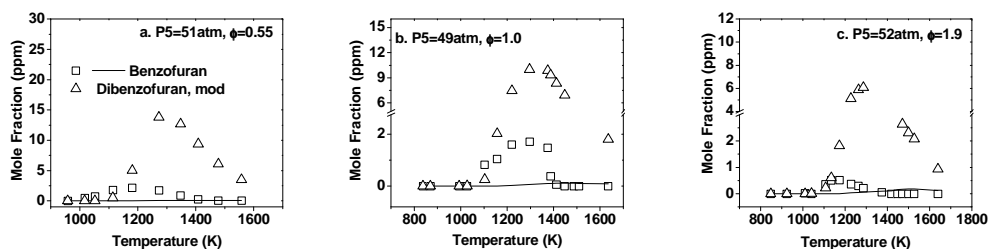


Fig 39. Comparison between experimental mole fraction profiles of benzofuran from the shock tube oxidation experiments of *n*-propylbenzene and model predictions of benzofuran and dibenzofuran, [\square] – benzofuran experimental profiles, [–] – benzofuran modeling profiles, [Δ] – dibenzofuran modeling profiles, a) average $P5 = 51$ atm, $\Phi = 0.55$ b) average $P5 = 49$ atm, $\Phi = 1.0$ c) average $P5 = 52$ atm, $\Phi = 1.9$

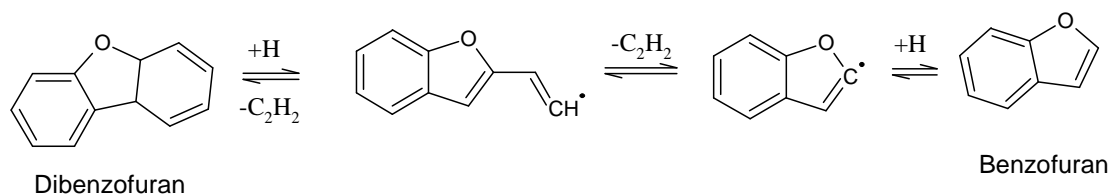


Fig 40. Reaction mechanism for the formation of benzofuran from dibenzofuran⁸⁵

4.3.4. Comparison with Other Experimental Data Available in Literature

The UIC n-Propylbenzene Oxidation Model has been compared against the flow reactor oxidation data of Litzinger et al.⁶⁰ and the jet stirred reactor data of Dagaut et al.⁶¹ and the results are discussed in sections 4.3.4.1 and 4.3.4.2 respectively. Published ignition delay data available in the literature is limited to the study by Roubaud et al.⁶³. This data is at a lower temperature (600 – 900 K) than our experimental data. It was further discussed in a later publication by these authors⁸⁶ that including the low temperature chemistry is crucial in predicting their ignition delay data. Since the fuel decay for our experimental conditions occurs at higher temperatures (> 1000 K), the low temperature chemistry for n-propylbenzene oxidation was not included. Hence the model is not compared against the ignition delay data of Roubaud et al.⁶³. Validation of the flame speed data⁶² requires additional evaluation of new thermochemical parameters as well as transport parameters which is beyond the scope of the current work.

4.3.4.1. Modeling of Major Intermediates from the Flow Reactor Data

The experimental data from Litzinger et al.⁶⁰ and the modeling profiles of the fuel and the major intermediates are shown in Fig 41 (a – i). The model shows very good agreement with the fuel decay for all the experimental data sets. It also shows fairly good agreement with most of the major intermediates like styrene, toluene, ethylbenzene and ethene. From the profiles it can be noticed that a majority of styrene was formed when compared to toluene for the experimental conditions of Litzinger et al.⁶⁰ and the model could capture the fuel decay and the formation of toluene and styrene satisfactorily.

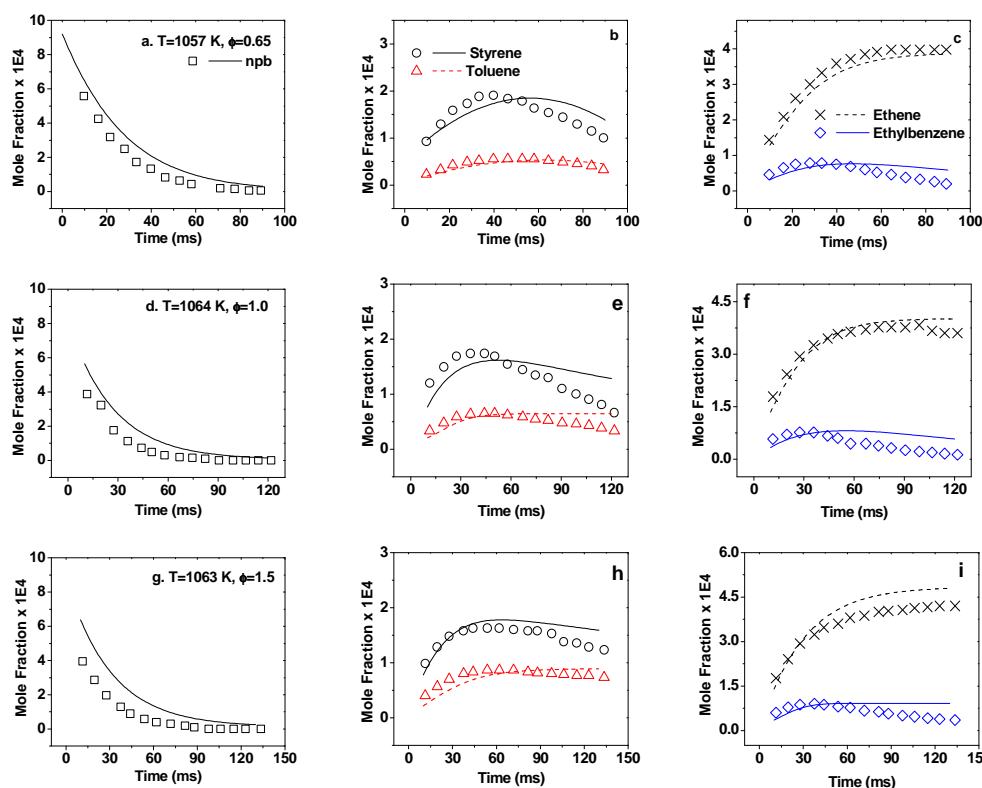


Fig 41. Experimental and modeling profiles of stable intermediates from the atmospheric pressure flow reactor oxidation experiments of *n*-propylbenzene⁶⁰, [\square , -]-*n*-Propylbenzene, [Δ , --]-Toluene, [\circ , -]- Styrene, [\diamond , -]- Ethylbenzene, [\times , ---]- Ethene, [a - c] – $T = 1057\text{ K}$, $\Phi = 0.65$, [d - f] – $T = 1064\text{ K}$, $\Phi = 1.0$, [g - i] – $T = 1063\text{ K}$, $\Phi = 1.5$, time shift = 0 ms.

4.3.4.2. Modeling of Major Intermediates from the Jet-stirred Reactor Data

The UIC *n*-Propylbenzene Oxidation Modeling results are plotted against Dagaut et al.⁶¹ experimental data in Fig 42. The model shows fairly good agreement with the fuel decay and styrene formation. The model under predicts the formation of toluene, ethylbenzene and ethene. The agreement between experimental and the modeling profiles for these species improves considerably as the equivalence ratio is increased.

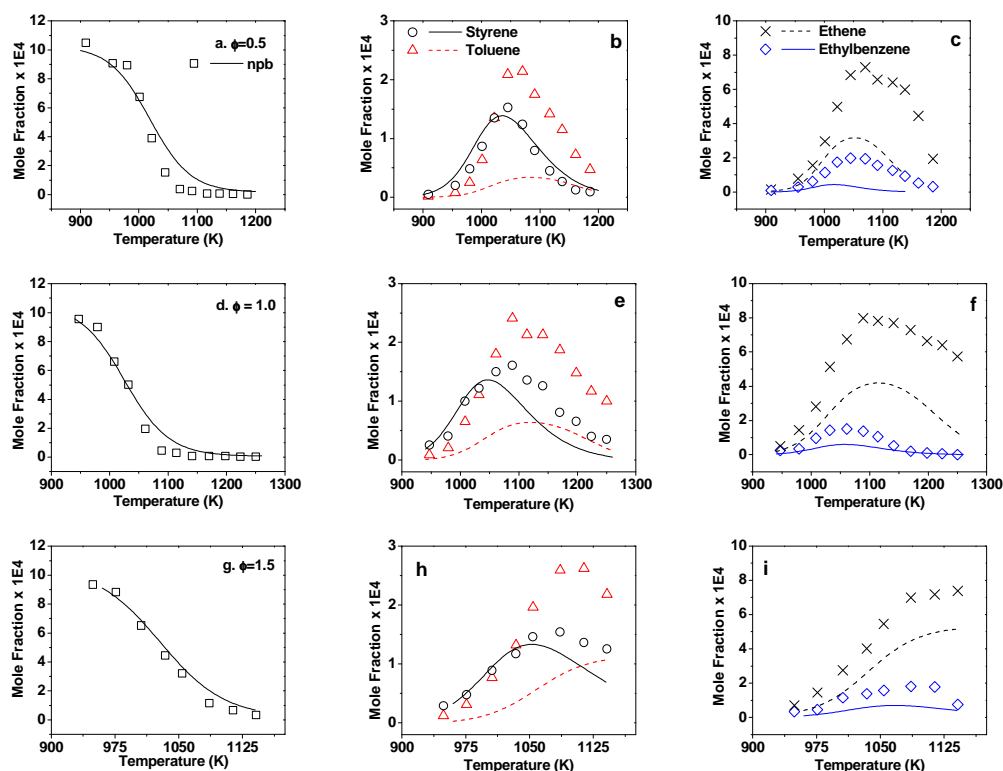


Fig 42. *Experimental and modeling profiles of stable intermediates from the atmospheric jet-stirred reactor oxidation experiments of n-propylbenzene⁶¹, n-Propylbenzene [\square , -], Toluene [Δ , --], Styrene [O , -], Ethylbenzene [\diamond , -], Ethene [\times , ---], [a – c] – $\Phi = 0.5$, [d - f] – $\Phi = 1.0$, [g - i] – $\Phi = 1.5$*

Considerable agreement between the experimental and the modeling results for the fuel decay indicates that the overall kinetics for n-propylbenzene decay is accurate. We have discussed in the previous sections about the major pathways responsible for n-propylbenzene decay and the important role played by the hydrogen abstraction and the homolysis reaction in the fuel decay and the formation of the intermediate species. Comparison of the total rate constants for the hydrogen abstraction reactions in Fig 27 (a – c) showed that the largest deviation between our estimated rate constants and the rate constants estimated by Dagaut et al. is within a factor of two. However, the branching ratios for the abstraction of hydrogen atoms from different sites of the n-propylbenzene

side chain by H, O and OH radicals differ significantly and these plots are shown in Fig 43 (a-c). The branching ratios calculated using our estimated rate constants are shown by symbols and the branching ratios calculated using Dagaut et al.⁶¹ rate constants are shown as straight lines.

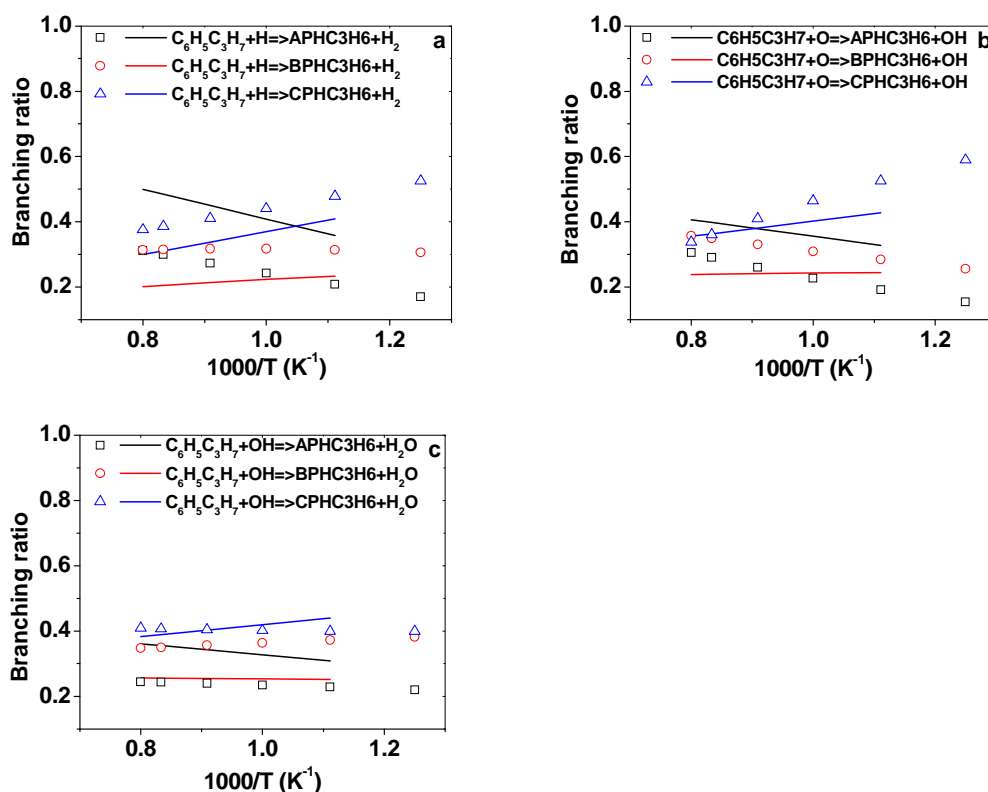


Fig 43. Branching ratios for the formation of 3-phenyl-1-propyl (APHC3H6), 1-phenyl-2-propyl (BPHC3H6) and 1-phenyl-1-propyl radicals (CPHC3H6) by hydrogen abstraction reactions with (a) H (b) O and (c) OH radicals computed using rate constants estimated by Dagaut et al.⁶¹ (lines) and in our present work (open symbols). [\square , -]- $C_6H_5C_3H_7+R=APHC3H6+RH$, [\circ , -]- $C_6H_5C_3H_7+R=BPHC3H6+RH$, [\triangle , -]- $C_6H_5C_3H_7+R=CPHC3H6+RH$

From Fig 43 (a) we can observe from that the Dagaut et al. branching ratios for the abstraction of hydrogen atom from the primary sites ($\text{C}_6\text{H}_5\text{C}_3\text{H}_7 + \text{H} \Rightarrow \text{APHC}_3\text{H}_6 + \text{H}_2$) by H radical are consistently higher and the branching ratios for the abstraction of hydrogen atom from the benzylic sites by H radical ($\text{C}_6\text{H}_5\text{C}_3\text{H}_7 + \text{H} \Rightarrow \text{CPHC}_3\text{H}_6 + \text{H}_2$) are consistently lower than that of the present work. This difference in the branching ratios results in greater formation of toluene, ethylbenzene and ethene when Dagaut et al. model is used. Comparison of the homolysis rate constants also showed that the rate constant proposed by Dagaut et al. is a factor of 3 higher than the rate constant used by us, which was taken from an experimental study⁶⁷. However if we use similar branching ratios and the same rate constant for homolysis reaction as that of Dagaut et al., the predictions of toluene, ethene and ethylbenzene can be improved but there will also be a disagreement in predicting not only our experimental data but also the flow reactor data of Litzinger et al. The UIC n-Propylbenzene Oxidation Model thus provides an optimum agreement between all the three experimental datasets and any variation in the rate constants would result in either under predicting or over predicting the major intermediates for the other two datasets. Hence, the rate constants were not modified.

4.3.5. Interpretation of the Experimental Data using the UIC n-Propylbenzene Oxidation Model

Two different fuel decay behaviors could be observed from our shock tube experiments and the flow reactor experiments of Litzinger et al.⁶⁰. Within the range of fuel decay, the shock tube experiments show increasing relative maxima of toluene when compared to styrene with increasing Φ . In contrast, the flow reactor experiments of Litzinger et al.⁶⁰ show slightly increasing contributions of toluene with Φ and a dominance by styrene. In order to gain some insight into this difference in the species distribution, all the experimental data available in literature have been

compiled and analyzed in the following sections. Since the UIC n-Propylbenzene Oxidation Model shows fairly good predictions against our experimental data and the flow reactor data of Litzinger et al.⁶⁰, it has been used to perform a reaction path analysis of the fuel, to reveal the important pathways from the fuel to the formation of these intermediates.

4.3.5.1. Low Temperature Datasets

Litzinger et al.⁶⁰ performed n-propylbenzene oxidation at 1060 K, for $\Phi = 0.65$ to 1.5 and at atmospheric pressures. The authors have observed increased amounts of styrene when compared to toluene for their experimental conditions. The ratio of toluene to styrene increases from 0.34 to 0.45 for $\Phi = 0.65$ to 1.5 and a residence time of 40 ms. Qi Chen and Froment⁷⁴ studied the thermal cracking of n-propylbenzene at a pressure of 1.3 bar for a temperature range of 893 – 1063 K. The authors have reported greater yield of styrene when compared to toluene over their range of experimental conditions. Dagaut et al.⁶¹ has also observed lower amounts of toluene being formed when compared to styrene at temperatures less than 1050 K from their experimental data. Our experiments also showed similar results at lower temperatures. The toluene to styrene ratio from our experiments increased from 0.10 to 0.34 for $\Phi = 0.5$ to 1.9 and these ratios were computed at 1107 K, a nominal pressure of 50 atm and reaction time of 1.71 ms.

Since the model shows fairly good agreement for the production of styrene and toluene, both at atmospheric and high pressures, it can be used to perform a reaction path analysis of the fuel, to gain insight into the important pathways from the fuel to the formation of these intermediates. The cumulative percentage contributions of different pathways to the fuel decay forming 1-phenyl-1-propyl (CPHC3H6), 2-phenyl-1-propyl (BPHC3H6) and 3-phenyl-1-propyl radical (APHC3H6) and benzyl radicals (homolysis pathway) are shown as a function of equivalence ratio in Fig 44 (a). This

analysis was performed for a temperature of 1108 K, pressure of 56 atm and a reaction time of 1.71 ms for three different equivalence ratios, $\Phi = 0.55, 1$ and 1.9. From the figure it can be noticed that the contribution of the hydrogen abstraction pathways decreases slightly with an increase in equivalence ratio and the contribution of the homolysis route increases slightly. The formation of 1-phenyl-1-propyl and 2-phenyl-1-propyl radicals leads to the formation of styrene, the formation of 3-phenyl-1-propyl radicals and the homolysis route produce toluene. Even though there is a cumulative 8 % increase in the benzyl radical production routes from fuel lean to fuel rich conditions, the formation of benzyl radicals at such low temperatures leads to increase in bibenzyl concentrations rather than increase in toluene. Based on this analysis and the experimental results we can conclude that irrespective of the pressure and equivalence ratio, styrene is always found to be the major intermediate for temperatures around 1060 K.

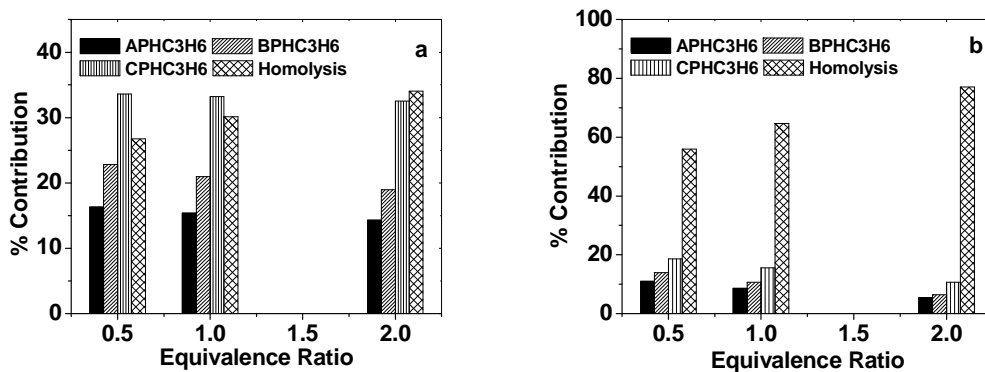


Fig 44. Percentage contribution of different pathways to fuel decay as a function of equivalence ratio, (a) $P_5 = 55.9$ atm, $T_5 = 1108$ K and reaction time = 1.71 ms, (b) $P_5 = 55.9$ atm, $T_5 = 1250$ K and reaction time = 1.71 ms

The sensitivity analysis of the fuel is shown in Fig 45 and it was performed for a temperature of 1250 K, a pressure of 55.9 atm and a reaction time of 1.71 ms. At lower temperatures the fuel decay is sensitive to the formation phenylpropyl radicals by hydrogen abstraction reactions and benzyl radicals by the homolysis route (reactions 1000, 1009, 998, 1006, 1004 and 989).

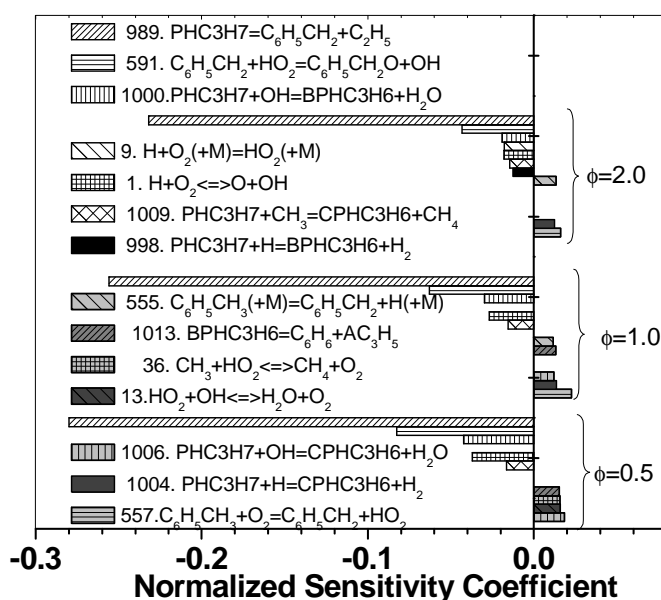


Fig 45. Sensitivity analysis of the fuel at $P5 = 55.9 \text{ atm}$, $T5 = 1108 \text{ K}$ and reaction time = 1.71 ms.

4.3.5.2. High Temperature Datasets

At high temperatures the relative maximum of toluene or styrene at a particular temperature depends on the Φ . For our experimental datasets, the ratio of toluene to styrene increases from 0.57

to 2.75 for $\Phi = 0.5$ to 1.9, for a temperature of about 1275 K and a nominal pressure of 50 atm. This increase in toluene concentrations with temperature was also observed in a few other experimental studies available in literature. Dagaut et al.⁶¹, observed higher amounts of toluene being formed when compared to styrene at higher temperatures from their experimental data. The only other available high temperature study of n-propylbenzene is that of Anderson et al.⁸⁷. The authors studied the naphthalene formation pathways in non-premixed methane flames doped with alkylbenzenes. High concentrations of toluene when compared to styrene were observed in the n-propylbenzene flames, at temperatures of about 1600 K.

The cumulative percentage contributions of different pathways to the fuel decay forming 1-phenyl-1-propyl (CPHC3H6), 2-phenyl-1-propyl (BPHC3H6) and 3-phenyl-1-propyl radical (APHC3H6) and benzyl radicals (homolysis pathway) are shown as a function of equivalence ratio in Fig 44 (b). This analysis was performed for a temperature of 1250 K, pressure of 56 atm and a reaction time of 1.71 ms for three different equivalence ratios, $\Phi = 0.55$, 1 and 1.9. From the figure, we can notice that the contribution of the homolysis route to the fuel decay increases significantly with an increase in equivalence ratio, which results in the increased formation of toluene at stoichiometric and fuel rich conditions and this was observed from both the experimental and the modeling results. However, at fuel lean conditions, even though the contribution of the routes for the formation of benzyl radical (homolysis and 3-phenyl-1-propyl radical) is almost twice greater than the routes forming styrene, the benzyl radicals oxidize to form benzaldehyde (a maximum of 10 ppm measured in the fuel lean dataset), thereby resulting in lower amounts of toluene being formed when compared to styrene. As the concentration of oxidizer decreases a lower amount of benzaldehyde is formed and this results in increased formation of toluene. Based on this analysis and the experimental results discussed above, we can infer why the relative maximum of toluene or styrene for temperatures above 1200 K depends on the concentration of the oxidizer. The sensitivity

analysis of the fuel is shown in Fig 46 and it was performed for a temperature of 1250 K, a pressure of 55.9 atm and a reaction time of 1.71 ms. At higher temperatures, considerable increase in normalized sensitivity coefficients, from about 0.3 to 5 can be observed for the formation of benzyl radicals by the homolysis route, when compared to the normalized sensitivity coefficients at lower temperatures (compare reaction 989 in Fig 45 and Fig 46).

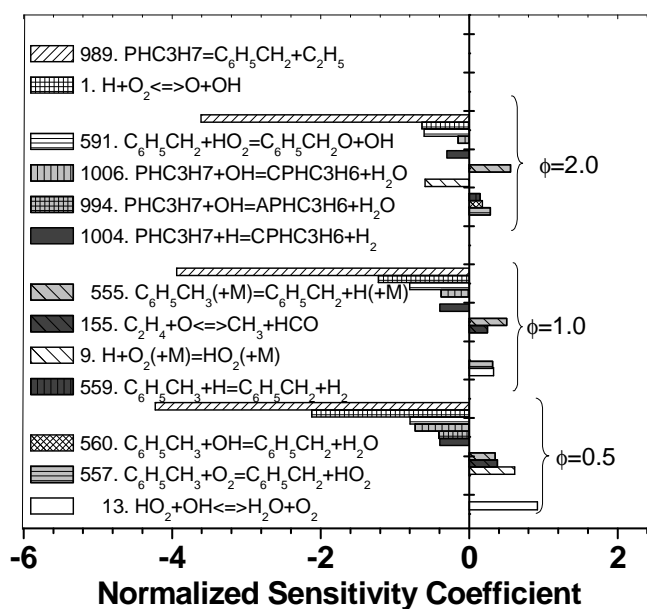


Fig 46. Sensitivity analysis of the fuel at $P_5 = 55.9 \text{ atm}$, $T_5 = 1250 \text{ K}$ and reaction time = 1.71 ms.

4.4. Conclusions

The oxidation of n-propylbenzene has been studied at nominal reflected shock pressures of 25 and 50 atm, for a temperature range of 838-1669 K at fuel lean, stoichiometric and fuel rich

conditions. Species concentrations of small hydrocarbons, mono-aromatic and multi-ringed aromatic species were obtained as a function of temperature. A kinetic model was assembled to describe the decay of n-propylbenzene and the formation of the stable intermediates, as measured from the experiments. The fuel decay pathways depended on the temperature. At low temperatures the majority of the fuel decayed by hydrogen abstraction reactions from the n-alkyl side chain. At high temperatures the majority of the fuel is consumed primarily by the homolysis route. A direct pathway from the fuel was identified to be responsible for minor amounts of indene being formed. The model simulates the fuel decay and formation of most of the intermediates accurately for all the experimental data sets. The model has also been validated against the flow reactor oxidation data and jet stirred reactor oxidation data available in literature.

5. DISCUSSION OF EXPERIMENTS AND MODELING RESULTS OF N-PROPYLBENZENE PYROLYSIS

5.1. Introduction

The detailed pyrolysis, i.e. oxygen free, chemical kinetics of n-propylbenzene compound has been investigated. Previous studies on n-propylbenzene kinetics were limited to oxidation^{60–63}. The oxidation studies provided valuable information regarding the influence of oxygen on the reactivity of the fuel and the formation of the intermediates for varied concentrations of oxygen. However, pyrolytic studies are also important in analyzing the fuel decay behavior without the influence of oxygen in regimes of combustion where thermal processes dominate. The pyrolytic reaction chemistry then becomes an important subset of combustion models. Hence, developing accurate kinetics for the pyrolytic reactions is critical in developing fully comprehensive combustion models. Therefore, we studied the pyrolysis of n-propylbenzene at conditions pertinent to combustion in practical devices, at an average pressure of 54 atm and temperatures from 1027-1678 K.

5.2. Experimental Results

n-Propylbenzene pyrolysis experiments were conducted at an average pressure of 54 atm and for a temperatures range of 1027-1678 K. These experiments were performed to extend the experimental validation database for n-propylbenzene kinetics to pyrolysis and to confirm that the hypothesized pyrolytic steps in our oxidation model⁸⁸ are accurate and sufficient. Most of the species measured for this set of experiments were similar to those measured in the shock tube oxidation experiments⁸⁸, except for a few species such as triacetylene, 1-ethynyl naphthalene, methylfluorene, diphenylethyne, methylanthracene, phenyl naphthalene, m-, p-terphenyl and

acenaphthylene. Since, it was not possible to distinguish, between the three ringed species, anthracene and phenanthrene, with the current experimental set-up, both these species were lumped into one species, which is referred to as anthracene in this paper. These species have been measured for the first time during the pyrolysis of n-propylbenzene. Leigh and Szwarc⁸⁹ investigated the pyrolysis of n-propylbenzene, but the authors' measured only ethylene concentrations from their experiments. Chen and Froment⁷⁴ studied the thermal cracking of n-propylbenzene and they measured only single ringed aromatic hydrocarbons from their experiments. Hence, the current study is of importance because of the measurement of species, a number of which, were not observed from the previous experimental studies reported in the literature.

The observed species distribution depended on the temperature range. At lower temperatures, of about 1052 K where the fuel starts to decay, several species such as ethane, ethene, propene, benzene, toluene, ethylbenzene, bibenzyl and styrene are formed. The fuel decay, formation and consumption profiles of these intermediates are shown in Fig 47 (a) and (b). The hydrogen abstraction reactions and the homolysis reactions of the side chain, lead to the above mentioned species and the specific pathways for the formation of these species will be discussed in the subsequent sections. Hence, at lower temperatures, the n-propyl side chain chemistry appears to be dominant and the reactions that occur are similar to the reactions of n-propane. These similarities were discussed in detail in Section 4.2.2.

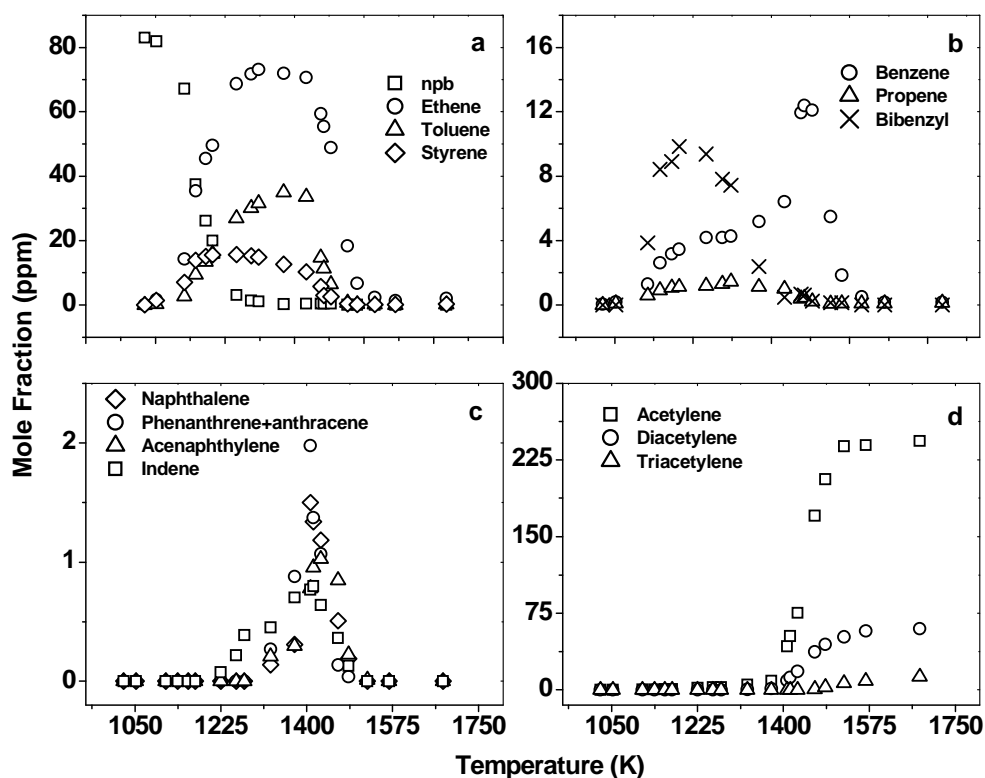


Fig 47. *n*-Propylbenzene decay and the formation of products.

Reactions at higher temperatures, greater than 1326 K, lead to the formation of two ringed and three ringed aromatic hydrocarbons, which can be attributed to the aromatic characteristic to *n*-propylbenzene. For example, considerable concentrations of species such as indene, naphthalene, anthracene and acenaphthylene are observed at a temperature of about 1326 K and these species profiles are shown in Fig 47 (c). At temperatures greater than 1400 K, the polycyclic aromatic hydrocarbons decay to form acetylene, diacetylene and triacetylene. The species profiles of these intermediates are shown as a function of reflected shock temperatures in Fig 47 (d). In fact, most of the polycyclic aromatic hydrocarbons observed in the pyrolysis experiments of *n*-propylbenzene, such as indene, naphthalene, anthracene and acenaphthylene are also formed from the high

temperature pyrolysis of toluene^{18,19,90,91}. This observation indicates that since toluene is the major intermediate formed from the side chain reactions of n-propylbenzene the subsequent reactions of the benzyl radical that results from toluene could be responsible for the formation of the polycyclic aromatic hydrocarbons. The specific pathways that are responsible for the formation of the major polycyclic aromatic hydrocarbons will be discussed in the subsequent sections.

5.3. Modeling

The UIC n-Propylbenzene Oxidation Model⁸⁸ has been used as the basis to simulate the experimental data since it contains within it a pyrolysis subset of reactions. The Oxidation Model has been validated for oxidation experiments, which included the speciation data from our shock tube⁸⁸, flow reactor data of Litzinger et al.⁶⁰ and jet stirred reactor data of Dagaut et al.⁶¹. The model showed excellent agreement with the fuel decay and the formation of the major intermediates, for these three different oxidation experimental datasets. Hence this model has been used as the initial basis for interpretation of the pyrolysis experiments. Only the oxygen free reaction subset of the UIC n-Propylbenzene Oxidation Model is considered to simulate the pyrolysis experimental data. This model which is devoid of any reactions involving oxygen containing compounds is the initial version of the UIC n-Propylbenzene Pyrolysis Model and is referred to as Mod1.

CHEMKIN 4.1.1⁵⁸ suite of programs was used to simulate our experimental data initially with Mod1. For the modeling calculations, the exact reaction time, temperature and pressure are specified for each shock along with the initial conditions of the fuel, oxidizer and the diluent. The simulations are performed assuming an adiabatic constant pressure process.

5.3.1. Modeling Results and Discussion

The experimental and modeling profiles of the fuel and the major intermediates such as ethene, toluene, styrene, bibenzyl, ethane, benzene and propene are shown in Fig 48 (a) and (b). The modeling profiles were generated using Mod1. The experiments are denoted by symbols and the modeling profiles are shown by the corresponding symbol and connecting line. The model, shows excellent agreement with the fuel decay and shows fairly good agreement with the formation of the other intermediates over the temperature range of the fuel decay i.e., from 1052 to 1257 K, which indicates that the reactions included in the Mod1 for fuel decay are sufficient and accurate. The percentage contribution of each reaction to the net rate of destruction of the fuel is shown in Fig 48 (c). This analysis was performed at a temperature of 1158 K and reaction time of 1.8 ms, which corresponds to the experimental conditions at which almost 50 % of the fuel has decayed. From the plot, Fig 48 (c), it is evident that about 60 % of the fuel decays by the homolysis reaction (reaction R6) and about 40 % of the fuel decays by hydrogen abstraction reactions from the propylbenzene side chain, producing radical species such as CPHC3H6 (1-phenyl-1-propyl radical), BPHC3H6 (1-phenyl-2-propyl radical) and APHC3H6 (3-phenyl-1-propyl radical). The sensitivity analysis of the fuel, which was also performed at the same experimental conditions shows that the fuel decay is most sensitive to the homolysis pathway (reaction R6). Previous studies^{60–62,88} have shown that the hydrogen abstraction pathways are important to the fuel decay in the presence of oxygen and at temperatures below 1060 K. In this pyrolysis study we have identified the homolysis pathway to be the dominant route for fuel consumption, irrespective of the temperature.

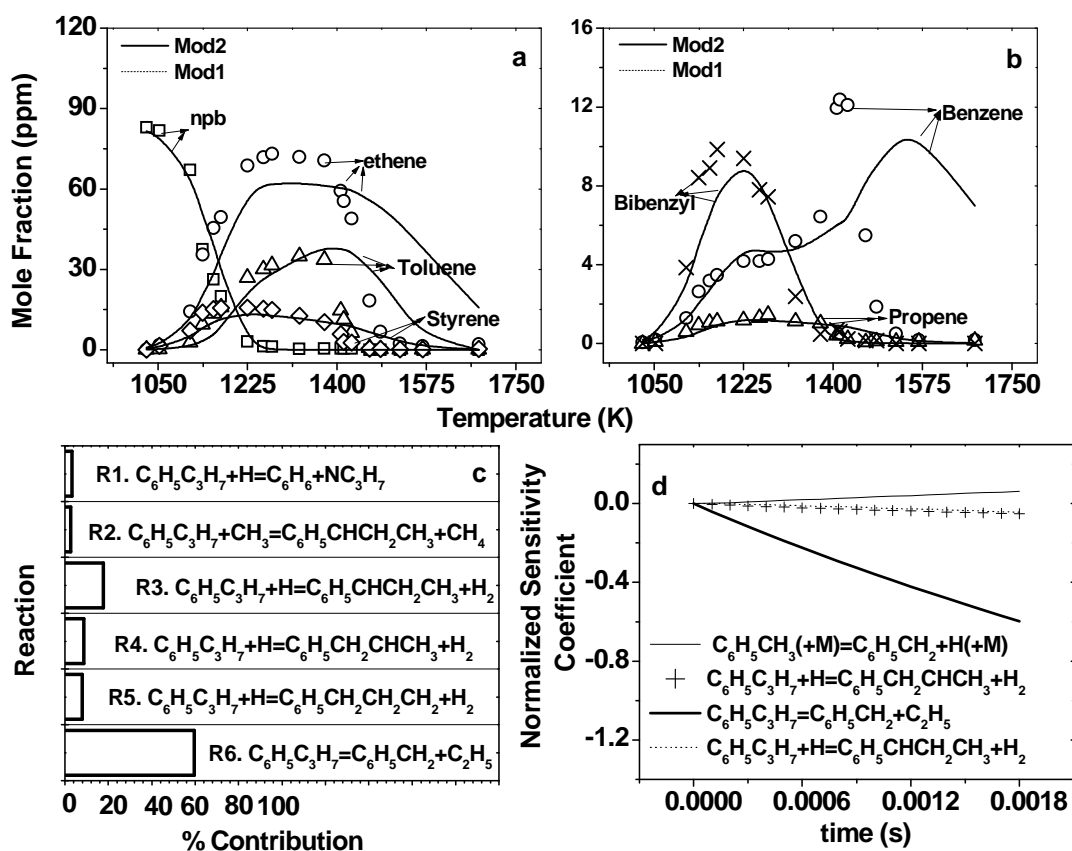


Fig 48. Experimental and modeling profiles of species using Mod1.

Bibenzyl is the major intermediate among the two ring aromatic hydrocarbon products. This species is formed by the recombination of benzyl radicals (reaction R18 in Table 9).

Table 9. Reactions in Mod1 responsible for the formation of naphthalene, indene and anthracene

Number	Reaction ^a	A	n	Ea
R16 ⁷⁵	$2C_5H_5 \Rightarrow A2+2H$	4.30E+13	0	9713
R18 ⁸	$C_6H_5CH_2+C_6H_5CH_2=C_{14}H_{14}$	5.00E+12	0	454
R19 ¹⁹	$R22C9H9=INDENE+H$	1.00E+13	0	37158
R20 ⁷⁵	$INDENYL+C_5H_5\Rightarrow A3+2H$	4.30E+13	0	9713
R21 ⁷⁵	$A2-+C_4H_4=A3+H$	3.30E+33	-5.7	25334

^a $k = AT^n \exp(-Ea/RT)$: rate constant (units: mol, s, cm³, cal).

From Fig 48 (b) it can be observed that the Mod1 shows fairly good prediction for the formation of bibenzyl. Among the polycyclic aromatic hydrocarbons the major species formed were indene, naphthalene, anthracene and acenaphthylene. The predictions of Mod1 are shown against the experiments in Fig 49, denoted by symbols and dashed lines. Mod1 over predicts the formation of naphthalene and under predicts the formation of indene and anthracene. Reaction path analysis of naphthalene was performed at a temperature of 1568 K, the temperature at which the maximum concentrations were predicted by Mod1. The reaction path analysis showed that naphthalene (A2) is formed primarily from the recombination of cyclopentadienyl radicals (R16 in Table 9). Reaction path analysis of indene at a temperature of about 1225 K showed that indene is formed from C₉H₉ radical, which is produced from 1-phenyl-2-propyl radical by subsequent hydrogen abstraction reactions⁸⁸ (R19 in Table 9). Modeling profiles showed the formation of anthracene (A3) at higher temperatures, which is produced as a result of recombination of indenyl and cyclopentadienyl radical and naphthyl radical (A2-) and vinylacetylene (R20 and R21 in Table 9). Since Mod1 did not quantitatively capture many of the polycyclic aromatic temperature profiles, the modifications,

as described in the following paragraph, were made to the model to predict the formation and consumption these major polycyclic aromatic hydrocarbons with greater agreement. In addition to this, the reactions for the formation of a number of other minor polycyclic aromatic hydrocarbons, which were not originally present in the Mod1, were also included, from various references^{76,92,93}. The references to this set of reactions are also provided in the model. This updated version of Mod1 is the final version of the UIC n-Propylbenzene Pyrolysis Model and is referred to as Mod2.

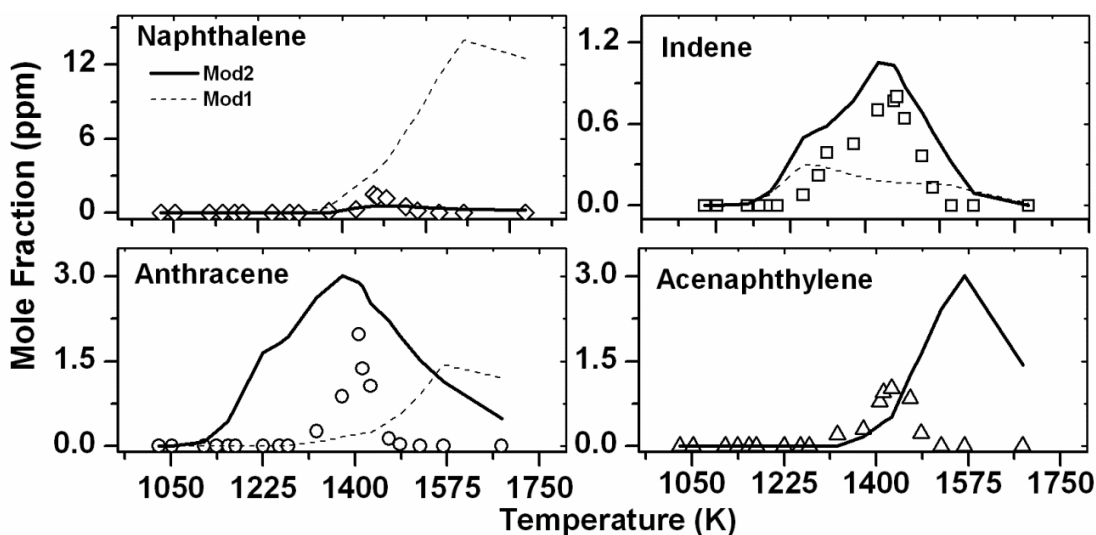


Fig 49. Experimental profiles and modeling predictions of polycyclic aromatic hydrocarbons, [Symbols]-Experiments

Since naphthalene is primarily formed from the recombination of the cyclopentadienyl radicals, in order to decrease the formation of naphthalene a number of the rate constants for the decay of cyclopentadiene and cyclopentadienyl radicals were updated from the recent publication of Robinson and Lindstedt⁹⁴ (R23, R24, R17 and R26 in Table 10). The authors theoretically

investigated the chemical kinetics of cyclopentadiene oxidation and pyrolysis. Inclusion of updated kinetics for these reactions has significantly reduced the formation of naphthalene in the modeling profiles, from 14 ppm to about 0.5 ppm and also increased the production of acetylene and diacetylene by about 40 ppm and 7 ppm, respectively (see Fig 49 and Fig 50).

Table 10. Reactions in Mod2 which are discussed in the text

Number	Reaction ^a	A	n	E
R14 ⁹²	$C_6H_5CH_2 + C_2H_2 = INDENE + H$	6.00E+11	0	9995
R23 ⁹⁴	$C_5H_5 + CH_3 = C_5H_4CH_3 + H$	2.00E+13	0	6214
R24 ⁹⁴	$C_5H_4CH_3 = C_5H_4CH_2 + H$	1.00E+17	0	51864
R17 ⁹⁴	$H_2CCCH + C_2H_2 = C_5H_5$	6.87E+55	-12.5	42017
R26 ⁹⁴	$C_5H_6 = C_5H_5 + H$	1.61E+16	0.86	89579
R27 ⁹³	$C_5H_5 + C_5H_5 = INDENYL + CH_3$	2.50E+12	0	9560
R28 ⁹¹	$C_{14}H_{12} \Rightarrow A3 + H_2$	2.50E+15	2	84700

^a $k = AT^n \exp(-Ea/RT)$: rate constant (units: mol, s, cm³, cal).

Updated rate constant for the formation of indene from the reaction of benzyl radical and acetylene⁹² has considerably increased the indene formation at temperatures greater than 1300 K (R27 in Table 10). The formation of anthracene at lower temperatures could not be reproduced by any of the reactions from the included references^{76,92,93}, which comprised of recombination

reactions among indenyl and cyclopentadienyl radicals, naphthyl radicals and diacetylene, vinylacetylene, phenylacetylene and phenyl radical, 1-ethynyl naphthyl radical and acetylene and biphenyl radicals and acetylene. The formation of anthracene at lower temperatures could be predicted, from stilbene through reaction, $C_{14}H_{12} \Rightarrow C_{14}H_{10} + H_2$ ⁹¹ (R28 in Table 10). The formation and consumption reactions of acenaphthylene were included from the atmospheric pressure soot model of Slavinskaya and Frank⁹². The predictions of Mod2 are shown in Fig 49 for the major polycyclic aromatic hydrocarbons and are denoted by symbols and lines. Mod2 also showed fairly good predictions for the formation of other minor intermediates.

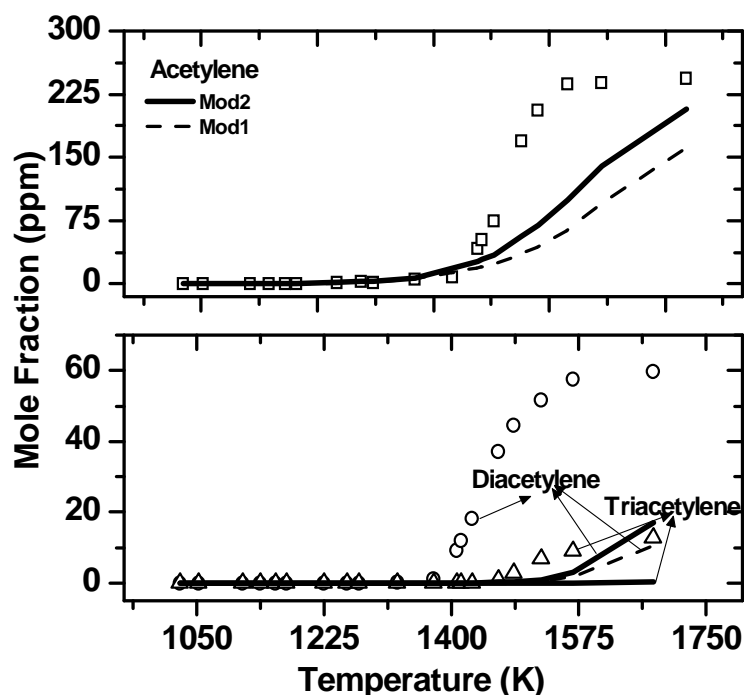


Fig 50. Experimental and modeling profiles of [□] -Acetylene, [○] - Diacetylene, [△] - Triacetylene, [Symbols]-Experiments

Based on the development of Mod2 two important observations could be made with regard to the formation of the polycyclic aromatic hydrocarbon species. The formation pathways of few of the intermediates like indene are dependent on the temperature. The sensitivity analysis of indene is shown in Fig 51 (a) and (b) at low and high temperatures respectively.

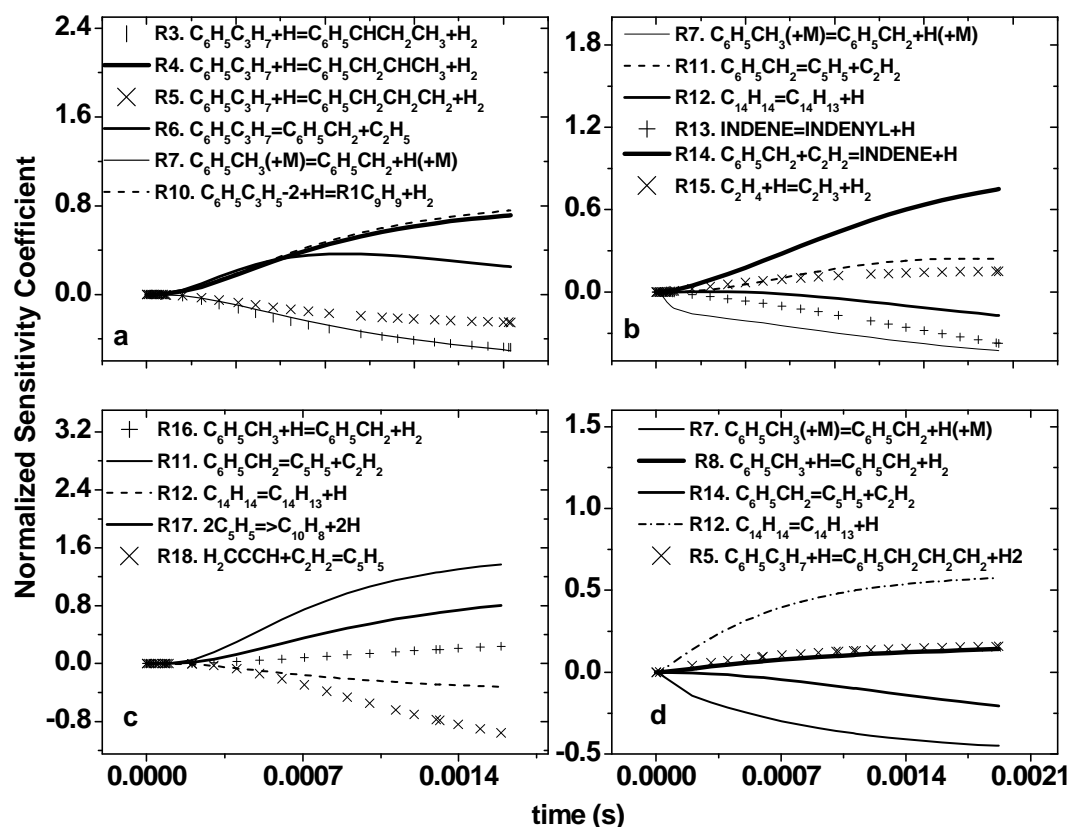


Fig 51. Sensitivity analysis of (a) Indene, $T_5 = 1225$ K, $P_5 = 56$ atm, $t = 2.04$ ms (b) Indene, $T_5 = 1375$ K, $P_5 = 52$ atm, $t = 1.92$ ms (c) Naphthalene, $T_5 = 1407$ K, $P_5 = 56$ atm, time = 1.59 ms (d) Anthracene, $P_5 = 52$ atm, $t = 1.92$ ms using Mod2

At low temperature the formation of indene is sensitive to the production of R1C9H9 and BPHC3H6 radicals (R4 and R10 in Fig 51 (a)). Both of these radicals are responsible for formation of indene at these low temperatures (also discussed in Section 4.3.3). At higher temperatures the formation of indene is sensitive to reaction of recombination of benzyl radical and acetylene and is also influenced by the production of benzyl and vinyl radicals (R11, R14 and R15 in Fig 51 (b)). The formation of a few of the polycyclic aromatic hydrocarbons is dependent on the radical pool formed from the breakdown of the fuel. For example, since the fuel decays primarily by homolysis pathway, the benzyl radical is one of the major intermediate species formed. We can observe from Fig 51 (c), that the formation of naphthalene is sensitive to the availability of benzyl radical and the intermediates produced from the decay of benzyl radicals, such as the cyclopentadienyl radical (R11, R16 and R17 in Fig 51 (c)). Benzyl radical also plays a role in the formation of indene (reaction R14) and is indirectly related to the formation of anthracene. The formation of anthracene is sensitive to the production of bibenzyl (R12 in Fig 51 (d)), which decays by hydrogen abstraction reactions to produce stilbene. Stilbene is responsible for the production of anthracene through reaction R28 in Table 10. Hence, the modeling results validate our initial hypothesis that the benzyl radicals could be responsible for the formation of the major polycyclic aromatic hydrocarbons.

The updated pyrolysis subset of reactions in Mod 2 has been included into the UIC n-Propylbenzene Oxidation Model. The revised UIC n-Propylbenzene Oxidation Model consisting of the updated pyrolysis subset of reactions showed similar predictions, when compared with the original oxidation data model, for the fuel decay and the formation of most of the intermediates which were primarily formed from the fuel decay such as toluene, styrene, bibenzyl, ethylbenzene, ethane, benzene and propene. However, the revised oxidation model showed increased consumption of oxygen and ethene by about 25 % and 40 % respectively, for temperatures greater than 1400 K and for fuel rich and stoichiometric conditions, when compared to the original model⁸⁸, resulting in

a greater agreement with the experimental data. The revised oxidation model also showed a significant increase in acetylene and indene concentrations for the experimental datasets at $\phi = 0.5$, 1 and 2, which results in the modeling profiles showing improved agreement with the experimental data. The revised model also showed the formation of anthracene at the right experimental temperatures and a decrease in the formation of naphthalene by about 90 %, irrespective of the equivalence ratio, which resulted in under predicted modeling concentrations of naphthalene for all the experimental datasets. Overall, including the updated pyrolytic subset of reactions into the UIC n-Propylbenzene Oxidation Model has also improved the predictions of a number of major species from the oxidation experiments such as oxygen, ethylene and acetylene, indene and anthracene.

5.4. Conclusions

The pyrolysis of n-propylbenzene has been investigated in the High Pressure Single Pulse Shock Tube (HPST) at University of Illinois at Chicago, for a nominal reflected shock pressure of 50 atm and for a temperature range of 1027 to 1678 K. Several stable intermediates have been measured from the experiments using gas chromatographic techniques. These intermediates included aliphatic, single ringed aromatic and polycyclic aromatic hydrocarbons. The subset of pyrolysis reactions in the UIC n-Propylbenzene Oxidation Model was utilized as a basis to model the formation of these stable intermediates. This model was further modified to include and update reactions for predicting the formation of polycyclic aromatic hydrocarbons, with greater agreement. From the final pyrolysis model, it was found for our experimental conditions, that the fuel decays primarily by a homolysis pathway which has been seen to be the dominant pathway, irrespective of the temperature range of the decay of the fuel. The formation pathways of indene were dependent on temperature. At low temperatures, indene formation was influenced by the presence of C_9H_9 radicals. At high temperatures,

indene was formed through the recombination pathway of benzyl radical and acetylene. Benzyl radical, cyclopentadienyl radical and propargyl radicals influenced the formation of other polycyclic aromatic hydrocarbons like naphthalene, anthracene and acenaphthylene.

6. DISCUSSION OF EXPERIMENTS AND MODELING RESULTS OF M-XYLENE OXIDATION

6.1. Introduction

The m-xylene experimental data available in literature fall into three categories: species profiles obtained from reactors^{64,95}, ignition delay time measurements in shock tubes^{96,97} and rapid compression machines⁶³ and laminar flame speeds⁹⁸. The temperature and pressure ranges over which these experiments were performed are shown in Table 11. Despite the number of experimental studies conducted there is a lack of experimental data simultaneously at high temperature and high pressure conditions, which are characteristic of combustion environments. To address this lack of data, as well as the absence of a validated chemical kinetic model at high temperature and pressure, the oxidation of m-xylene was studied in our high pressure single pulse shock tube (HPST).

Table 11. Experimental conditions of the m-xylene studies available in literature

Measurement	Pressure/atm	Temperature/K	Experimental Apparatus
species profiles ⁹⁵	1	~1160	Flow reactor
species profiles ⁶⁴	1	1050-1400	Jet-stirred reactor
ignition delay times ⁹⁶	7-9	1336-1712	Shock tube
ignition delay times ⁹⁷	9-45	941-1408	Shock tube
ignition delay times ⁶³	20	600-900	Rapid compression machine
burning velocities ⁹⁸	3	450	Spherical vessel
species profiles	27-53	1024-1584	Shock tube (this work)

6.2. Experimental Results

m-Xylene oxidation experiments were performed at fuel lean, stoichiometric and fuel rich conditions ($\Phi = 0.53, 1, 2.35$), for a temperature range of 1024-1583 K. Experiments at fuel lean and fuel rich conditions were done at two nominal reflected shock pressures of 25 and 50 atm, whereas all the experiments at stoichiometric conditions are at an average pressure of 51 atm. The diaphragm opening process causes minor variations ($\pm 20\%$) in the final pressure; consequently the experiments are referred to as being performed at “nominal” pressures as quoted above. The reaction times for these experiments are in the range of 1.5 ± 0.5 ms. The experimental conditions are listed in Table 12.

Table 12. m-Xylene experimental conditions

Average Shock Pressure /atm	Fuel /ppm	Temperature Range /K	Φ	Reaction Time /ms
27	102	1025-1561	0.62	1.37-2.01
52	103	1056-1569	0.55	1.28-1.97
50	61	1080-1514	1.2	1.35-2.1
27	90	898-1632	2.1	1.3-1.96
49	93	1131-1583	2.3	1.38-1.92
54	54	1060-1579	∞	1.28-1.91
50	102	1025-1741	∞	1.17-1.92

6.2.1. Effect of Pressure on m-Xylene Decay

The profiles of the fuel are shown as a function of temperature in Fig 52, for two different reflected shock pressures and similar equivalence ratios. Over the pressure and temperature range of the current experiments, no significant pressure dependence was seen for the decay of the fuel, oxidizer and for the formation of the intermediates.

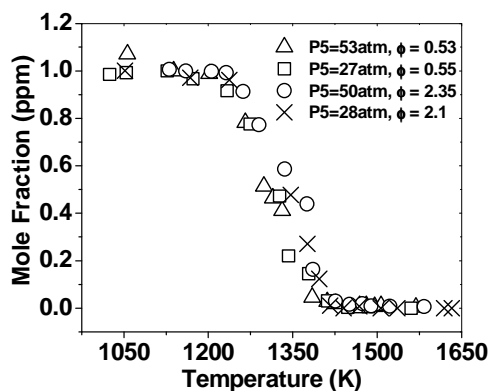


Fig 52. m-Xylene decay, [Δ]-average $P5 = 53 \text{ atm}$, $\Phi = 0.53$, [\square]-average $P5 = 27 \text{ atm}$, $\Phi = 0.55$, [\circ]-average $P5 = 50 \text{ atm}$, $\Phi = 2.35$, [\times]- average $P5 = 28 \text{ atm}$, $\Phi = 2.1$, nominal reaction time = 1.5 ms

6.2.2. Effect of Oxygen Concentration on the Fuel Decay

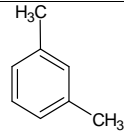
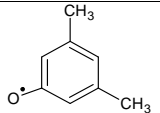
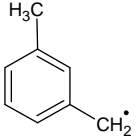
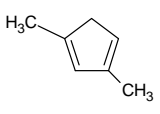
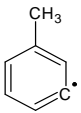
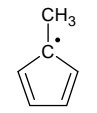
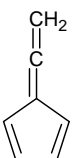
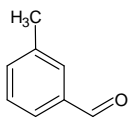
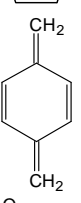
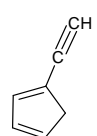
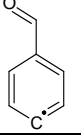
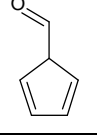
As seen in Fig 52, for similar temperatures a lower amount of m-xylene is consumed at fuel rich conditions when compared to the fuel lean conditions. The species distribution also varied for different equivalence ratios with greater number of polycyclic aromatic hydrocarbons being formed

for the experiments at fuel rich conditions when compared to the fuel lean and stoichiometric conditions. The structures of a few of these polycyclic aromatic hydrocarbons and other relevant species mentioned below can be found in Table 13 (T13) and Table 14 (T14). Note: Following the initial mention of species not thought to be of common knowledge a T13 or T14 is placed to provide the reader with a guide to location of the species structure.

Table 13. Structures of major polycyclic aromatic hydrocarbons measured in the m-xylene oxidation experiments

Species	Structure	Species	Structure
3, 3'- Dimethylbibenzyl (C ₁₆ H ₁₈)		di-m- Tolylmethane (C ₁₅ H ₁₆)	
m-Tolyl-p- tolylmethane (C ₁₅ H ₁₆)		Indene (C ₉ H ₈)	
Naphthalene (C ₁₀ H ₈)		Fluorene (C ₁₃ H ₁₀)	
Biphenylene (C ₁₂ H ₈)		Pyrene (C ₁₆ H ₁₀)	
Acenaphthylene (C ₁₂ H ₈)		Anthracene (C ₁₄ H ₁₀)	

Table 14. Structures of the species, whose reactions are discussed in this publication

Species	Structure	Species	Structure
m-Xylene ($C_6H_4(CH_3)_2$)		3,5-Dimethylphenoxy radical ($OC_6H_3(CH_3)_2$)	
m-Xylyl radical or m-methylbenzyl radical ($CH_3C_6H_4CH_2\cdot$)		1,3-Dimethylcyclopentadiene ($C_5H_4(CH_3)_2$)	
m-Methylphenyl radical ($C_6H_4CH_3\cdot$)		1-Methylcyclopentadienyl radical ($C_5H_4CH_3\cdot$)	
Fulvenallene (C_7H_6)		3-Methylbenzaldehyde ($CH_3C_6H_4CHO$)	
p-Xylylene ($CH_2C_6H_4CH_2$)		1-Ethynylcyclopentadiene ($C_5H_5C_2H$)	
m-Formylphenyl radical ($C_6H_4CHO\cdot$)		Formyl cyclopentadiene (C_5H_5CHO)	

6.2.2.1. Fuel Lean Oxidation ($\Phi = 0.53$)

Fuel lean oxidation experiments were performed for a temperature range from 1025 to 1560 K and nominal post reflected shock pressures of 25 and 50 atm.

Apart from the fuel and oxidizer, several other intermediates were also measured, among which the major small hydrocarbon intermediates formed were CO, CO₂, benzene (C₆H₆), toluene (C₆H₅CH₃), 3-methylbenzaldehyde (CH₃C₆H₄CHO)T14, methane (CH₄), acetylene (C₂H₂), and ethene (C₂H₄). Small amounts (<3 ppm) of 1-ethyl-3-methylbenzene (CH₃C₆H₄C₂H₅), styrene

($C_6H_5C_2H_3$), phenylacetylene ($C_6H_5C_2H$), 1, 3-cyclopentadiene (C_5H_6), vinylacetylene (C_4H_4), and ethane (C_2H_6) and trace amounts of allene (C_3H_4), propyne (C_3H_4), 1,3-butadiene (C_4H_6), 1,3-hexadiene (C_6H_{10}), p-xylene (C_8H_{10}), 1,3,5-cycloheptatriene (C_7H_8), 5-methylcyclopentadiene ($C_5H_5CH_3$), benzaldehyde (C_6H_5CHO) and 1-ethenyl-4-methyl-benzene ($CH_3C_6H_4C_2H_3$) were also measured.

The major species profiles are shown in Fig 53 and Fig 54 as a function of temperature. Above 1350 K, O_2 decays rapidly and CO and CO_2 start to build up. The aliphatic and aromatic intermediates reach their peak concentrations around 1350 K.

Dimeric species like bibenzyl ($C_{14}H_{14}$), 3,3'-dimethylbibenzyl ($C_{16}H_{18}$)T13, di-m-tolylmethane ($C_{15}H_{16}$)T13 and m-tolyl-p-tolyl-methane ($C_{15}H_{16}$)T13 were also formed from the interactions of benzyl, methylbenzyl (m-xylyl) and methylphenyl radicals. It can be seen from Fig 55 that 3,3'-dimethylbibenzyl and bibenzyl reach their maximum concentrations around 1250 K, which corresponds to the temperature at which almost 25% of the fuel has decayed. This observation suggests since 3,3'-dimethylbibenzyl, for example, is a recombination product of m-xylyl radical, that the fuel decays primarily to m-xylyl radical at temperatures below 1300 K. Above 1300 K the methylphenyl radicals are formed leading to the formation of small amounts of di-m-tolylmethane and m-tolyl-p-tolylmethane.

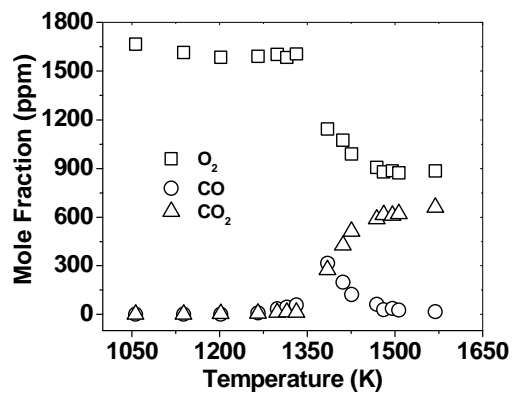


Fig 53. *m*-Xylene oxidation species profiles , average $P5 = 53 \text{ atm}$, $\Phi = 0.53$, nominal reaction time = 1.5 ms , $[\square]$ - O_2 , $[o]$ - CO , $[\Delta]$ - CO_2 ,

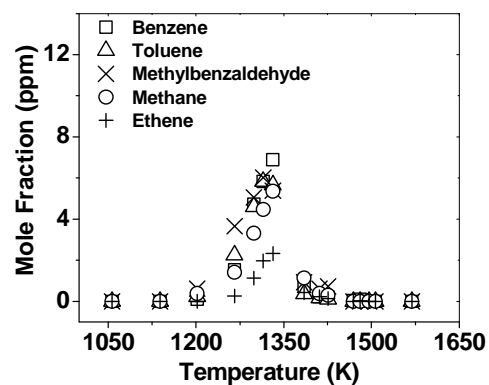


Fig 54. *m*-Xylene oxidation species profiles, average $P5 = 53 \text{ atm}$, $\Phi = 0.53$, nominal reaction time = 1.5 ms, $[\square]$ -Benzene, $[\Delta]$ -Toluene, $[X]$ - 3-Methylbenzaldehyde, $[o]$ -Methane, $[+]$ -Ethene

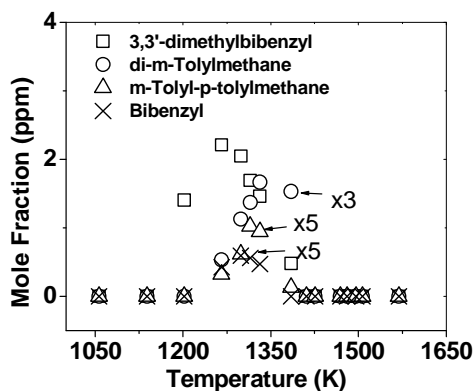


Fig 55. *m*-Xylene oxidation species profiles, average $P5 = 53$ atm, $\Phi = 0.53$, nominal reaction time = 1.5 ms [\square]-3,3'-Dimethylbibenzyl, [o]-di-*m*-Tolylmethane, [Δ]-*m*-Tolyl-*p*-tolylmethane, [X]-Bibenzyl

Other multi-ring aromatic hydrocarbons which were measured include indene (C_9H_8)T13, naphthalene ($C_{10}H_8$)T13, fluorene ($C_{13}H_{10}$)T13 and biphenylene ($C_{12}H_8$)T13.

The carbon totals were calculated for this set of experiments and are shown in Fig 56. Almost 95 % of the carbon was recovered for this set of experiments. Except for the oxygenated species like 3-methylbenzaldehyde and benzaldehyde, all the other aromatic and aliphatic species observed in this set of experiments were also measured in experiments at stoichiometric and fuel rich conditions.

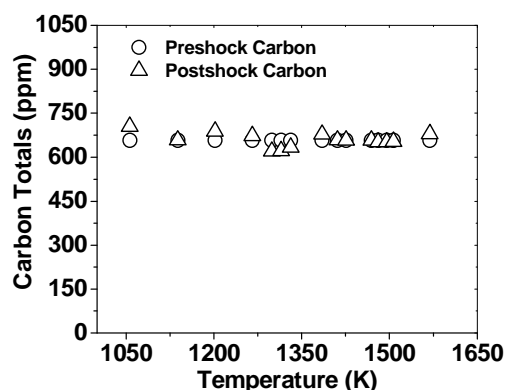


Fig 56. *m*-Xylene oxidation carbon totals, average $P_5 = 53$ atm, nominal reaction time = 1.5 ms, $\Phi = 0.53$, [o]-Preshock carbon, [Δ]-Postshock carbon

6.2.2.2. Stoichiometric Oxidation ($\Phi = 1.2$)

Stoichiometric oxidation experiments were performed for a temperature range from 1079 to 1514 K and an average post reflected shock pressure of 49 atm. New species which were measured in this set were diacetylene (C_4H_2), triacetylene (C_6H_2), 1-methylindene ($C_{10}H_{10}$), acenaphthylene ($C_{12}H_8$)T13, anthracene ($C_{14}H_{10}$)T13, 2-ethynylnaphthalene ($C_{12}H_8$), 4-methylfluorene ($C_{14}H_{12}$) and diphenylethyne ($C_{14}H_{10}$).

6.2.2.3 Fuel Rich Oxidation ($\Phi = 2.35$)

Fuel rich oxidation experiments were performed for a temperature range from 1079 to 1583 K and an average post reflected shock pressures of 28 and 50 atm at fuel rich conditions

Fig 57 shows the carbon totals as a function of temperature for this set of experiments.

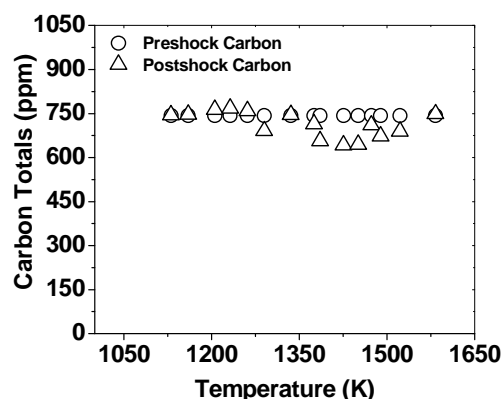


Fig 57. *m*-Xylene oxidation carbon totals, average $P5 = 50 \text{ atm}$, $\Phi = 2.35$, nominal reaction time = 1.5 ms, [o]-Preshock carbon, [Δ]-Postshock carbon

More than 95% of carbon is recovered for temperatures up to 1385 K which corresponds to the temperature for which almost 85% of the fuel is consumed. In between 1385 K and 1450 K about 86% of the carbon is recovered. For temperatures below 1385 K maximum mole fractions of the polycyclic aromatic hydrocarbon intermediates were formed, which explains the good carbon balance at these temperatures. Some of these PAH intermediates are shown in Fig 58 and Fig 59. At temperatures in between 1385 and 1450 K these intermediates decay, possibly forming heavier aromatics which were not identified in the present set up. Heavy aromatics up to pyrene ($C_{16}H_{10}$)T13 were measured in the current experiments. It was found to be important to measure even sub-ppm levels of these polycyclic aromatic hydrocarbons so as to attain better carbon recovery. The highest carbon number hydrocarbon measured for these sets of experiments was pyrene ($C_{16}H_{10}$); even 0.5 ppm of measured pyrene will have an 8 carbon count which accounts for 1% loss of carbon.

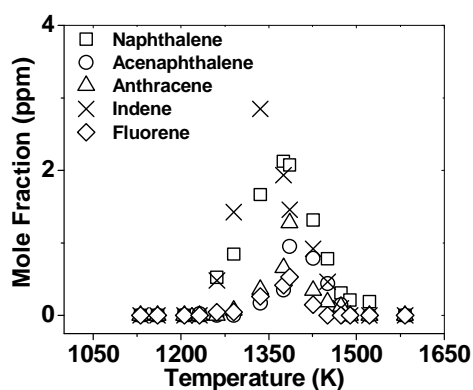


Fig 58. *m*-Xylene oxidation species profiles, average $P5 = 50$ atm, $\Phi = 2.35$, nominal reaction time = 1.5 ms, [□]-Naphthalene, [Δ]-Anthracene, [X]-Indene, [o]-Acenaphthylene, [◇]-Fluorene

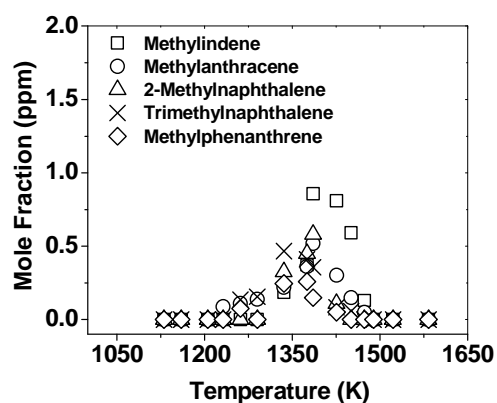


Fig 59. *m*-Xylene oxidation species profiles, average $P5 = 50$ atm, $\Phi = 2.35$, nominal reaction time = 1.5 ms, [□]-1-Methylindene [Δ]-1-Methylnaphthalene, [X]- 1,3,6-Trimethylnaphthalene, [o]-2-Methylanthracene, [◇]-2-Methylphenanthrene

The pathways involving polyacetylenic species could be important in the decay and formation of polycyclic aromatic hydrocarbons⁹⁹. As shown in Fig 60, acetylene and diacetylene start building up around 1335 K and their maximum concentrations are attained at 1450 K, which is the same temperature window within which the maximum carbon loss is observed. Polyacetylenes

up to triacetylene (C_6H_2) were identified and quantified in the present experiments. Most of the carbon was recovered at temperatures above 1450 K since all the carbon is converted to CO and CO_2 in the oxidation experiments.

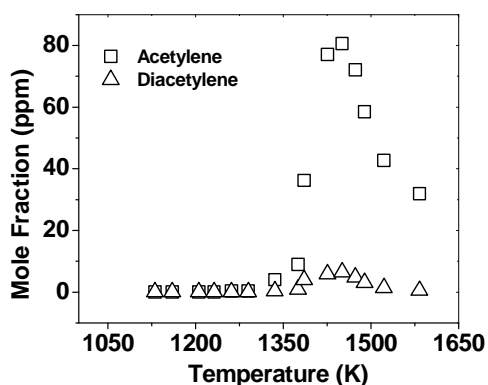


Fig 60. *m*-Xylene oxidation, species profiles, average $P_5 = 50$ atm, $\Phi = 2.35$, nominal reaction time = 1.5 ms, [\square]- Acetylene, [Δ]-Diacetylene

6.3. Modeling

As observed from the experiments, the oxidation of *m*-xylene produced both lower carbon number aromatics and aliphatics and higher carbon number aromatics than the fuel. This chapter discusses the modeling results up to the formation of the lower carbon number first aromatic ring. The modeling of the formation of higher carbon number multi-ring aromatic hydrocarbons from the fuel will be discussed in Chapter 8.

Three chemical kinetic models, the Gail and Dagaut model⁶⁴, the Battin-Leclerc et al. model⁹⁶, and Narayanaswamy et al. model⁹³ were initially used to simulate our experimental data.

The Battin-Leclerc et al. model had been validated against their shock tube ignition delay experiments of the xylenes, spanning a temperature range from 1300 to 1800 K and pressures from 6.7 to 9 atm. The Gail and Dagaut model was developed to simulate their m-xylene oxidation data in an atmospheric jet stirred reactor. The Narayanaswamy et al. model was validated against the experimental data available in literature and this includes the flow reactor experiments, shock tube ignition delay experiments and laminar burning velocities of m-xylene. Both the CHEMKIN 3.6.2⁵⁷ and CHEMKIN 4.1.1⁵⁸ suite of programs were used to simulate our experimental data with these models. For the modeling calculations, the exact reaction time, temperature and pressure are specified for each shock along with the initial conditions of the fuel, oxidizer and the diluent.

The Battin-Leclerc et al. model provides a better fit to the experimental data than the Gail and Dagaut model and the Narayanaswamy et al. model but all the three of them fail to predict the experimental data accurately. The Gail and Dagaut model and the Narayanaswamy et al. model show lower consumption of the fuel and oxygen and formation of the intermediates. The Battin-Leclerc et al. model shows fairly good consumption of fuel and oxygen but shows displaced profiles for the formation and consumption of the intermediates, like CO, benzene and toluene as seen in Fig 61 and Fig 62. Improved agreement of the Battin-Leclerc et al. model with the experimental data can be achieved by modifying or including the reactions to which the fuel decay and formation of intermediates is sensitive. This model has been built in a hierarchical fashion and consists of their toluene, benzene and C₀-C₅ oxidation mechanisms. However, as a result of greater familiarity with and confidence our own high pressure toluene oxidation and pyrolysis models, an independent m-xylene oxidation model has been developed based on our previous work.

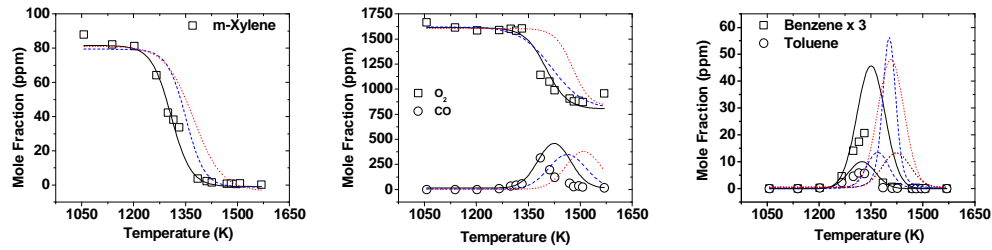


Fig 61. Comparison of experimental and modeling profiles for *m*-xylene oxidation, average $P5 = 53$ atm, $\Phi = 0.53$, nominal reaction time = 1.5 ms, $[\square]$ -Experiments, $[-]$ -Battin-Leclerc et al. model⁹⁶, $[\dots]$ -Gail and Dagaut model⁶⁴, $[- -]$ -Narayanaswamy et al. model⁹³

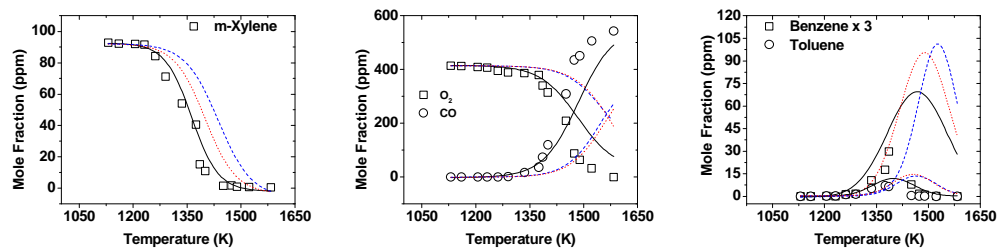


Fig 62. Comparison of experimental and modeling profiles for *m*-xylene oxidation, average $P5 = 51$ atm, $\Phi = 2.35$, nominal reaction time = 1.5 ms, $[\square]$ - Experiments, $[-]$ -Battin-Leclerc et al. model⁹⁶, $[\dots]$ -Gail and Dagaut model⁶⁴, $[- -]$ -Narayanaswamy et al. model⁹³

6.3.1. The High Pressure Toluene Oxidation Model

The high pressure toluene oxidation model¹⁰⁰ was used as the base model in constructing the *m*-xylene oxidation model. Hence, it was important to update the rate parameters and include additional pathways as available from the literature. The rate constants for the pyrolytic steps of toluene, CO/H₂ oxidation and ethane oxidation were updated from the references^{18,19,101,102}, all of which have been studied in our laboratory. In addition to this, rate constants for a few important reactions were updated based on the suggestions of Vasu et al.⁷². Recent experimental and

modeling work have highlighted the dominance of a few pathways in toluene oxidation such as, the decomposition of the benzyl radical^{103,104}, the benzyl+O₂, methylphenyl+O₂ and benzyl+HO₂ pathways^{105–108}. The benzyl radicals decays to form a seven carbon numbered intermediate, which has later been identified by theoretical calculations to be fulvenallene (C₇H₆)T14 by both Da Silva et al.¹⁰³ and Cavallotti et al.¹⁰⁴, and this further decays to form cyclopentadienyl radical and acetylene. Murakami et al.¹⁰⁹ investigated the potential energy surface for the reaction of benzyl radical with molecular oxygen, using ab initio calculations. Pressure dependent rate constants were calculated for the dissociation reactions of the benzylperoxy radicals, forming benzaldehyde and OH as the major products, along with minor amounts of phenoxy radical and formaldehyde. The addition of molecular oxygen to methylphenyl radicals forms methylphenoxy radical¹¹⁰ and fulvene, propyne, CO, CO₂ and ethenyl radical as products⁹³. All of the above reactions and subsequent reactions of fulvene forming benzene, phenyl¹¹¹ and propargyl radicals⁹³ have been included in the updated toluene oxidation model. The rate constants of the modified reactions and included pathways are shown in Table 15.

Table 15. Modifications and additions to the High Pressure Toluene Oxidation model referred to as Updated Toluene Oxidation Model 1

Reaction Number	Reaction ^a	A	n	E _a
R1 ⁷²	C ₆ H ₅ CH ₂ +C ₆ H ₅ CHO=C ₆ H ₅ CH ₃ +C ₆ H ₅ CO	2.18E+07	2.5	46045
R2 ⁷²	C ₆ H ₅ CH ₃ +OH=C ₆ H ₅ CH ₂ +H ₂ O	1.81E+05	2.39	-602
R3 ⁷²	C ₆ H ₅ CH ₃ +H=C ₆ H ₅ CH ₂ +H ₂	6.47E+00	3.98	3384
R4 ⁷²	C ₆ H ₅ CH ₃ +H=C ₆ H ₆ +CH ₃	3.90E+08	1.25	2371
R5 ⁹³	C ₆ H ₄ CH ₃ +O ₂ =OC ₆ H ₄ CH ₃ +O	8.57E+20	-2.27	7189.29
R6 ¹⁰⁰	C ₆ H ₅ CH ₂ +HO ₂ =>C ₆ H ₅ CHO+H+OH	3.67E+13	0	0
R7 ¹⁰⁰	C ₆ H ₅ CH ₂ +HO ₂ =>C ₆ H ₅ +CH ₂ O+OH	1.17E+13	0	0
R8¹⁰³	C₆H₅CH₂=>C₇H₆+H	6.28E+22	-2.056	93400
R9¹⁰³	C₇H₆+H=>C₆H₅CH₂	1.12E-06	6.25	6040

R10 ¹⁰⁹	C₆H₅CH₂+O₂=>C₆H₅CH₂OO	1.75E+09	-0.02	-7700
R11 ¹⁰⁹	C₆H₅CH₂OO=>C₆H₅CH₂+O₂	6.87E+11	0	17341
R12 ¹⁰⁹	C₆H₅CH₂OO=C₆H₅O+CH₂O	1.56E+07	0	33817
R13 ¹⁰⁹	C₆H₅CH₂OO=C₆H₅CHO+OH	1.65E+09	0	29040
R14 ⁹³	C₆H₄CH₃+O=OC₆H₄CH₃	1.00E+14	0	0
R15 ⁹³	C₆H₄CH₃+OH=OC₆H₄CH₃+H	3.00E+13	0	0
R16 ⁹³	C₆H₄CH₃+HO₂=OC₆H₄CH₃+OH	3.00E+13	0	0
R17 ⁹³	C₆H₄CH₃+O₂=>C₅H₄CH₂+CO₂+H	2.55E+13	-0.44	-1649.1
R18 ⁹³	C₆H₄CH₃+O₂=>PC₃H₄+C₂H₃+2CO	2.55E+13	-0.44	-1649.1
R19 ¹¹¹	C₅H₄CH₂=C₆H₆	2.95E+31	-4.97	175780
R20 ¹¹¹	C₅H₄CH₂=C₆H₅+H	8.51E+24	-2.505	225187
R21 ⁹³	H₂CCCH+H₂CCCH=C₅H₄CH₂	8.25E+46	-10.1	16959.9

^ak = ATⁿ exp(-Ea/RT): rate constant (units: mol, s, cm³, cal).

^bBolded reactions denote the reactions added to the model.

The benzyl+HO₂ chemistry has been accounted for previously in our High Pressure Toluene Oxidation model¹⁰⁰ by the global reactions, R6 and R7, as shown in Table 15 but were adjusted for the current work by being lowered by a factor of 10 when compared to the original High Pressure Toluene Oxidation Model. The updated High Pressure Toluene Oxidation Model consisting of all the changes mentioned in the above paragraphs is referred to as Updated Toluene Oxidation Model 1.

The high pressure toluene oxidation experimental data at $\Phi = 1$ and 543 atm¹⁰⁰ are compared against the original High Pressure Toluene Oxidation Model and the Updated Toluene Oxidation Model 1 in Fig 63. Both the models are also compared against ignition delay data of Vasu et al.⁷² in Fig 64. The Updated Toluene Oxidation Model 1 does a fairly good job in predicting the ignition delay times, when compared to the original High Pressure Toluene Oxidation Model.

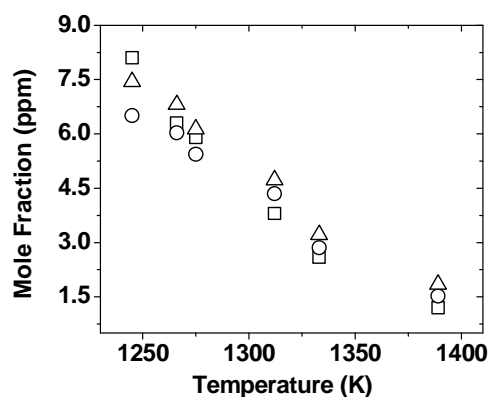


Fig 63. Comparison of the experimental data and the modeling results for toluene oxidation¹⁰⁰, average $P_5 = 543$ atm, $\Phi = 1$, nominal reaction time = 1.4 ms, $[\square]$ - Experiments, $[\Delta]$ -High Pressure Toluene Oxidation Model¹⁰⁰ $[o]$ -Updated Toluene Oxidation Model 1

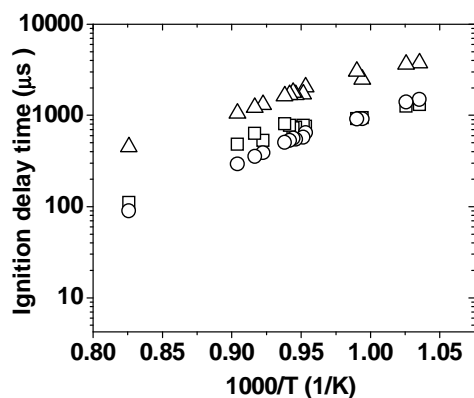


Fig 64. Toluene/air, $P_5 = 50$ atm, $\Phi = 1$, comparison of experimental ignition delay data of S.S. Vasu *et al.*⁷² and modeling results, $[\square]$ - Experiments, $[\Delta]$ -High Pressure Toluene Oxidation Model¹⁰⁰, $[o]$ -Updated Toluene Oxidation Model 1

Despite the good prediction abilities of the Updated Toluene Oxidation Model 1, before its inclusion in a xylene model would be warranted, further modification of the global steps, R6 and R7 were necessary in view of recent scientific developments. The global reactions R6 and R7 have now

been replaced by an elementary mechanism because of a recent computational study by Da Silva et al.¹¹²⁻¹¹⁴ on the benzyl+HO₂ reaction. These researchers have identified benzoyl radical and OH to be the major products of the reaction for temperatures greater than 800 K. The formation of benzylhydroperoxide molecules was seen to be dominant at lower temperatures and higher pressures. The decomposition kinetics of benzoyl radical was also studied by the same group with major product channels identified as benzaldehyde and H, benzene and HCO and phenyl and CH₂O, in decreasing order of importance. Benzoyl radical was identified to be the major product in benzylhydroperoxide decay. The reactions R6 and R7 in the Updated Toluene Oxidation Model 1 were consequently replaced by the elementary steps shown in Table 16. Pressure dependent rate constants were included, as available in the references found in Table 16, for the formation of benzylhydroperoxide and benzoyl radical and their subsequent reactions. For pressures above 1 atm, the high pressure limit rate constants are considered for the formation of benzylhydroperoxide and benzoyl radical from benzyl+HO₂ reaction and subsequent decay of benzylhydroperoxide to benzoyl radical. The Updated Toluene Oxidation Model 1 with reactions R6 and R7 replaced with elementary mechanism shown in Table 16, is now referred to as Updated Toluene Oxidation Model 2.

Table 16. Reactions R6 and R7 in Updated Toluene Oxidation Model 1 replaced by reactions R22 to R37, now referred to as Updated Toluene Oxidation Model 2

Reaction Number	Pressure (atm)	Reaction ^a	A	n	E _a
R22 ¹¹²	1	$C_6H_5CH_2+HO_2=C_6H_5CH_2OOH$	3.70E+37	-16.33	-67470
R23 ¹¹²	≥ 1	$C_6H_5CH_2+HO_2=C_6H_5CH_2OOH$	8.29E+04	2.20	-5130
R24 ¹¹³	1	$C_6H_5CH_2OOH=C_6H_5CH_2O+OH$	2.03E+47	-10.27	50710
R25 ¹¹²	≥ 1	$C_6H_5CH_2OOH=C_6H_5CH_2O+OH$	3.29E+13	0.42	39890
R26 ¹¹²	1	$C_6H_5CH_2+HO_2=C_6H_5CH_2O+OH$	1.19E+09	1.03	-2250
	≥ 1 (900 ≤ T ≤ 1300				
R27 ^{112,b}	K)	$C_6H_5CH_2+HO_2=C_6H_5CH_2O+OH$	1.24E+10	0	-1433
	≥ 1 (T > 1300				
R28 ^{112,b}	K)	$C_6H_5CH_2+HO_2=C_6H_5CH_2O+OH$	3.86E+10	0	1456
R29 ¹¹⁴	1	$C_6H_5CH_2O=C_6H_5CHO+H$	5.26E+28	-5.081	22250
R30 ¹¹⁴	10	$C_6H_5CH_2O=C_6H_5CHO+H$	1.68E+22	-2.901	20760
R31 ¹¹⁴	>100	$C_6H_5CH_2O=C_6H_5CHO+H$	5.07E+08	1.56	16850
R32 ¹¹⁴	1	$C_6H_5CH_2O=C_6H_5+CH_2O$	7.21E+33	-6.21	36850
R33 ¹¹⁴	10	$C_6H_5CH_2O=C_6H_5+CH_2O$	1.32E+27	-4.009	35070
R34 ¹¹⁴	>100	$C_6H_5CH_2O=C_6H_5+CH_2O$	1.09E+14	0.157	31160
R35 ¹¹⁴	1	$C_6H_5CH_2O=C_6H_6+HCO$	2.37E+32	-6.095	28810
R36 ¹¹⁴	10	$C_6H_5CH_2O=C_6H_6+HCO$	3.82E+31	-5.663	29840
R37 ¹¹⁴	>100	$C_6H_5CH_2O=C_6H_6+HCO$	1.81E+13	0	22717

^ak = ATⁿ exp(−E_a/RT): rate constant (units: mol, s, cm³, cal).

^bRate constant estimated utilizing steady state approximation for the benzylhydroperoxide adduct

The Updated Toluene Oxidation Model 2 is compared against the high pressure oxidation and the ignition delay data in Fig 65 and Fig 66. It can be seen that the model under predicts the toluene consumption and over predicts the ignition delay time. To achieve similar predictions of Updated Toluene Oxidation Model 2 as the Updated Toluene Oxidation Model 1, the rate constant for the formation of benzylhydroperoxide from benzyl+HO₂ reaction had to be modified to the value shown in Table 17. The Updated Toluene Oxidation Model 2 with the modified rate constant for the formation of benzylhydroperoxide from the benzyl+HO₂ reaction is now referred to as Updated Toluene Oxidation Model 3. The Updated Toluene Oxidation Model 3 shows a closer agreement

with the toluene high pressure experimental data and the ignition delay data when compared to the Updated Toluene Oxidation Model 2. To retain the consistency of the original High Pressure Toluene Oxidation Model predictions with the previous high pressure toluene experimental data¹⁰⁰, the Updated Toluene Oxidation Model 3 is considered to be the final version of the revised High Pressure Toluene Oxidation Model and is included in this form in the m-xylene oxidation models discussed below.

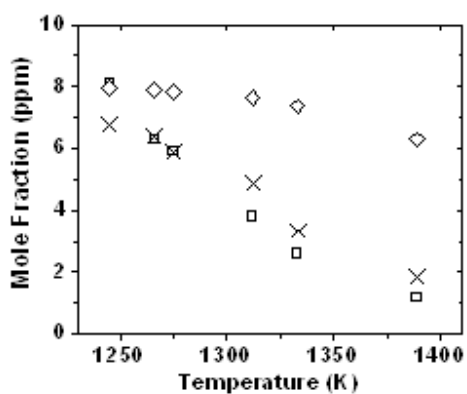


Fig 65. Comparison of the toluene oxidation experimental data and the modeling result¹⁰⁰, average $P_5 = 543$ atm, $\Phi = 1$, nominal reaction time = 1.4 ms, [□]- Experiments, [◇]- Updated Toluene Oxidation Model 2, [X]-Updated Toluene Oxidation Model 3.

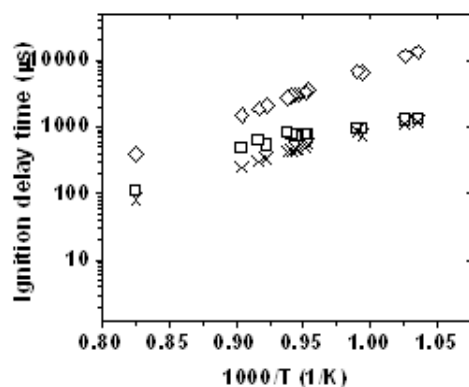


Fig 66. Toluene/air, $P_5 = 50 \text{ atm}$, $\Phi = 1$, comparison of the experimental data⁷² and the modeling results, [□]- Experiments, [◇]-Updated Toluene Oxidation Model 2, [X]-Updated Toluene Oxidation Model 3.

Table 17. Reactions R23 in the Updated Toluene Oxidation Model 2 replaced by reaction R38, now referred to as Updated Toluene Oxidation Model 3

Reaction Number	Pressure (atm)	Reaction ^a	A	n	E _a
R38 ^{Est}	≥ 1	$\text{C}_6\text{H}_5\text{CH}_2 + \text{HO}_2 = \text{C}_6\text{H}_5\text{CH}_2\text{OOH}$	$8.00\text{E}+13$	0.00	0

^a $k = AT^n \exp(-E_a/RT)$: rate constant (units: mol, s, cm³, cal).

^bEst, short notation of estimated

6.3.2. The High Pressure m-Xylene Oxidation Model

6.3.2. 1. The Preliminary m-Xylene Oxidation Model (UIC m-Xylene Oxidation Model 1)

The independent m-xylene oxidation model is built in a hierarchical fashion based on the Updated High Pressure Toluene Oxidation Model 3. The reaction mechanism of m-xylene oxidation was taken from Emdee et al.⁹⁵, which was proposed based on the product distribution seen in an

atmospheric flow reactor experiments, for a temperature range of 1093-1199 K and an equivalence ratio from 0.4 to 1.7. The oxidation of m-xylene was suggested to take place by sequential oxidation and removal of the methyl side chains producing, toluene, m-methylbenzyl alcohol, m-tolualdehyde, m-ethyltoluene, m-methylstyrene, methylcyclopentadiene, m-cresol and benzene as intermediates. Due to an absence in the literature of kinetic data for most of the reaction steps, the rate constants for their proposed mechanistic steps were assumed by us to be similar to analogous reactions of toluene^{18,19,100}. The thermochemistry of m-xylene and its oxygenated products was taken from the Gail and Dagaut model. Thermochemistry of dimethylphenoxy radical ($\text{OC}_6\text{H}_3(\text{CH}_3)_2$)T14, dimethylphenol ($\text{HOC}_6\text{H}_3(\text{CH}_3)_2$), methyltolyl (dimethylphenyl) radical ($\text{C}_6\text{H}_3(\text{CH}_3)_2$) and key reaction steps for the formation of methyltolyl were taken from the Battin-Leclerc et al. model.

The m-xylyl+HO₂ reactions and their rate constants have been assumed to be analogous to the benzyl+HO₂ ones. The m-xylyl+O₂ chemistry was included from theoretical study of Murakami et al.¹¹⁵ on the oxidation of o-, m- and p-xylyl radicals. They proposed pressure dependent rate constants for the formation and decay of o-xylylperoxy radicals ($\text{CH}_3\text{C}_6\text{H}_4\text{CH}_2\text{OO}$), yielding 2-methylbenzaldehyde ($\text{CH}_3\text{C}_6\text{H}_4\text{CHO}$), OH radical and other products. The authors also mentioned that the position of the methyl groups on the aromatic ring had little influence on the heats of reactions and the barrier heights of xylyl+O₂ reactions; hence pressure dependent rate expressions for the formation and consumption of m-xylylperoxy radicals were assumed to be same as that of corresponding o-xylylperoxy radical reactions.

Reaction path analyses and sensitivity analyses of the initial assembled model (referred to as Model 1 hereafter), revealed the pathways important to the fuel consumption and formation of the intermediates. The sensitivity analysis of the fuel for 50 atm fuel lean oxidation experiments at a nominal temperature of 1331 K and reaction time of 1.9 ms is shown in Fig 67. Reactions to which

m-xylene concentration shows considerable sensitivities have been plotted as a function of the normalized sensitivity coefficient. The fuel decay is sensitive to the formation of m-xylylhydroperoxide, methylbenzaldehyde, m-xylyperoxy radicals, m-xylyl and dimethylphenyl radicals, through the reactions shown in Fig 67. The consumption reactions for m-xylylhydroperoxide and m-xylyperoxy radicals are included in Model 1 and are shown in Table 18. The dimethylphenyl radicals are oxidized to dimethylcresol and dimethylcresoxy radicals⁹⁶. The dimethylcresoxy radical reaction mechanism has been assumed to be similar to the reaction mechanism of methylcresoxy radical. In addition to this, the reaction path analyses of the fuel showed that from $\Phi = 0.53$ to 2.35, most of the fuel decays by hydrogen abstraction reactions forming m-xylyl radicals and the percentage contribution of these reactions increase as the equivalence ratio is increased.

The sensitivity analyses and reaction path analyses of the fuel helped us to concentrate on the areas needing further improvement, which were:

- (1) The decomposition pathways for cresoxy radicals
- (2) The decomposition pathways for the methylcresoxy radicals.
- (3) The decomposition pathways for the m-xylyl radicals.

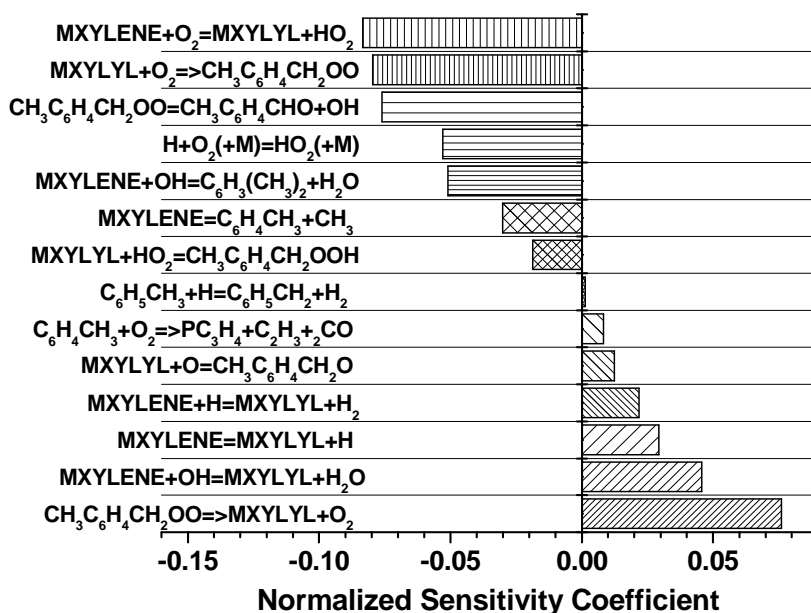


Fig 67. Sensitivity analysis of *m*-xylene, $P_5 = 53 \text{ atm}$, $\Phi = 0.53$, time = 1.9 ms using the UIC *m*-Xylene Oxidation Model 1.

Table 18. *m*-Xylyl+O₂ and *m*-Xylyl+HO₂ reactions in UIC *m*-Xylene Oxidation Model 1

Reaction Number	Reaction ^a	A	n	E _a
R39 ¹¹⁵	CH ₃ C ₆ H ₄ CH ₂ +O ₂ =>CH ₃ C ₆ H ₄ CH ₂ OO	1.17E+09	-0.05	-2414
R40 ¹¹⁵	CH ₃ C ₆ H ₄ CH ₂ OO=>CH ₃ C ₆ H ₄ CH ₂ +O ₂	1.56E+11	0	6502
R41 ¹¹⁵	CH ₃ C ₆ H ₄ CH ₂ OO=CH ₃ C ₆ H ₄ CHO+OH	1.11E+11	0	9401
R42 ¹¹⁵	CH ₃ C ₆ H ₄ CH ₂ OO=OC ₆ H ₄ CH ₃ +CH ₂ O	5.55E+09	0	17341
R43 ^{112,b}	CH ₃ C ₆ H ₄ CH ₂ +HO ₂ =CH ₃ C ₆ H ₄ CH ₂ OOH	3.70E+37	-16.33	-67470
R44 ^{112,b}	CH ₃ C ₆ H ₄ CH ₂ OOH=CH ₃ C ₆ H ₄ CH ₂ O+OH	2.03E+47	-10.27	50710
R45 ^{113,b}	CH ₃ C ₆ H ₄ CH ₂ +HO ₂ =CH ₃ C ₆ H ₄ CH ₂ O+OH	1.19E+09	1.03	-2250
R46 ^{114,b}	CH ₃ C ₆ H ₄ CH ₂ O=CH ₃ C ₆ H ₄ CHO+H	5.26E+28	-5.081	22250
R47 ^{114,b}	CH ₃ C ₆ H ₄ CH ₂ O=C ₆ H ₄ CH ₃ +CH ₂ O	7.21E+33	-6.21	36850
R48 ^{114,b}	CH ₃ C ₆ H ₄ CH ₂ O=C ₆ H ₅ CH ₃ +HCO	2.37E+32	-6.095	28810

^ak = ATⁿ exp(-E_a/RT): rate constant (units: mol, s, cm³, cal).

^bRate constants assumed same as analogous reactions from the benzyl+HO₂ mechanism, only the low pressure rate constants are shown in table, detailed reaction mechanism is present in the model.

6. 3.2.2 UIC *m*-Xylene Oxidation Model 2

The following sections describe the changes that have been made to UIC *m*-Xylene Oxidation Model 1 based on the sensitivity analyses and reaction path analyses of the fuel and major intermediates. The UIC *m*-Xylene Oxidation Model 1 with the added and modified reactions, presented in Table 19 and Table 20 is referred to as the UIC *m*-Xylene Oxidation Model 2.

Table 19. Reactions added to UIC *m*-Xylene Oxidation Model 1

Reaction Number	Reaction ^a	A	n	E _a
<i>Decomposition of m-Xylyl Radicals</i>				
R49 ¹¹⁶	$\text{CH}_3\text{C}_6\text{H}_4\text{CH}_2=\text{CH}_2\text{C}_6\text{H}_4\text{CH}_2+\text{H}$	3.26E+13	0.128	70300
R50 ¹¹⁶	$\text{CH}_3\text{C}_6\text{H}_4\text{CH}_2=\text{C}_7\text{H}_6+\text{CH}_3$	4.00E+15	0	76100
<i>Decomposition of Fulvenallene</i>				
R51 ¹¹⁷	$\text{C}_7\text{H}_6+\text{H}=>\text{C}_6\text{H}_5\text{CH}_2$	1.12E-06	6.25	6040
R52 ¹¹⁷	$\text{C}_7\text{H}_6+\text{H}=>\text{C}_5\text{H}_5+\text{C}_2\text{H}_2$	8.55E-21	10.35	12590
R53 ¹¹⁷	$\text{C}_7\text{H}_6+\text{H}=>\text{C}_5\text{H}_5\text{C}_2\text{H}+\text{H}$	2.72E-29	12.88	11510
R54 ¹¹⁷	$\text{C}_5\text{H}_5\text{C}_2\text{H}+\text{H}=>\text{C}_5\text{H}_5+\text{C}_2\text{H}_2$	4.44E+20	-1.82	14450
R55 ¹¹⁷	$\text{C}_5\text{H}_5+\text{C}_2\text{H}_2=>\text{C}_7\text{H}_6+\text{H}$	1.15E-44	17.07	22460
R56 ¹¹⁷	$\text{C}_5\text{H}_5\text{C}_2\text{H}+\text{H}=>\text{C}_7\text{H}_6+\text{H}$	8.56E-31	13.1	8670
R57 ¹¹⁷	$\text{C}_5\text{H}_5+\text{C}_2\text{H}_2=>\text{C}_5\text{H}_5\text{C}_2\text{H}+\text{H}$	7.24E+15	-0.61	34040
<i>Decomposition of p-Xylylene</i>				
R58 ¹¹⁸	$\text{CH}_2\text{C}_6\text{H}_4\text{CH}_2+\text{O}=\text{CHOC}_6\text{H}_4\text{CH}_2+\text{H}$	3.16E+13	0	0
R59 ⁶⁴	$\text{CHOC}_6\text{H}_4\text{CH}_2+\text{O}_2=\text{CHOC}_6\text{H}_4\text{CHO}+\text{OH}$	6.31E+12	0	3000
R60 ⁶⁴	$\text{CHOC}_6\text{H}_4\text{CHO}+\text{H}=\text{CHOC}_6\text{H}_4\text{CO}+\text{H}_2$	5.00E+13	0	4928
R61 ⁶⁴	$\text{CHOC}_6\text{H}_4\text{CHO}+\text{O}=\text{CHOC}_6\text{H}_4\text{CO}+\text{OH}$	9.04E+13	0	3080
R62 ⁶⁴	$\text{CHOC}_6\text{H}_4\text{CO}+\text{H}=\text{CHOC}_6\text{H}_4\text{CHO}$	3.00E+13	0	0
R63 ⁶⁴	$\text{CHOC}_6\text{H}_4\text{CO}=\text{C}_6\text{H}_4\text{CHO}+\text{CO}$	3.98E+14	0	29400
R64 ⁶⁴	$\text{C}_6\text{H}_4\text{CHO}+\text{H}=\text{C}_6\text{H}_5\text{CHO}$	3.98E+15	0	83701
R65 ⁶⁴	$\text{C}_6\text{H}_4\text{CHO}+\text{O}_2=\text{OC}_6\text{H}_4\text{CHO}+\text{O}$	2.09E+12	0	7470
R66 ⁶⁴	$\text{CHOC}_6\text{H}_4\text{CHO}+\text{CH}_3=\text{CHOC}_6\text{H}_4\text{CO}+\text{CH}_4$	2.77E+03	2.81	5773
R67 ⁶⁴	$\text{OC}_6\text{H}_4\text{CHO}=\text{C}_5\text{H}_4\text{CHO}+\text{CO}$	3.98E+14	0	29400
R68 ⁶⁴	$\text{C}_5\text{H}_4\text{CHO}=\text{C}_5\text{H}_5\text{CO}$	1.00E+12	0	0

R69 ⁶⁴	$C_5H_5CO=C_5H_5+CO$	2.00E+12	0	0
	<i>OC₆H₄CH₃→Products</i>			
R70 ¹¹⁹	$OC_6H_4CH_3=CO+C_5H_4CH_3$	2.51E+11	0	43900
R71 ⁵¹	$C_5H_4CH_3=C_5H_5CH_2$	3.00E+12	0	50400
R72 ⁵¹	$C_5H_4CH_3=n-C_6H_7$	8.00E+13	0	50000
R73 ⁵¹	$n-C_6H_7=C_2H_2+n-C_4H_5$	3.16E+13	0	43100
R74 ⁵¹	$C_5H_5CH_2=c-C_6H_7$	1.40E+13	0	17400
R75 ⁵¹	$c-C_6H_7=C_6H_6+H$	7.45E+13	0	28500
R76 ⁵¹	$c-C_6H_7=n-C_4H_5+C_2H_2$	2.00E+15	0	92000
	<i>OC₆H₃(CH₃)₂→Products</i>			
R77 ^{119,b}	$OC_6H_3(CH_3)_2=CO+C_5H_3(CH_3)_2$	2.51E+11	0	43900
R78 ^{51,c}	$C_5H_3(CH_3)_2=C_5H_4CH_3CH_2$	6.00E+12	0	50400
R79 ^{Est}	$C_5H_4CH_3CH_2=C_6H_6CH_3$	1.40E+13	0	17400
R80 ¹²⁰	$CH_3+C_6H_6=>C_6H_6CH_3$	2.60E+03	2.84	8502
R81 ¹²⁰	$C_6H_6CH_3=>CH_3+C_6H_6$	1.10E+14	0	22425
R82 ¹²⁰	$C_6H_6CH_3=>C_6H_5CH_3+H$	3.76E+13	0	27321
R83 ¹²⁰	$C_6H_5CH_3+H=>C_6H_6CH_3$	1.93E+06	2.17	4163
	<i>m-Xylene+O->Products</i>			
R84 ^{71,121,122,d}	$C_6H_4(CH_3)_2+O=HOC_6H_3(CH_3)_2$	1.54E+13	0	2710
R85 ^{71,121,122,d}	$C_6H_4(CH_3)_2+O=C_5H_4(CH_3)_2+CO$	1.04E+12	0	2710
R86 ¹²³	$C_6H_6+O=C_6H_5OH$	5.84E+35	-5.89	34534
R87 ¹²³	$C_6H_6+O=C_6H_5OH$	2.53E+13	0	6565
R88 ¹²³	$C_6H_6+O=C_5H_6+CO$	1.56E+31	-4.73	33568
R89 ¹²³	$C_6H_6+O=C_5H_6+CO$	4.83E+03	0	14929

^ak = ATⁿ exp(-Ea/RT): rate constant (units: mol, s, cm³, cal).

^bRate constants assumed to be same as the analogous reactions of cresoxyl radical

^cRate constants assumed to be same as the analogous reactions of methylcyclopentadienyl radical

^dBranching ratios for C₆H₄(CH₃)₂+O reactions estimated from the analogous reactions of C₆H₆+O

Table 20. Reactions whose rate constants were modified in UIC m-Xylene Oxidation Model 1

Reaction Number	Reaction ^a	A	n	E _a
R89 ^{73,b}	$\text{C}_6\text{H}_4(\text{CH}_3)_2 + \text{O}_2 = \text{CH}_3\text{C}_6\text{H}_4\text{CH}_2 + \text{HO}_2$	5.23E+07	2.5	46045
R90 ^{72,b}	$\text{C}_6\text{H}_4(\text{CH}_3)_2 + \text{H} = \text{C}_6\text{H}_5\text{CH}_3 + \text{CH}_3$	6.47E+00	3.98	3384
R91 ^{72,b}	$\text{C}_6\text{H}_4(\text{CH}_3)_2 + \text{H} = \text{CH}_3\text{C}_6\text{H}_4\text{CH}_2 + \text{H}_2$	3.90E+08	1.25	2371
R92 ^{71,121,122,c}	$\text{C}_6\text{H}_4(\text{CH}_3)_2 + \text{O} = \text{OC}_6\text{H}_3(\text{CH}_3)_2 + \text{H}$	1.80E+13	0	2710
R93 ¹²⁴	$\text{OC}_6\text{H}_4\text{CH}_3 + \text{H} = \text{HOC}_6\text{H}_4\text{CH}_3$	1.00E+14	0	0
R94 ^{124,b}	$\text{OC}_6\text{H}_3(\text{CH}_3)_2 + \text{H} = \text{HOC}_6\text{H}_3(\text{CH}_3)_2$	1.00E+14	0	0
R95 ¹²³	$\text{C}_6\text{H}_6 + \text{O} = \text{C}_6\text{H}_5\text{O} + \text{H}$	3.55E+10	0.91	6323
R96 ^{72,b}	$\text{C}_6\text{H}_4(\text{CH}_3)_2 + \text{OH} = \text{CH}_3\text{C}_6\text{H}_4\text{CH}_2 + \text{H}_2\text{O}$	3.62E+05	2.39	-602

^a $k = \text{AT}^n \exp(-E_a/RT)$: rate constant (units: mol, s, cm³, cal).

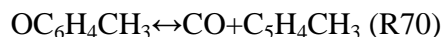
^bRate constants estimated from analogous reactions of toluene

^cBranching ratios for $\text{C}_6\text{H}_4(\text{CH}_3)_2 + \text{O}$ reactions estimated from the analogous reactions of $\text{C}_6\text{H}_6 + \text{O}$

6.3.2.2.1. $\text{OC}_6\text{H}_4\text{CH}_3 \rightarrow \text{Products}$

The decomposition of cresoxyl radical ($\text{OC}_6\text{H}_4\text{CH}_3$) in UIC m-Xylene Oxidation Model 1 takes place by forming benzene, H and CO in a single step. This reaction has been replaced by a series of reactions, shown as reactions (R70) to (R76) in Table 19. According to this reaction mechanism, the cresoxyl radicals not only produce benzene and CO but also $\text{n-C}_4\text{H}_5$ and C_2H_2 as products.

The decomposition of the phenoxy radical to form CO and cyclopentadienyl radical is the model reaction for the decomposition of cresoxyl radical. The cresoxyl radical decomposes to methyl cyclopentadienyl radical and CO⁶⁴. The rate constant of this step, (R70), was estimated from Emdee et al.¹¹⁹.



Further consumption reactions of methylcyclopentadiene, produce both open chain intermediates ($\text{n-C}_4\text{H}_5$ and C_2H_2) and closed ring compounds (C_6H_6), whose rate constants were taken from Lifshitz et al.⁵¹.

6.3.2.2.2. $\text{OC}_6\text{H}_3(\text{CH}_3)_2 \rightarrow \text{Products}$

The decomposition of dimethylphenoxy radical ($\text{OC}_6\text{H}_3(\text{CH}_3)_2$) in UIC m-Xylene Oxidation Model 1 takes place by forming toluene, H and CO in a single step. This step has been replaced by a series of steps, shown as reactions (R77) to (R83) in Table 19. According to this reaction mechanism, the dimethylphenoxy radicals produce both benzene and toluene as products.

This mechanism is similar to the decomposition mechanism proposed by Gregory et al.¹²⁵ and is shown in Fig 68. The dimethylphenoxy radical decays to dimethylcyclopentadienyl radical, the rate constant of this reaction was estimated from analogous reaction of phenoxy radical decay to cyclopentadienyl radical¹¹⁹. The dimethylcyclopentadienyl radical isomerizes to form a cyclic compound $\text{C}_6\text{H}_6\text{CH}_3$, the rate constant of this reaction was estimated from analogous methylcyclopentadienyl reaction of Lifshitz et al.⁵¹. The rate constants for decay of $\text{C}_6\text{H}_6\text{CH}_3$ to toluene and benzene by fast dehydrogenation and demethylation were taken from the theoretical work of Tokmakov and Lin on the addition of H atoms to toluene and benzene¹²⁰.

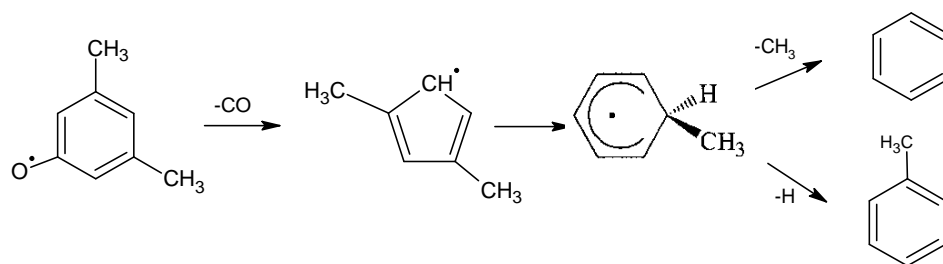


Fig 68. Reaction mechanism of dimethylphenoxy radical

6.3.2.2.3. Decomposition of m-Xylyl Radicals

Emdee et al.⁹⁵ suggested two routes for the decay of m-xylyl radicals ($\text{CH}_3\text{C}_6\text{H}_4\text{CH}_2$)T14, the oxidation of the methylene side chain and the addition of methyl group to the methylene side chain. These routes have been included in UIC m-Xylene Oxidation Model 1.

Due to the similarities in the chemical structures and decomposition activation energies of m-xylyl and benzyl radicals, later studies hypothesized that these two species decay similarly. Gail and Dagaut⁶⁴ hypothesized that the thermal decomposition of m-xylyl radical yields acetylene and methylcyclopentadienyl radical or propargyl radical and 1,3-cyclopentadiene. The rate constants for these two reaction pathways for methylbenzyl radical were assumed to be similar to corresponding reactions of benzyl radical decay forming either cyclopentadiene, acetylene or vinylacetylene, propargyl radical, respectively⁹⁰. Similar reactions have been considered in the Battin-Leclerc et al. model⁹⁶ and Narayanaswamy et al. model⁹³, where m-methylbenzyl decays to form a C_6H_7 intermediate and acetylene. In a recent study, Da Silva et al.¹¹⁶ investigated the kinetics of m-methylbenzyl radicals by high level theoretical calculations and proposed that these radicals decay by forming fulvenallene (C_7H_6)T14 and p-xylylene ($\text{CH}_2\text{C}_6\text{H}_4\text{CH}_2$)T14 as intermediates at low temperatures. Their estimated rate constant of m-xylyl radical forming p-xylylene+H, was in good

agreement with the experimental C_8H_8+H measurements of Fernandes et al.¹²⁶. Therefore, these two channels along with their calculated high pressure limit rate parameters were included in the model as taken from Da Silva et al.¹¹⁶.

The major products of fulvenallene decay were found to be benzyl radical, cyclopentadienyl radical, acetylene and 1-ethynylcyclopentadiene ($C_5H_5C_2H$)T14 by Cavallotti et al.¹⁰⁴ and Da Silva et al.¹¹⁷ These steps along with their rate constants were taken from Da Silva et al.¹¹⁷ and were included in UIC m-Xylene Oxidation Model 1, shown as steps (R51) to (R57) in Table 19. The oxidation of p-xylylene leads, as proposed by Emdee et al.⁹⁵, to the formation of p-phthalaldehyde, m-formylphenyl radical (C_6H_4CHO)T14, formylcyclopentadiene (C_5H_4CHO)T14 and cyclopentadienyl radicals as intermediates. The steps describing these pathways, shown as reactions (R58) to (R69) in Table 19, were included in Model 1 with their rate constants taken from Brezinsky et al.¹¹⁸ and Dagaut et al.⁶⁴.

6.3.3. Modeling Results and Discussion

The UIC m-Xylene Oxidation Model 2 has been validated against a wide range of experimental data. The experimental data can be categorized into high pressure, intermediate pressure and low pressure datasets. The high pressure dataset (40- 50 atm) includes species profiles from our high pressure shock tube m-xylene oxidation experiments and the ignition delay measurements of Shen and Oehlschlaeger⁹⁷. The intermediate pressure range (10 - 25 atm) includes species profiles from our m-xylene oxidation experiments and the ignition delay measurements from Battin-Leclerc et al.⁹⁶ and Shen and Oehlschlaeger⁹⁷. The low pressure datasets (1 atm) include the species profiles measurements of Emdee et al.⁹⁵ and Gail and Dagaut⁶⁴ in a flow reactor and a jet stirred reactor respectively. The UIC high pressure shock tube m-xylene oxidation

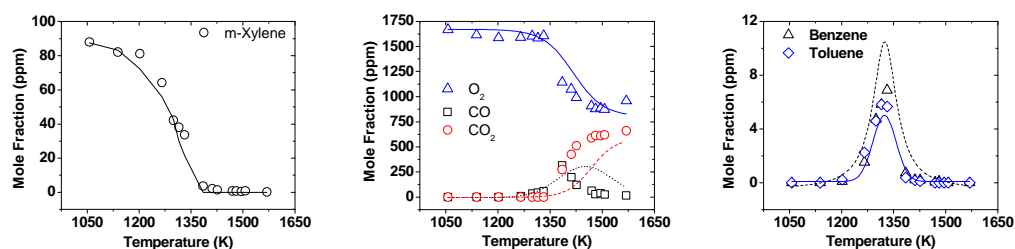
experiments complete the species profile spectrum across all pressures and temperatures and play a crucial role in analyzing the fuel behavior over these wide range of experimental conditions.

Ignition delay time measurements were modeled using CHEMKIN 4.1.1⁵⁸, with an adiabatic constant volume constraint. Maximum slope of the OH concentration traced to the baseline defined the modeling ignition delay time. The plug flow reactor experiments were modeled as isobaric homogenous reactors. The jet stirred reactor experiments were modeled using the PSR code in CHEMKIN 4.1.1.

6.3.3.1. High Pressure Experimental Datasets

6.3.3.1.1. Species Profiles

The experimental and modeling profiles for $\Phi = 0.53$, 1 and 2.35, at nominal reflected shock pressures of 50 atm are shown in Fig 69 through Fig 71. The model shows good agreement with fuel decay for different equivalence ratios. Lower consumption of the O_2 and formation of the intermediates is observed for experimental datasets with $\Phi \geq 1$.



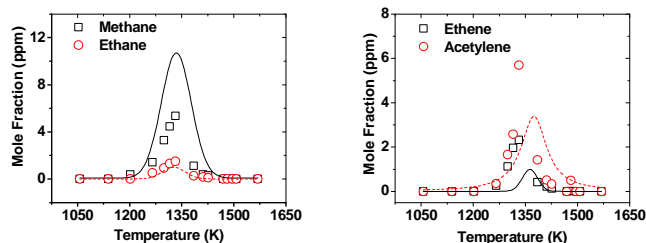


Fig 69. Comparison of experimental and modeling profiles for *m*-xylene oxidation, average $P5 = 53$ atm, $\Phi = 0.53$, nominal reaction time = 1.5 ms, [□]- Experiments, [-]-UIC *m*-Xylene Model 2

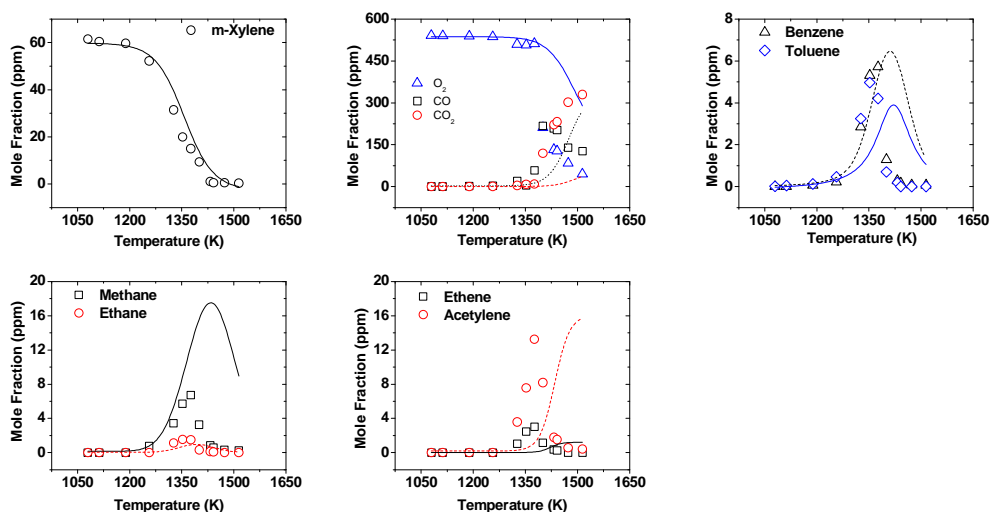
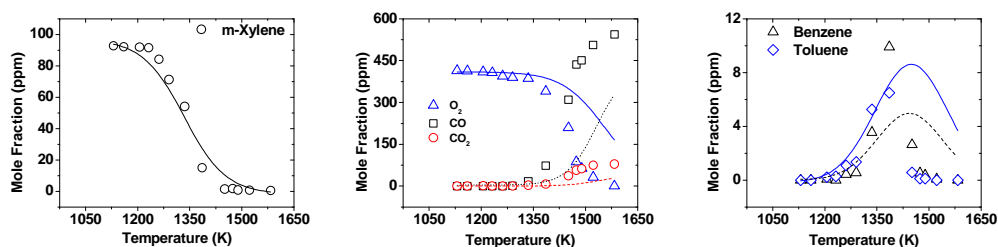


Fig 70. Comparison of experimental and modeling profiles for *m*-xylene oxidation, average $P5 = 51$ atm, $\Phi = 1.19$, nominal reaction time = 1.5 ms, [□]- Experiments, [-]-UIC *m*-Xylene Model 2



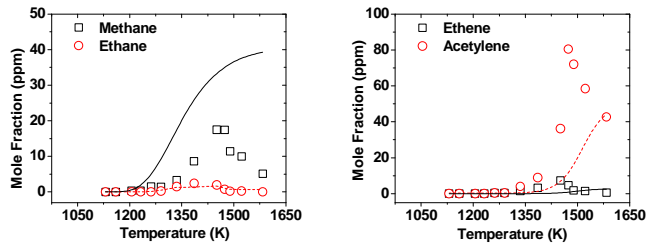


Fig 71. Comparison of experimental and modeling profiles for *m*-xylene oxidation, average $P_5 = 50$ atm, $\Phi = 2.35$, $P_5 = 53$ atm, $\Phi = 0.53$, nominal reaction time = 1.5 ms, $[\square]$ - Experiments, $[-]$ -UIC *m*-Xylene Model 2

6.3.3.1.2. Ignition Delay Measurements

The model has been compared against the ignition delay data of Shen and Oehlschlaeger⁹⁷. These measurements were made at a nominal pressure of 45 atm, for a temperature range from 1023-1269 K and $\Phi = 0.5$ and 1. The model shows excellent agreement with the ignition delay time measurements for the fuel lean data set as shown in Fig 72 (A). It shows fairly good agreement with the experiments for the stoichiometric conditions, Fig 72 (B), with the maximum deviation in the modeling ignition delay times being lower than a factor of 2 at very low temperatures.

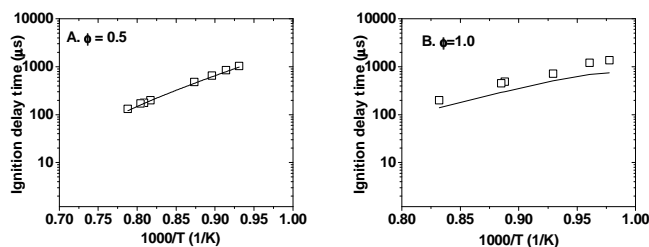


Fig 72. *m*-Xylene/air, $P = 45$ atm, (A) $\Phi = 0.5$, (B) $\Phi = 1$, comparison of experimental ignition delay data of Shen and Oehlschlaeger⁹⁷ and modeling results, $[\square]$ - Experiments, $[-]$ -UIC *m*-Xylene Model 2

6.3.3.2. Intermediate Pressure Experimental Datasets

6.3.3.2.1. Species Profiles

The experimental and modeling profiles for $\Phi = 0.5$ and 2.1, at nominal reflected shock pressures of 25 atm are shown in Fig 73 and Fig 74. The model shows good agreement with fuel decay for different equivalence ratios. Lower consumption of the O_2 and formation of the intermediates is observed for $\Phi \geq 1$.

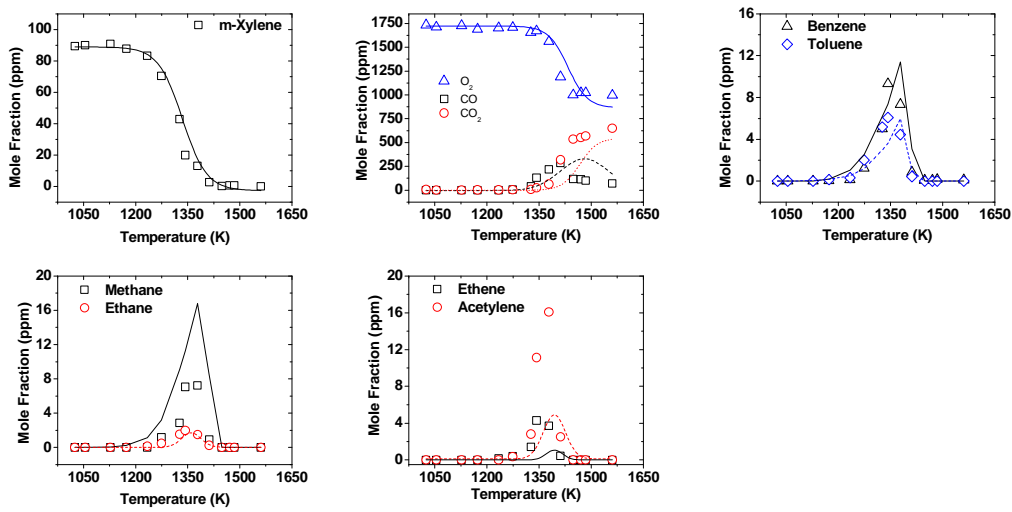


Fig 73. Comparison of experimental and modeling profiles for *m*-xylene oxidation, average $P_5 = 27$ atm, $\Phi = 0.55$, nominal reaction time = 1.5 ms, $[\square]$ - Experiments, $[-]$ -UIC *m*-Xylene Model 2

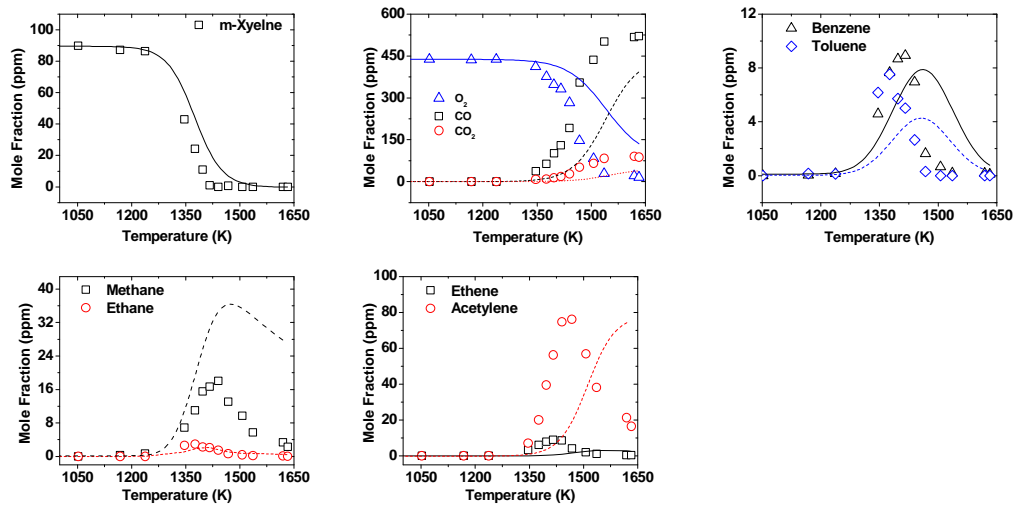


Fig 74. Comparison of experimental and modeling profiles for *m*-xylene oxidation, average $P5 = 28$ atm, $\Phi = 2.1$, nominal reaction time = 1.5 ms, [□]- Experiments, [-]-UIC *m*-Xylene Model 2

6.3.3.2.2. Ignition Delay Measurements

The model has been compared with the ignition delay measurements of Battin-Leclerc et al.⁹⁶ and Shen and Oehlschlaeger⁹⁷. Ignition measurements by Battin-Leclerc et al. were performed at very high temperature range of 1399 to 1880 K for $\Phi = 0.5$, 1 and 2, for a nominal pressure of 9 atm. Ignition measurements by Shen and Oehlschlaeger⁹⁷ were performed for a temperature range of 1153 to 1408 K for a nominal pressure of 10 atm and $\Phi = 0.5$ and 1.

The experimental ignition delay times and the modeling predictions are shown in Fig 75. The model shows excellent agreement with the ignition delay time measurements for the fuel lean data set of Shen and Oehlschlaeger and shows ignition delay times with a maximum deviation by a factor of 3 for temperatures greater than 1590 K for the Battin-Leclerc et al. data sets. For the stoichiometric and fuel rich datasets, the maximum deviation in the modeling ignition delay times

are lower by a factor of 2 for both high temperature datasets of Battin-Leclerc et al. and low temperature datasets of Shen and Oehlschlaeger.

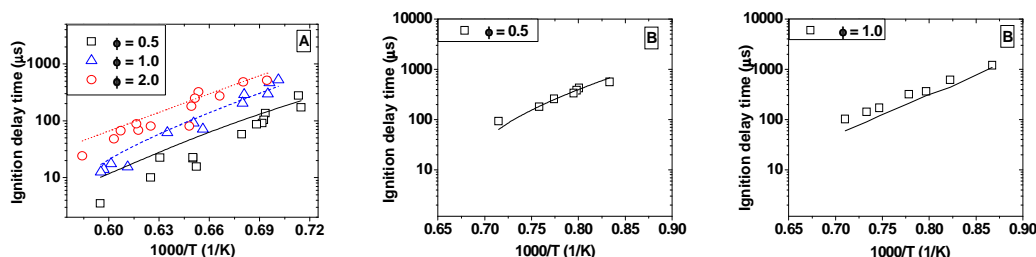


Fig 75. Comparison of experimental and modeling predictions of the *m*-xylene ignition delay times, (A) $P = 9$ atm, Battin-Leclerc et al.⁹⁶, (B) $P = 9$ atm, Shen and Oehlschlaeger⁹⁷, [□]-Experiments, [-]-UIC *m*-Xylene Model 2

6.3.3.3. Low Pressure Datasets

6.3.3.3.1. Species Profiles

Flow reactor experiments of Emdee et al.⁹⁵ were performed for three different equivalence ratios ($\Phi = 0.5, 1$ and 2), an average temperature of 1160 K. The model predictions and the low pressure experimental datasets are shown in Fig 76. For the stoichiometric conditions, the model predicts good profiles for the decay of the fuel, O_2 and the formation of intermediates like toluene, benzene, methane, methylstyrene and benzylalcohol. However, it shows twice as much methylbenzaldehyde and much lower amounts of ethyltoluene.

The jet stirred reactor experiments by Gail and Dagaut⁶⁴ were performed for a temperature range of 1049 - 1399 K and for three different equivalence ratios ($\Phi = 0.5, 1$ and 2). For the jet

stirred reactor data at stoichiometric conditions the model shows greater consumption of fuel, oxygen and earlier formation of the intermediates when compared to the experimental data, which is shown in Fig 77.

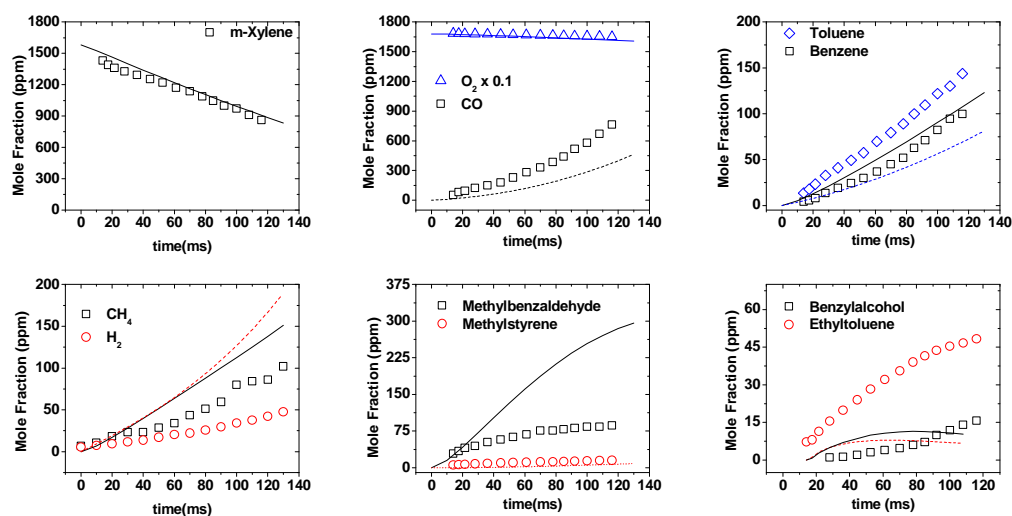


Fig 76. *m*-Xylene oxidation flow reactor experiments at atmospheric pressure, Emdee et al.⁹⁵ time shift = 10 ms, comparison of experimental and modeling predictions [□]- Experiments, [-]-UIC *m*-Xylene Model 2

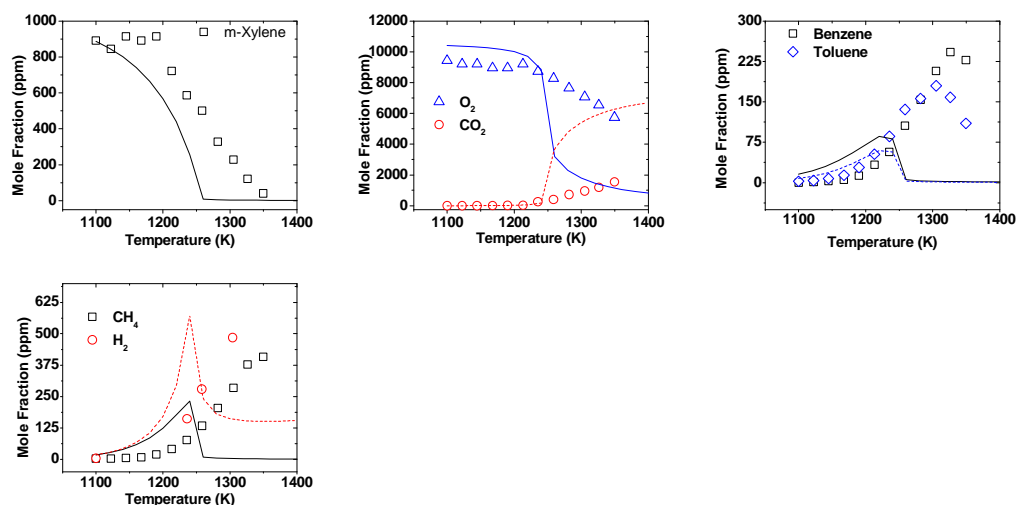


Fig 77. *m*-Xylene oxidation jet stirred reactor experiments at atmospheric pressure, Gail and Dagaut⁶⁴, comparison of experimental and modeling predictions [□]- Experiments, [-]-UIC *m*-Xylene Model 2

6.3.4. Sensitivity Analysis of *m*-Xylene

Sensitivity analyses of the fuel were performed to verify the contribution of the added and modified pathways to the fuel decay. Sensitivity analysis of the fuel was performed at fuel lean conditions for three different cases, which are described in detail below. The analyses were performed using closed homogenous batch reactor subroutine in CHEMKIN 4.1 and the normalized sensitivity coefficients are plotted against the corresponding reaction.

6.3.4.1. High Pressure (40-50 atm)

The sensitivity analysis of the fuel was performed at a temperature of 1265 K, pressure of 45 atm and a reaction time of 1.9ms and is shown in Fig 78. The temperature and pressure of the analysis were chosen such that it encompasses the temperature and pressure range of both high pressure shock tube and ignition delay experiments. The fuel decay is seen to be sensitive to the

formation of m-xylyl radical by hydrogen abstraction reactions, followed by the formation of dimethylphenyl radical, methylcresol and methylcresoxy radicals through reactions of m-xylene with O, OH and HO₂. Reactions of m-xylyl radical with O₂ and HO₂ leading to the formation of m-xylylperoxy and m-xylylhydroperoxide radicals are also important in this regime. At these temperatures less than 74% of the fuel has been consumed, so these temperatures are low enough and at high enough pressures to see noticeable formation of m-xylylperoxy and m-xylylhydroperoxide in the simulations.

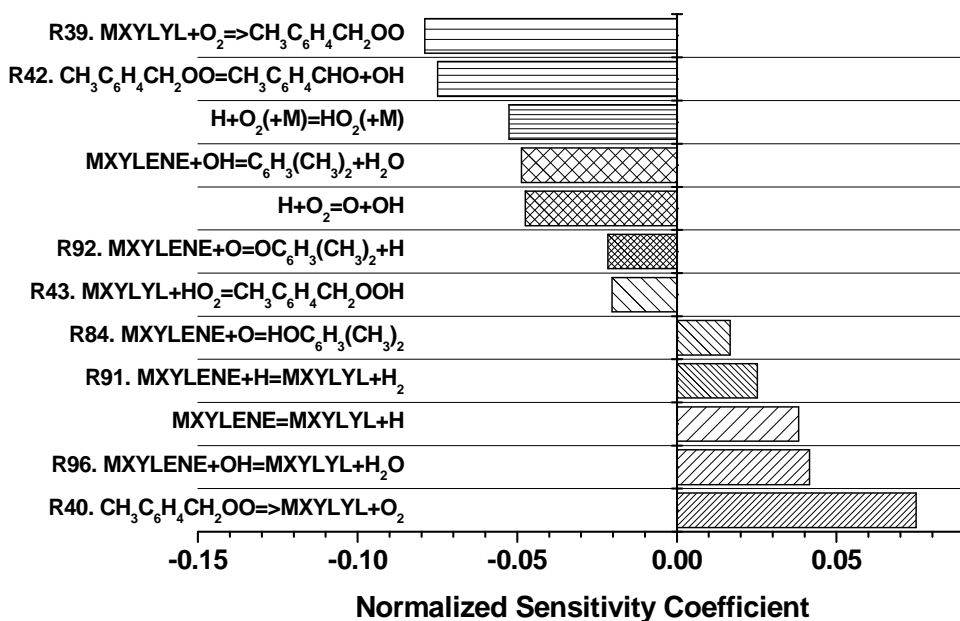


Fig 78. Sensitivity analysis of m-xylene performed for $T = 1265\text{ K}$, $P = 45\text{ atm}$ and time = 1.9 ms, using UIC m-Xylene Oxidation Model 2

6.3.4.2. Intermediate Pressure (10-25 atm)

The sensitivity analysis of the fuel was performed at a temperature of 1399 K, pressure of 16 atm and a reaction time of 1.9ms. The temperature and pressure of the analysis were chosen such that it encompasses the temperature range of both high pressure shock tube and ignition delay experiments. The pressure chosen was the average pressure for all the experimental datasets. The fuel decay was seen to be sensitive to the formation of m-xylylhydroperoxide, methylphenyl radicals and the consumption of methylphenyl radical with oxygen through reactions shown in Fig 79. At higher temperatures the C-C scission pathway becomes important which explains the fuel decay being sensitive to the consumption reaction of methylphenyl radicals. At these high enough temperatures (100 % fuel decay), the methylphenyl radical chemistry seems to be more important than the m-xylylperoxy radical chemistry.

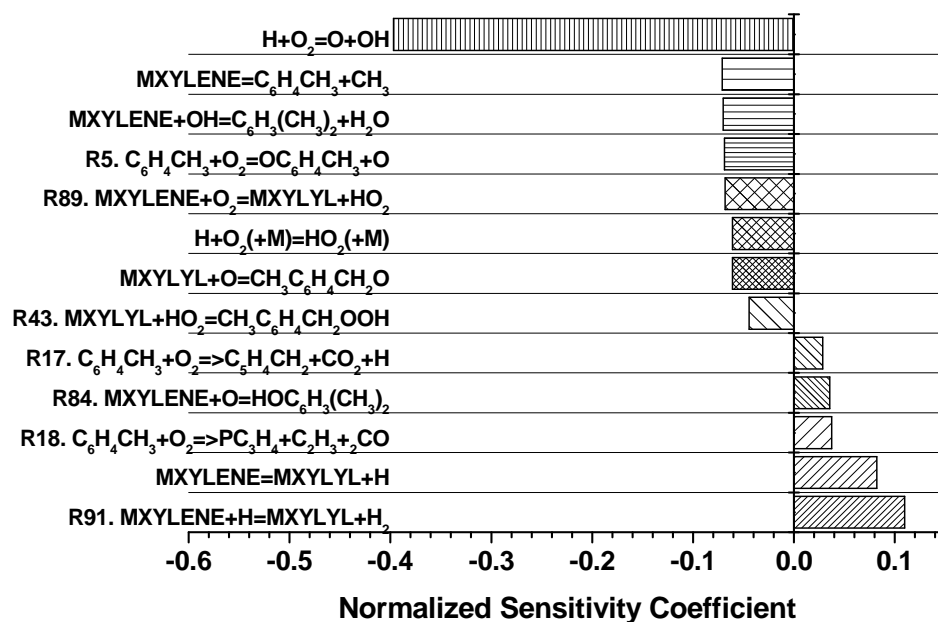


Fig 79. Sensitivity analysis of m-xylene performed for $T = 1399 \text{ K}$, $P = 16 \text{ atm}$ and time = 1.9 ms, using UIC m-Xylene Oxidation Model 2

6.3.4.3. Low Pressure(1 atm)

The sensitivity analysis of the fuel was performed at a temperature of 1161 K, pressure of 1 atm and a reaction time of 0.1s, which are the typical reaction times for complete conversion of the fuel in a plug flow reactor or the residence time in a jet stirred reactor, and it is shown in Fig 80.

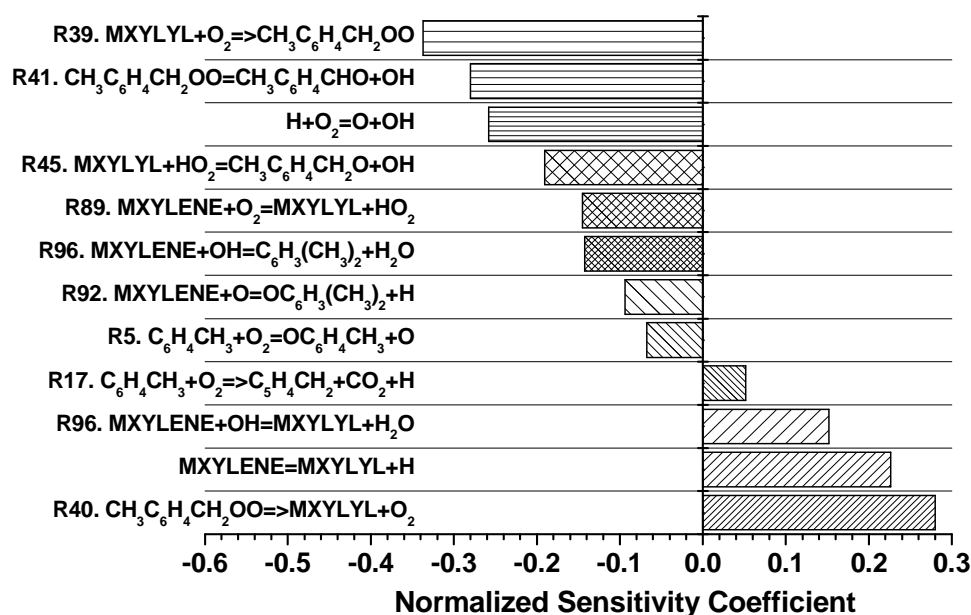


Fig 80. Sensitivity analysis of *m*-xylene performed for $T = 1161 \text{ K}$, $P = 1 \text{ atm}$ and time = 0.1s, using UIC *m*-Xylene Oxidation Model 2.

The fuel decay is most sensitive to the formation of *m*-xylylperoxy radicals through *m*-xylyl+O₂ reaction and the formation of methylbenzoxyl radical from the benzyl+HO₂ reaction. The fuel decay is also sensitive to the formation of dimethylphenyl radical, methylcresoxy and cresoxyl radical. A significant observation which can be made for the low pressure datasets is the shift in the benzyl+HO₂ chemistry. At low pressures the fuel decay is seen to be sensitive to the formation of methylbenzoxyl radical whereas at high pressures it is sensitive to the formation of *m*-xylylhydroperoxide. The temperatures and the pressures are low enough for this system, for the fuel decay to be dominated by the consumption reactions of methylbenzoxyl and *m*-xylylperoxy radical reactions. The increased amount of methylbenzaldehyde, shown by the model is due to the

formation of methylbenzoxyl and m-xylylperoxy radicals, both of which subsequently form methylbenzaldehyde.

The m-xylene oxidation chemistry is controlled by the formation of m-xylylhydroperoxide and m-xylylperoxy radicals at high pressures and low temperatures. At high pressures and high temperatures the methylphenyl radical oxidation and pyrolytic chemistry becomes important. At low pressures and low temperatures the m-xylyl oxidation chemistry is controlled by the formation of methylbenzoxyl radicals and m-xylylperoxy radicals.

6.3.4.4. Implications for Soot Formation

The experimental and modeling profiles of O₂, CO, CO₂, toluene, benzene, methane and acetylene at fuel lean, stoichiometric and fuel rich conditions are shown in Fig 69, Fig 70, Fig 71 and in Fig 73, Fig 74. The model predicts the consumption of oxygen and formation of the intermediates CO and CO₂, fairly well for fuel lean conditions. The model shows maximum concentrations of intermediates at the right experimental temperatures. For the fuel rich conditions, the modeling profiles show higher oxygen and correspondingly lower CO and CO₂. The modeling profiles show lower consumption of oxygen above 1385 K. For the consumption of the intermediates shown in Fig 71 and Fig 74, there is a shift in the modeling profiles when compared to the experimental data at higher temperatures. The temperatures at which the modeling profiles of intermediates are different from the experiments are the temperatures at which polycyclic aromatic hydrocarbons are being formed and decayed. This suggests that these intermediates, toluene, benzene, methane and acetylene, play a crucial role in the formation and consumption of the multi-ring compounds. Hence it is important to include in future development, the channels for the formation of polycyclic aromatic hydrocarbons to predict the experimental data more accurately.

However, the model at this stage, is sufficiently developed to be combined with a soot model that includes PAH formation and decay, for attempts at simulating the experimentally measured formation of soot from m-xylene. Nevertheless, for better soot modeling an extension of this current work to include pyrolytic experiments on m-xylene were conducted, in order to better identify the pathways leading to the formation of polycyclic aromatic hydrocarbons from the fuel under these shock tube conditions. The pyrolysis experiments and the modeling of the PAH formed in the m-xylene oxidation experiments are discussed in Chapter 8.

6.5. Conclusions

The oxidation of m-xylene has been studied at nominal reflected shock pressures of 25 and 50 atm, for a temperature range of 1050-1584 K at fuel lean, stoichiometric and fuel rich conditions. Species profiles of small hydrocarbons, mono-aromatic and multi-ring aromatic species were obtained as a function of temperature. A model was assembled to describe the decay of m-xylene and the formation of lower carbon number hydrocarbons, as measured from the experiments. The formation of dimethylphenoxy radicals and dimethylphenol are seen to be dominant in modeling the m-xylene decay for fuel lean conditions. The m-xylene oxidation chemistry is seen to be dependent on the consumption of m-xylyl radical through $\text{m-xylyl} + \text{O}_2$ and $\text{m-xylyl} + \text{HO}_2$ reactions. The model simulates the fuel decay accurately for all the experimental data sets and fairly good agreement is seen in modeling profiles of the intermediates when compared to the experimental data for fuel lean and stoichiometric conditions. The model has also been tested against experimental data obtained in other laboratories with satisfactory results. This chapter is focused only on the formation of single ring and substituted mono-aromatic species from the fuel.

7. DISCUSSION OF EXPERIMENTS AND MODELING RESULTS OF 1,3,5-TRIMETHYLBENZENE OXIDATION

7.1. Introduction

Prior experimental studies on 1,3,5-trimethylbenzene oxidation were limited to ignition delay times^{63,127}, diffusion flame extinction limits⁶² and measurement of rate constants for hydrodealkylation of the side chains¹²⁸ and reaction with the hydroxyl radical^{129,130}. Experimental data are also limited to low temperatures and pressures: temperatures of about 300 to 1000 K and pressures up to 21 atm. Detailed product distribution and mechanism of 1,3,5-trimethylbenzene oxidation is also not available in literature. Hence the focus of this study is to provide the ‘speciation’ data for 1,3,5-trimethylbenzene oxidation for pressures between 25 – 55 atm and for temperatures up to 1650 K and to develop a kinetic model to simulate our experimental data. 1,3,5-Trimethylbenzene oxidation experiments were performed in the High Pressure Single Pulse Shock Tube (HPST) at UIC.

7.2. Experimental Results

1,3,5-Trimethylbenzene oxidation experiments were performed at fuel lean, stoichiometric and fuel rich conditions, for a combined temperature range of 1017-1645 K. Experiments at fuel lean and fuel rich conditions were performed at two nominal reflected shock pressures of 20 and 50 atm. All the experiments at stoichiometric conditions were conducted at an average pressure of 50 atm. The experimental conditions are provided in Table 21.

Table 21. 1,3,5-Trimethylbenzene oxidation experimental conditions

Average Shock Pressure /atm	Fuel /ppm	Temperature Range /K	Φ	Reaction Time /ms
20	76	845-1515	0.46	1.55-4.6
50	87	1018-1561	0.51	1.26-2.8
50	73	1036-1639	0.95	1.13-1.7
20	82	1035-1620	1.79	1.4-3.2
45	86	938-1645	1.86	1.11-2.1

7.2.1. Effect of Pressure on the Fuel and Oxidizer Decay

The profiles of the fuel and oxidizer are shown as a function of temperature and concentration in Fig 81, for two different nominal reflected shock pressures of 20 and 50 atm and similar equivalence ratios. Over the pressure and temperature range of the current experiments, no significant pressure dependence was seen for the decay of the fuel, oxidizer and for the formation of the major intermediates.

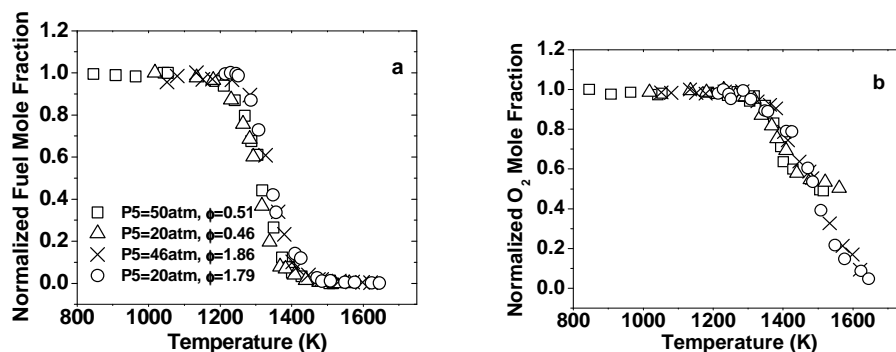


Fig 81. a) Fuel (1,3,5-trimethylbenzene) and b) oxidizer decay, [Δ]-average pressure = 49.7 atm, $\Phi = 0.51$, reaction times = 1.26-2.8 ms, [\square]-average pressure = 20 atm, $\Phi = 0.46$, reaction times = 1.55-2.55 ms, [\circ]-average pressure = 45.6 atm, $\Phi = 1.86$, reaction times = 1.11-2.11 ms, [\times]-average pressure = 19.69 atm, $\Phi = 1.79$, reaction times=1.40-2.47 ms

7.2.2. Development of 1,3,5-Trimethylbenzene Oxidation Mechanism based on the Product Distribution

As per the authors knowledge detailed mechanism or a chemical kinetic model for oxidation of 1,3,5-trimethylbenzene is not available in literature. However, mechanisms and chemical kinetic models are available for the oxidation of trimethylbenzenes. In these cases, the 1,2,3-, 1,2,4- and 1,3,5- trimethylbenzenes were lumped into a single species^{131–133}. Since a detailed mechanism for the oxidation of 1,3,5-trimethylbenzene was not available in literature, the primary task was to develop a mechanism based on the product distribution observed from our experiments. The secondary task was to develop a chemical kinetic model based on the mechanism developed by us. In this section we explain the procedure followed in developing a mechanism for oxidation of the fuel based on the product distribution. In section 7.4 we explain the rationale behind choosing the rate constants for the reactions discussed in the mechanism.

Since there was minor influence of the equivalence ratio on the species distribution, the oxidation experiments at $\phi = 0.5$, have been chosen to define the reaction mechanism of the fuel based on the species observed at different temperatures. The concentration profiles of the fuel and the major intermediates are provided in Fig 82 (a-d). The proposed mechanism for the oxidation of 1,3,5-trimethylbenzene is shown in Fig 83. The structures of the stable intermediates are bolded in Fig 83, to make identification of these species easier for the reader.

At lower temperatures ($T_5 = 1134$ K) of the decay of 1,3,5-trimethylbenzene we observed the formation of 1-[2-(3,5-dimethylphenyl)ethyl]-3,5-dimethylbenzene ($C_{18}H_{22}$), which could be formed from the recombination of 1,3,5-trimethylbenzene and 1,3,5-trimethylbenzyl radicals (Fig 82 (a) and pathway I in Fig 83). The latter species is formed from 1,3,5-trimethylbenzene via hydrogen abstraction reactions (pathway II in Fig 83). At temperature of about 1181 K we observed the formation of 3,5-dimethylbenzaldehyde (see Fig 82 (a)). This species could be formed from oxidation reactions of 1,3,5-trimethylbenzyl radical (reaction mechanism in the box labeled as III in Fig 83). At slightly higher temperatures ($T_5 = 1264$ K) we observed the formation of m-xylene, methane, ethane, 1-ethyl-3,5-dimethylbenzene, 1-ethenyl-3,5-dimethylbenzene, toluene and benzene (see Fig 82 (b-d)). m-Xylene could be formed from the fuel by displacement of the methyl side chain by a hydrogen atom (Fig 82 (b) and pathway IV in Fig 83). The methyl radical could recombine with a hydrogen atom and other methyl radicals and produce methane and ethane (profiles shown in Fig 82 (b) and pathways not shown in Fig 83). Subsequent displacement reactions of methyl radicals from m-xylene by hydrogen atom could lead to the formation of toluene and benzene (Fig 82 (c) and pathways V and VI in Fig 83). Another possibility for the formation of these species is through a sequence of steps involving oxidation of 3,5-dimethylbenzaldehyde (reaction mechanism in box labeled as VII, where DIMCPD radical is the dimethylcyclopentadienyl radical). 1-Ethyl-3,5-dimethylbenzene could be formed from recombination reactions of 1,3,5-

trimethylbenzyl radical with methyl radical (Fig 82 (d) and pathway VIII in Fig 83) and subsequent hydrogen abstraction reactions could lead to the formation of 1-ethenyl-3,5-dimethylbenzene (Fig 82 (d) and pathway IX in Fig 83).

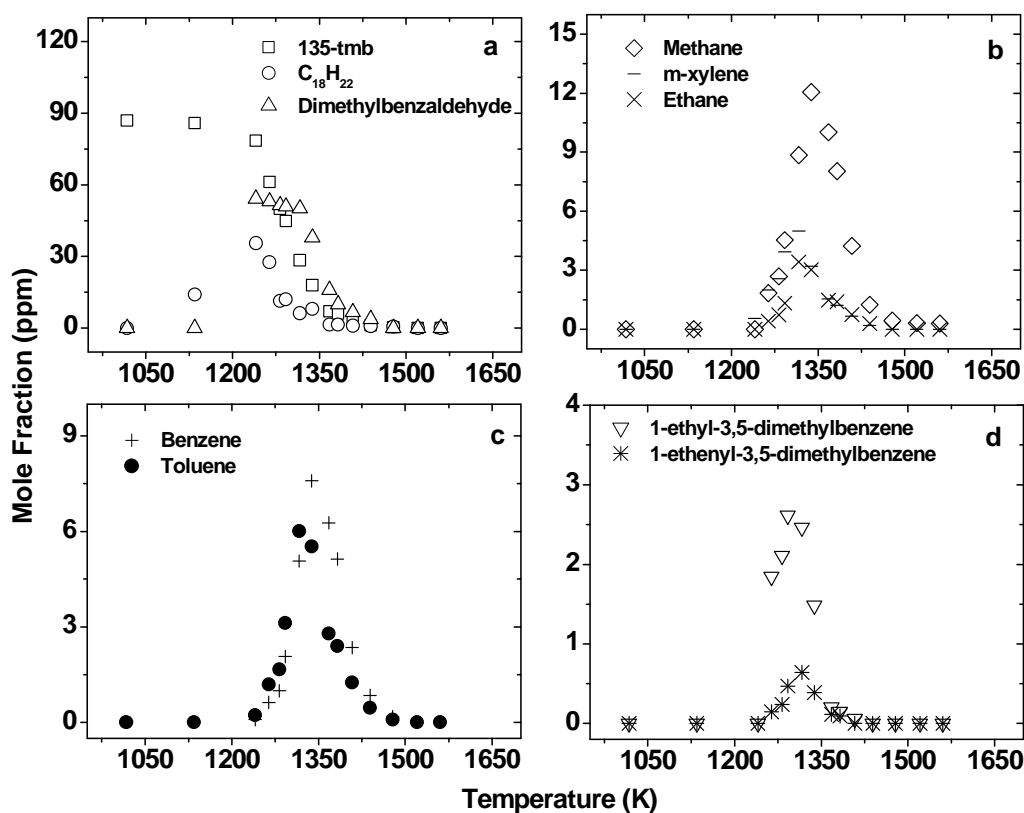


Fig 82. Fuel decay and the formation of major intermediates, average $P5 = 49.7$ atm, $\phi = 0.51$, reaction times = 1.26 to 2.8 ms. (a) [\square]-1,3,5-Trimethylbenzene, [\circ]- $C_{18}H_{22}$, [Δ]-3,5-Dimethylbenzaldehyde, (b) [-]-m-Xylene, [\diamond]-Methane, [\times]-Ethane, (c) [\bullet]-Toluene, [$+$]-Benzene, (d) [∇]-1-Ethyl-3,5-Dimethylbenzene, [$*$]-1-Ethenyl-3,5-Dimethylbenzene,

The procedure followed by us, in developing the chemical kinetic model for the oxidation of 1,3,5-trimethylbenzene is mentioned in the following section (Section 7.3). In Section 7.4, the modeling results are compared against the experimental data and a sensitivity and reaction path analysis is performed to get a better understanding of the decay of the fuel and formation of the intermediates and it also serves as a means to validate our proposed mechanism.

7.3. UIC 1,3,5-Trimethylbenzene Oxidation Model

7.3.1. Kinetics for 1,3,5-Trimethylbenzene Decay and Formation of Major Single Ringed Aromatic Intermediates

The UIC 1,3,5-Trimethylbenzene Oxidation Model is developed by adding reactions of methyl side chains oxidation and abstraction to our UIC m-Xylene Oxidation Model¹³⁴. Rate constants for the oxidation of 1,3,5-trimethylbenzene were directly taken from literature, if they are available, and when not available, the rate constants were estimated from analogous reactions of toluene and were adjusted for degeneracy. For example, the rate constant for abstraction of the methyl side chain hydrogen atoms of 1,3,5-trimethylbenzene by a methyl radical was estimated from the analogous reaction of a methyl radical abstracting a hydrogen atom from toluene. The pre-exponential factor was multiplied by a factor of 3, in order to account for the number of abstractable hydrogen atoms from the side chains; nine hydrogen atoms in the case of 1,3,5-trimethylbenzene and only three hydrogen atoms in the case of Toluene. Toluene has been chosen as the reference species because the oxidation and pyrolytic kinetics of toluene has been extensively studied and direct experimental measurements are available for most of the reactions for oxidation of toluene.

The rate constants for the oxidation of 1,3,5-trimethylbenzene and the formation of the intermediates discussed and shown in the mechanism in Fig 83, are listed in Table 22. The rate constants for the pathways shown in Fig 83 are bolded. Additional pathways were also included to develop a comprehensive kinetic model. The structures of the italicized species in Table 22 could be found in

Table 23. The source from which the rate constant has been estimated is provided in the superscripts beside the reaction and the letter beside superscript will direct the reader towards the footnotes where any modifications made to the rate constants are listed.

Table 22. Rate constants for the decay of the fuel and the formation and consumption of other major intermediates

Rxn	Reaction^a	A	n	Ea
R1 ¹³⁵	<i>C₉H₁₂=C₉H₁₁+H</i>	2.24E+16	0	87237
R-1 ¹³⁵	Reverse	7.80E+13	0	0
R2 ^{65,b}	<i>C₉H₁₂=C₆H₃(CH₃)₂+CH₃</i>	3.37E+17	0	100437
R-2 ^{136,c}	Reverse	1.38E+13	0	45
R3 ¹³⁷	<i>C₉H₁₂+H=C₉H₁₁+H₂</i>	3.70E+14	0	8628
R-3 ^{138,d}	Reverse	2.82E+12	0	14500
R4 ^{90,e}	<i>C₉H₁₂+CH₃=C₉H₁₁+CH₄</i>	3.51E+11	0	7700
R-4 ^{90,f}	Reverse	1.20E+13	0	27100
R5 ^{70,g}	<i>C₉H₁₂+OH=C₉H₁₁+H₂O</i>	1.56E+10	1	874
R-5 ^{70,h}	Reverse	1.23E+10	0.70	29538
R6 ^{70,i}	<i>C₉H₁₂+O₂=C₉H₁₁+HO₂</i>	3.42E+07	2.5	44946
R-6 ^{70,j}	Reverse	1.44E+07	1.974	4085
R7 ¹³⁹	<i>C₉H₁₂+H=MXYLENE+CH₃</i>	6.70E+13	0	6468
R-7 ^{140,k}	Reverse	8.00E+11	0	15900
R8 ^{135,l}	<i>C₉H₁₁+CH₃=DIMETB</i>	1.10E+12	0	0
R-8 ^{135,b}	Reverse	8.00E+14	0	80922
R9 ^{70,m}	<i>DIMETB+H=DIMCHCH3+H2</i>	7.26E+07	2	5345
R-9 ^{70,n}	Reverse	1.98E+06	2.2	22404
R10 ^{70,o}	<i>DIMETB+H=DIMCH2CH2+H2</i>	1.59E+08	1.5	7412

R-10 ^{70,p}	Reverse	6.51E+05	1.564	8720
R11 ^{70,q}	<i>DIMETB</i> +O= <i>DIMCHCH3</i> +OH	4.91E+13	0	3795
R-11 ^{70,r}	Reverse	3.19E+11	0.18	19027
R12 ^{70,s}	<i>DIMETB</i> +HO ₂ = <i>DIMCHCH3</i> +H ₂ O ₂	1.36E+05	2.5	13522
R-12 ^{70,t}	Reverse	9.75E+05	2.04	14045
R13 ^{70,u}	<i>DIMETB</i> +HO ₂ = <i>DIMCH2CH2</i> +H ₂ O ₂	7.81E+04	2.5	16849
R-13 ⁷⁰	Reverse	2.98E+03	1.901	1621
R14 ^{70,w}	<i>DIMETB</i> +OH= <i>DIMCH2CH2</i> +H ₂ O	4.80E+12	0	0
R-14 ^{70,x}	Reverse	8.51E+10	-0.03	16598
R15 ^{70,y}	<i>C</i> ₆ <i>H</i> ₃ (<i>CH</i> ₃) ₂ + <i>C</i> ₂ <i>H</i> ₄ = <i>DIMCH2CH2</i>	4.04E+03	2.64	1459
R-15 ^{141,z}	Reverse	1.72E+11	0.78	38704
R16 ^{141,aa}	<i>DIMCH2CH2</i> = <i>DIMSTYR</i> +H	1.83E+06	2.081	33207
R-16 ^{141,ab}	Reverse	1.63E+06	2.158	1994
R17 ^{141,ac}	<i>DIMCH2CH2</i> = <i>DIMCHCH3</i>	5.96E+05	2.074	29582
R-17 ^{141,ad}	Reverse	2.30E+07	1.737	44456
R18 ^{141,ae}	<i>DIMCHCH3</i> = <i>DIMSTYR</i> +H	3.74E+08	1.55	44609
R-18 ^{141,af}	Reverse	1.19E+07	1.925	-108
R19 ^{81,ag}	<i>DIMSTYR</i> +H= <i>DIMCHCH</i> +H ₂	1.99E+06	2.53	12239
R-19 ^{70,ah}	Reverse	1.98E+06	2.2	22404
R20 ^{81,ai}	<i>DIMSTYR</i> +O= <i>C</i> ₆ <i>H</i> ₃ (<i>CH</i> ₃) ₂ +CH ₂ HCO	3.50E+13	0	2832
R21 ^{142,aj}	<i>C</i> ₆ <i>H</i> ₃ (<i>CH</i> ₃) ₂ + <i>C</i> ₂ <i>H</i> ₂ = <i>DIMCHCH</i>	2.69E+06	2.05	3720
R-21 ^{142,ak}	Reverse	1.35E+14	0.34	45710
R22 ¹³¹	<i>DIMETB</i> +H= <i>MCPHC2H5</i> +CH ₃	5.80E+13	0	8100
R-22 ¹³¹	Reverse	1.20E+12	0	15900
R23 ^{131,al}	<i>DIMSTYR</i> +H= <i>MCSTYREN</i> +CH ₃	5.80E+13	0	8100
R-23 ^{131,am}	Reverse	1.20E+12	0	15900
R24 ¹³¹	<i>DIMETB</i> +H= <i>MXYLENE</i> +C ₂ H ₅	5.20E+13	0	4100
R-24 ¹³¹	Reverse	1.20E+11	0	15900
R25 ^{131,an}	<i>DIMSTYR</i> +H= <i>MXYLENE</i> +C ₂ H ₃	5.20E+13	0	4100
R-25 ^{131,ao}	Reverse	1.20E+11	0	15900
		3.076E+1		
R26 ^{115,ap}	<i>C</i> ₉ <i>H</i> ₁₁ +O ₂ = <i>C</i> ₉ <i>H</i> ₁₁ OO	1	-0.01	751.8
R-26 ^{115,aq}	Reverse	7.85E+13	0	10224
		1.795E+1		
R27 ^{115,ar}	<i>C</i> ₉ <i>H</i> ₁₁ OO= <i>DIMPHHCO</i> +OH	2	0	10066
R28 ^{115,as}	<i>C</i> ₉ <i>H</i> ₁₁ OO= <i>OC</i> ₆ <i>H</i> ₃ (<i>CH</i> ₃) ₂ +CH ₂ O	5.55E+09	0	17341
R-28 ^{68,b}	Reverse	1.00E+13	0	0
R29 ^{143,b}	<i>DIMPHHCO</i> = <i>DIMPHCO</i> +H	3.98E+15	0	83661
R-29 ^{68,b}	Reverse	3.00E+13	0	0
R30 ^{144,au}	<i>DIMPHCO</i> = <i>C</i> ₆ <i>H</i> ₃ (<i>CH</i> ₃) ₂ +CO	1.25E+15	0	27646
R-30 ^{145,av}	Reverse	1.17E+12	0	2778
R31 ^{119,aw}	<i>DIMPHHCO</i> +O ₂ = <i>DIMPHCO</i> +HO ₂	7.14E+13	0	38950
R-31 ^{146,ax}	Reverse	3.01E+13	0	0
R32 ^{119,ay}	<i>DIMPHHCO</i> +OH= <i>DIMPHCO</i> +H ₂ O	1.20E+10	1.18	-447

R-32 ^{146,az}	Reverse	5.14E+11	1.35	26000
R33 ^{119,ba}	$DIMPHHCO+H=DIMPHCO+H_2$	3.50E+14	0	4928
R-33 ^{146,bb}	Reverse	1.31E+11	1.82	17600
R34 ^{119,bc}	$DIMPHHCO+O=DIMPHCO+OH$	6.33E+13	0	3080
R-34 ^{146,bd}	Reverse	4.22E+13	0	0
R35 ^{131,al}	$DIMPHHCO+H=MCPHHCO+CH_3$	5.80E+13	0	8100
R-35 ^{131,am}	Reverse	1.20E+12	0	15900
R36 ^{147,be}	$C_9H_{11}+O=DIMPHHCO+H$	4.00E+13	0	0
R-36 ^{148,bf}	Reverse	3.98E+13	0	102540
R37 ^{147,bg}	$C_9H_{11}+OH=DIMPHCH_2OH$	2.00E+13	0	0
	$DIMPHCH_2OH+OH=DIMPHCH_2O$			
R38 ^{147,bh}	$+H_2O$	5.00E+12	0	0
	$DIMPHCH_2OH+H=MCPCH_2OH+CH_3$			
R39 ^{131,al}		5.80E+13	0	8100
R-39 ^{131,am}	Reverse	1.20E+12	0	15900
R40 ^{112,bi}	$C_9H_{11}+HO_2=C_9H_{11}OOH$	8.00E+13	0	0
R41 ^{112,bj}	$C_9H_{11}OOH=DIMPHCH_2O+OH$	3.29E+13	0.42	39890
R42 ^{113,bk}	$C_9H_{11}+HO_2=DIMPHCH_2O+OH$	3.86E+10	0	1456
R43 ^{114,bl}	$DIMPHCH_2O=DIMPHHCO+H$	5.07E+08	1.56	16850
R44 ^{114,bm}	$DIMPHCH_2O=C_6H_3(CH_3)_2+CH_2O$	1.09E+14	0.157	31160
R45 ^{114,bn}	$DIMPHCH_2O=MXYLENE+HCO$	1.81E+13	0	22717
R47 ^{114,bo}	$C_6H_3(CH_3)_2+O_2=OC_6H_3(CH_3)_2+O$	8.57E+18	-2.27	7189
R-47 ^{114,bp}	Reverse	2.21E+25	-3.39	16945
R48 ¹³¹	$MCPHC_2H_5+H=\phi C_2H_5+CH_3$	1.70E+14	0	8100
R-48 ¹³¹	Reverse	1.20E+12	0	15900
R49 ^{131,bq}	$MCSTYREN+H=\phi CH_3+C_2H_3$	5.20E+13	0	4100
R-49 ^{131,br}	Reverse	1.20E+11	0	15900
R50 ^{131,bs}	$MCSTYREN+H=\phi C_2H_3+CH_3$	1.70E+14	0	8100
R-50 ^{131,bt}	Reverse	1.20E+12	0	15900
R51 ^{65,b}	$MCSTYREN=C_6H_4CH_3+C_2H_3$	8.00E+15	0	114177
R-51 ^{68,b}	Reverse	2.00E+13	0	0
R53 ^{65,b}	$MCPHC_2H_5=C_6H_4CH_3+C_2H_5$	8.00E+15	0	100907
R-52 ^{68,b}	Reverse	2.00E+13	0	0
R53 ^{131,bq}	$DIMPHHCO+H=MXYLENE+HCO$	5.20E+13	0	4100
R-53 ^{131,br}	Reverse	1.20E+11	0	15900
R55 ^{65,b}	$DIMPHHCO=C_6H_3(CH_3)_2+HCO$	8.00E+15	0	147206
R-55 ^{68,b}	Reverse	2.00E+13	0	0
R56 ^{65,b}	$DIMPHCH_2OH=C_6H_3(CH_3)_2+CH_2OH$	8.00E+15	0	148412
R-56 ^{68,b}	Reverse	2.00E+13	0	0
R57 ^{68,b}	$C_6H_3(CH_3)_2+H=>MXYLENE$	1.00E+14	0	0
R58 ^{68,b}	$C_6H_3(CH_3)_2+O=>OC_6H_3(CH_3)_2$	1.00E+14	0	0
R59 ^{68,b}	$C_6H_3(CH_3)_2+OH=>HOC_6H_3(CH_3)_2$	1.00E+13	0	0

^arate constant, $k = AT^n \exp(-E_a/RT)$: rate constant (units:

mol, s, cm³, cal), ϕ denotes the phenyl ring

^bEstimated using rate rules proposed by Dean⁶⁵ and Allara and Shaw⁶⁸

^ck same as $\phi + \text{CH}_3 = \phi\text{CH}_3$

^dk same as $\phi\text{CH}_2 + \text{H}_2 = \phi\text{CH}_3 + \text{H}$

^eA-factor x 3 of $\text{CH}_3 + \phi\text{CH}_3 = \text{CH}_4 + \phi\text{CH}_2$

^fk same as $\phi\text{CH}_2 + \text{CH}_4 = \phi\text{CH}_3 + \text{CH}_3$

^gA-factor x 3 of $\text{OH} + \phi\text{CH}_3 = \text{H}_2\text{O} + \phi\text{CH}_2$

^hk same as $\phi\text{CH}_2 + \text{H}_2\text{O} = \phi\text{CH}_3 + \text{OH}$

ⁱA-factor x 3 of $\text{O}_2 + \phi\text{CH}_3 = \text{HO}_2 + \phi\text{CH}_2$

^jk same as $\phi\text{CH}_2 + \text{HO}_2 = \phi\text{CH}_3 + \text{O}_2$

^kA-factor x (2/3) of $\text{CH}_3 + \text{C}_6\text{H}_6 = \phi\text{CH}_3 + \text{H}$

^lA-factor x (1/10) of $\phi\text{CH}_2 + \text{CH}_3 = \phi\text{C}_2\text{H}_5$, adjusted based on the agreement of the modeling results with the experimental data

^mA-factor x 2.2 of $\phi\text{C}_2\text{H}_5 + \text{H} = \phi\text{CHCH}_3 + \text{H}_2$

ⁿk same as $\phi\text{CHCH}_3 + \text{H}_2 = \phi\text{C}_2\text{H}_5 + \text{H}$

^oA-factor x 2.2 of $\phi\text{C}_2\text{H}_5 + \text{H} = \phi\text{CH}_2\text{CH}_2 + \text{H}_2$

^pk same as $\phi\text{CH}_2\text{CH}_2 + \text{H}_2 = \phi\text{C}_2\text{H}_5 + \text{H}$

^qA-factor x 2.2 of $\phi\text{C}_2\text{H}_5 + \text{O} = \phi\text{CHCH}_3 + \text{OH}$

^rk same as $\phi\text{CHCH}_3 + \text{OH} = \phi\text{C}_2\text{H}_5 + \text{O}$

^sA-factor x 2.2 of $\phi\text{C}_2\text{H}_5 + \text{HO}_2 = \phi\text{CHCH}_3 + \text{H}_2\text{O}_2$

^tk same as $\phi\text{CHCH}_3 + \text{HO}_2 = \phi\text{C}_2\text{H}_5 + \text{HO}_2$

^uA-factor x 2.2 of $\phi\text{C}_2\text{H}_5 + \text{HO}_2 = \phi\text{CH}_2\text{CH}_2 + \text{H}_2\text{O}_2$

^vk same as $\phi\text{C}_2\text{H}_5 + \text{HO}_2 = \phi\text{CHCH}_3 + \text{HO}_2$

^wk same as $\phi\text{C}_2\text{H}_5 + \text{OH} = \text{products}$

^xk same as $\phi\text{CH}_2\text{CH}_2 + \text{HO}_2 = \phi\text{C}_2\text{H}_5 + \text{OH}$

^yk same as $\phi + \text{C}_2\text{H}_4 = \phi\text{CH}_2\text{CH}_2$

^zk same as $\phi\text{CH}_2\text{CH}_2 = \phi + \text{C}_2\text{H}_4$

^{aa}k same as $\phi\text{CH}_2\text{CH}_2 = \phi\text{C}_2\text{H}_3 + \text{H}$

^{ab}k same as $\phi\text{C}_2\text{H}_3 + \text{H} = \phi\text{CH}_2\text{CH}_2$

^{ac}k same as $\phi\text{CH}_2\text{CH}_2 = \phi\text{CHCH}_3$

^{ad}k same as $\phi\text{CHCH}_3 = \phi\text{CH}_2\text{CH}_2$

^{ae}k same as $\phi\text{CHCH}_3 = \phi\text{C}_2\text{H}_3 + \text{H}$

^{af}k same as $\phi\text{C}_2\text{H}_3 + \text{H} = \phi\text{CHCH}_3$

^{ag}A-factor x 3 of $\phi\text{C}_2\text{H}_3 + \text{H} = \phi\text{CHCH} + \text{H}_2$

^{ah}k same as $\phi\text{CH}_2\text{CH}_2 + \text{H}_2 = \phi\text{C}_2\text{H}_5 + \text{H}$

^{ai}k same as $\phi\text{C}_2\text{H}_3 + \text{O} = \phi + \text{CH}_2\text{HCO}$

^{aj}k same as $\phi + \text{C}_2\text{H}_2 = \phi\text{C}_2\text{H}_3$

^{ak}k same as $\phi\text{C}_2\text{H}_3 = \phi + \text{C}_2\text{H}_2$

^{al}k same as $\text{DIMETB} + \text{H} = \text{MCPHC}_2\text{H}_5 + \text{CH}_3$

^{am}k same as $\text{MCPHC}_2\text{H}_5 + \text{CH}_3 = \text{DIMETB} + \text{H}$

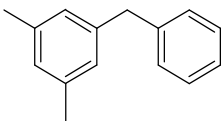
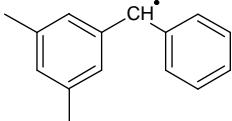
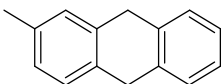
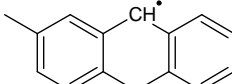
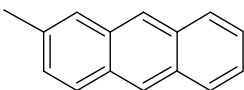
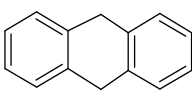
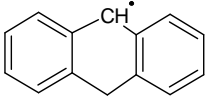
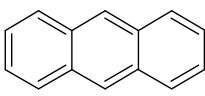
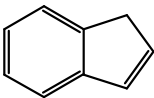
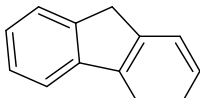
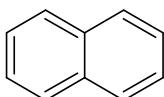
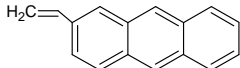
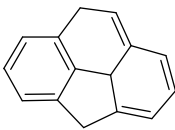
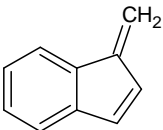
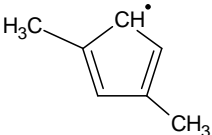
^{an}k same as $\text{DIMETB} + \text{H} = \text{MXYLENE} + \text{C}_2\text{H}_5$

^{ao}k same as $\text{MXYLENE} + \text{C}_2\text{H}_5 = \text{DIMETB} + \text{H}$

^{ap}k same as $C_8H_9 + O_2 = C_8H_9OO$
^{aq}k same as $C_8H_9OO = C_8H_9 + O_2$
^{ar}A-factor x (1/10) of $C_8H_9OO = CH_3C_6H_4CHO + OH$, adjusted based on the agreement of the modeling results with the experimental data
^{as}k same as $OC_6H_3(CH_3)_2 + CH_2O = C_9H_{11}OO$
^{at}k same as $\phi CHO = \phi CO + H$
^{au}k same as $\phi CO = \phi + CO$
^{av}k same as $\phi + CO = \phi CO$
^{aw}A-factor x 7 of $\phi CHO + O_2 = \phi CO + HO_2$
^{ax}k same as $HCO + HO_2 = \text{products}$
^{ay}A-factor x 7 of $\phi CHO + OH = \phi CO + H_2O$
^{az}k same as $HCO + HO_2 = CH_2O + OH$
^{ba}A-factor x 7 of $\phi CHO + H = \phi CO + H_2$
^{bb}k same as $CH_3CO + H_2 = CH_3CHO + H$
^{bc}A-factor x 7 of $\phi CHO + O = \phi CO + OH$
^{bd}k same as $CH_3CO + OH = \text{products}$
^{be}k same as $\phi CH_2 + O = \phi CHO + H$
^{bf}k same as $HCO + H = O + CH_2$
^{bg}k same as $\phi CH_2 + OH = \phi CH_2OH$
^{bh}k same as $\phi CH_2OH + OH = \phi CH_2O + H_2O$
^{bi}k same as $\phi CH_2 + HO_2 = \phi CH_2OOH$
^{bj}k same as $\phi CH_2OOH = \phi CH_2O + OH$
^{bk}k same as $\phi CH_2 + HO_2 = \phi CH_2O + OH$
^{bl}k same as $\phi CH_2O = \phi CHO + H$
^{bm}k same as $\phi CH_2O = \phi + CH_2O$
^{bn}k same as $\phi CH_2O = C_6H_6 + CHO$
^{bo}A-factor x (1/100) of $C_6H_4CH_3 + O_2 = OC_6H_4CH_3 + O$, adjusted based on the agreement of the modeling results with the experimental data
^{bp}A-factor x (1/100) of $OC_6H_4CH_3 + O = C_6H_4CH_3 + O_2$, adjusted based on the agreement of the modeling results with the experimental data
^{bq}k same as $MCPHCH_5 + H = \phi CH_3 + C_2H_5$
^{br}k same as $\phi CH_3 + C_2H_5 = MCPHCH_5 + H$
^{bs}k same as $MCPHC_2H_5 + H = \phi C_2H_5 + CH_3$
^{bt}k same as $\phi C_2H_5 + CH_3 = MCPHC_2H_5 + H$

Table 23. Structures of species present in reactions in Table 22 and Table 24, discussed in the text

Species name in model	Species Structure	Species name in model	Species Structure
C_9H_{12}		$C_6H_3(CH_3)_2$	
C_9H_{11}		DIMETB	
DIMCHCH3		DIMCH2CH2	
DIMSTYR		MCPHC2H5	
MCSTYREN		$C_9H_{11}OO$	
DIMPHHCO		$OC_6H_3(CH_3)_2$	
DIMPHCO		MCPHHCO	
DIMPHCH2OH		DIMPHCH2O	
MCPCH2OH		$C_9H_{11}OOH$	
$C_{18}H_{22}$		$HOC_6H_3(CH_3)_2$	

DIMERS196		RDIMERS196a	
PTRIARO192		PTRIARO192a	
A3CH3		PTRIARO178	
RPTRIARO178		A3	
INDENE		FLUORENE	
A2		A3C2H	
Cyclopentaphenanthrene		Methyleneindene	
Dimethylcyclopentadienyl radical (DIMCPD)			

7.3.2. Kinetics for the Formation of Major Two Ringed, Three Ringed and Four Ringed Intermediates from 1,3,5-Trimethylbenzene

The major two ringed aromatic hydrocarbons measured in our experiments were 1-(phenylmethyl)-3,5-dimethylbenzene (DIMERS196), 1-[2-(3,5-dimethylphenyl)ethyl]-3,5-dimethylbenzene ($C_{18}H_{22}$). The major polycyclic aromatic hydrocarbon intermediates measured in our experiments were indene (INDENE), naphthalene (A2), anthracene (A3) and methylantracene

(A3CH₃) for all the oxidation experiments. Considerable concentrations of fluorene, cyclopentaphenanthrene, methyleneindene and ethenylantracene were measured for the fuel rich oxidation experiments ($\phi = 2$). The profiles for the formation of the major polycyclic aromatic hydrocarbon intermediates are provided in Fig 84.

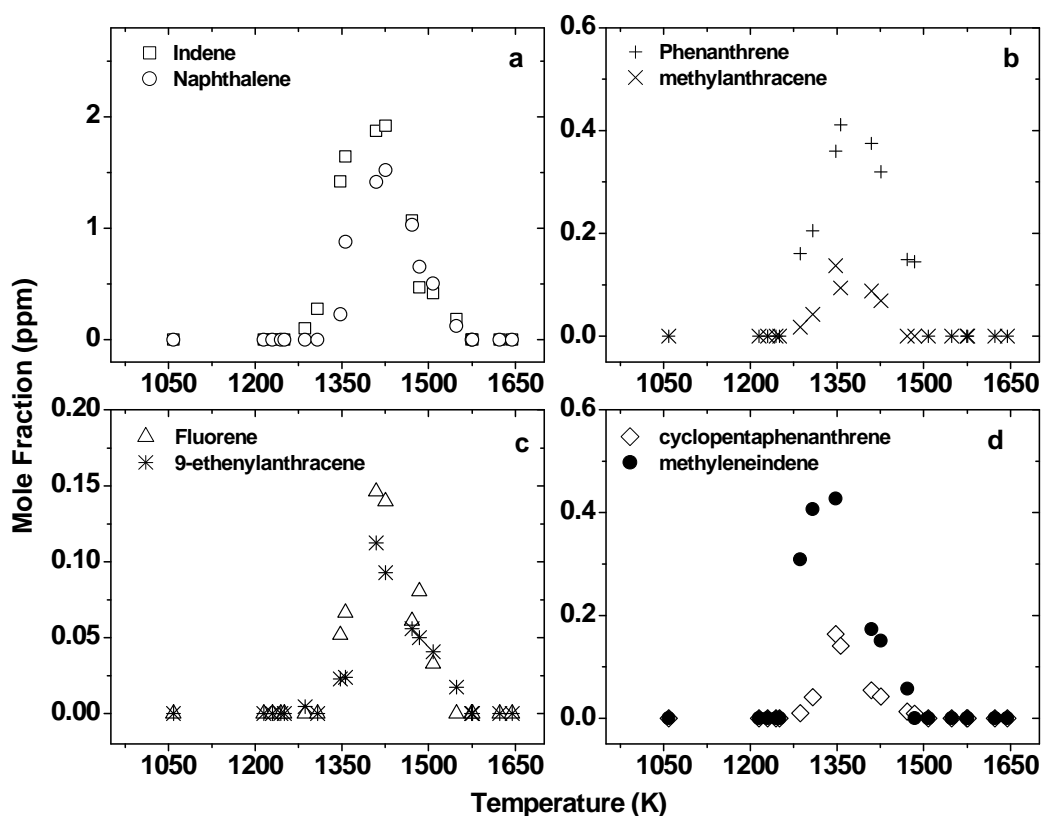


Fig 84. Major polycyclic aromatic hydrocarbons formed in 1,3,5-trimethylbenzene oxidation experiments, average $P_5 = 45.6$ atm, $\phi = 1.86$ and reaction time = 1.11 to 2.11 ms, (a) [\square]-Indene, [\circ]-Naphthalene, (b) [$+$]-Anthracene, [\times]-Methylanthracene, (c) [Δ]-Fluorene, [$*$]-Ethenylantracene, (d) [\diamond]-cyclopentaphenanthrene, [\bullet]-methyleneindene

A list of all the other polycyclic aromatic hydrocarbon intermediates which were identified is provided in the supplementary information. The concentrations of these intermediates were considerably small, so we were not successful in obtaining profiles for the formation and consumption of these intermediates. Nevertheless, the identification of these intermediates provides valuable information about the polycyclic aromatic hydrocarbons that are formed from the oxidation of 1,3,5-trimethylbenzene, for our experimental conditions. With the current experimental apparatus, it was not possible to differentiate between various isomers of three ringed aromatic hydrocarbons. Hence, the three ringed aromatic hydrocarbons have been assumed to be anthracene and methylated anthracene species.

The reaction mechanism and the rate constants for the formation of three ringed aromatic hydrocarbons were included from the publication of Fusetti et al.¹³¹ In this paper, the authors studied the pathways leading to the formation of methane from methylated monoaromatics, which includes 1,2,4-Trimethylbenzene by conducting pyrolysis experiments at a temperature range of 668-723 K and a pressure of 100 bar. The authors proposed the mechanism for the formation of various three ringed aromatic hydrocarbons (anthracene) with different degrees of alkylation from a trimethylbenzene (and not specifically 1,2,4-, 1,2,3- or 1,3,5-Trimethylbenzene). Hence these pathways have been incorporated into our kinetic model. The rate constants for the formation of anthracene and methyl anthracene from trimethylbenzene which were adapted from the work of Fusetti et al.¹³¹ are provided in Table 24. The reactions for the formation of other major polycyclic aromatic hydrocarbons like indene, naphthalene, acenaphthylene and ethenylantracene were included from the atmospheric pressure soot model of Slavinskaya et al.⁹², Slavinskaya and Frank⁷⁵, MIT atmospheric pressure soot model¹⁴⁹ and High Temperature Mechanism of the Heavy Hydrocarbons from Ranzi's group⁷⁶. This reaction subset is provided in Table 25. It was not

possible to include reactions for the formation of methylene indene and cyclopentaphenanthrene in the model due to the limited information available in the literature for the formation and consumption of these species.

Table 24. Reactions for the formation of $C_{18}H_{22}$, DIMERS196, anthracene and methyl anthracene

Rxn	Reaction ^a	A	n	Ea
R46 ^{150,b}	$C_9H_{11}+C_9H_{11}=C_{18}H_{22}$	1.58E+12	0.4	0
R-46 ^{150,c}	Reverse	7.94E+14	0	57361
R54 ^{151,d}	$C_9H_{11}+C_9H_{12}=C_{18}H_{22}+H$	1.99E+11	0	3994
R-54 ^{152,e}	Reverse	1.99E+14	0	29400
R60 ^{151,f}	$C_9H_{11}+C_6H_6=DIMERS196+H$	1.99E+11	0	3994
R-60 ¹⁵²	Reverse	1.99E+14	0	29400
R61 ¹³¹	$DIMERS196+C_9H_{11}=RDIMERS196a+C_9H_{12}$	1.60E+11	0	12800
R-61 ¹³¹	Reverse	1.60E+09	0	12800
R62 ¹³¹	$DIMERS196+H=RDIMERS196a+H_2$	4.00E+15	0	8400
R-62 ¹³¹	Reverse	2.80E+11	0	14500
R63 ¹³¹	$DIMERS196+CH_3=RDIMERS196a+CH_4$	1.60E+12	0	8800
R-63 ¹³¹	Reverse	6.60E+11	0	27500
R64 ¹³¹	$RDIMERS196a=PTRIARO192+H$	4.20E+11	0	23500
R-64 ¹³¹	Reverse	5.80E+13	0	29400
R65 ¹³¹	$RDIMERS196a=PTRIARO178+CH_3$	8.40E+11	0	23500
R-65 ¹³¹	Reverse	1.20E+12	0	29400
R66 ¹³¹	$PTRIARO192+H=RPTRIARO192a+H_2$	4.00E+15	0	8400
R-66 ¹³¹	Reverse	2.80E+11	0	14500
R67 ¹³¹	$PTRIARO178+H=RPTRIARO178a+H_2$	4.00E+15	0	8400
R-67 ¹³¹	Reverse	2.80E+11	0	14500
R68 ¹³¹	$PTRIARO192+CH_3=RPTRIARO192a+CH_4$	1.60E+12	0	8800
R-68 ¹³¹	Reverse	6.60E+11	0	27500
R69 ¹³¹	$PTRIARO178+CH_3=RPTRIARO178a+CH_4$	1.60E+12	0	8800
R-69 ¹³¹	Reverse	6.60E+11	0	27500
R70 ¹³¹	$RPTRIARO178a=A3+H$	3.50E+13	0	28400
R-70 ¹³¹	Reverse	4.30E+13	0	4500
R71 ¹³¹	$RPTRIARO192a=A3CH_3+H$	3.50E+13	0	28400
R-71 ¹³¹	Reverse	4.30E+13	0	4500
R72 ^{153,g}	$A3CH_3+H=A3+CH_3$	6.70E+13	0	6468
R-72 ^{131,h}	Reverse	1.20E+12	0	15900

R73 ^{154,g}	<i>DIMERS196</i> +H= <i>DIMERS182</i> +CH ₃	6.70E+13	0	6468
R-73 ¹³¹	Reverse	1.20E+12	0	15900
R74 ^{154,g}	<i>DIMERS196</i> +H= <i>DIMERS182</i> +CH ₃	6.70E+13	0	6468
R75 ¹³¹	Reverse	1.20E+12	0	15900
R76 ^{154,g}	<i>DIMERS182</i> +H=C ₆ H ₅ CH ₂ C ₆ H ₅ +CH ₃	6.70E+13	0	6468
R-76 ¹³¹	Reverse	1.20E+12	0	15900

^aA-factor x 5 of $\phi\text{CH}_2+\phi\text{CH}_2=\text{C}_{14}\text{H}_{14}$, adjusted based on the agreement of the modeling results with the experimental data

^bk same as $\text{C}_{14}\text{H}_{14}=\phi\text{CH}_2+\phi\text{CH}_2$

^cA-factor x (1/2) of $\phi+\text{C}_6\text{H}_6=\text{C}_{12}\text{H}_{10}+\text{H}$

^dA-factor x (1/2) $\text{C}_{12}\text{H}_{10}+\text{H}=\phi+\text{C}_6\text{H}_6$

^eA-factor x (1/2) of $\text{C}_6\text{H}_6+\text{C}_6\text{H}_5=\text{C}_{12}\text{H}_{10}+\text{H}$

^fRate constant same as $\text{C}_9\text{H}_{12}+\text{H}=\text{MXYLENE}+\text{CH}_3$

^gk same as $\phi\text{C}_2\text{H}_5+\text{CH}_3=\text{MCPHC2H5}+\text{H}$

Table 25. Reactions for the decay of anthracene and formation of acenaphthylene, indene and naphthalene

Rxn	Reaction ^a	A	n	Ea
R77 ⁹²	A3+H=A3-+H2	2.50E+14	0	15896
R78 ⁹²	A3+OH=A3-+H2O	1.70E+12	1.42	1496
R79 ⁹²	A3-+H=A3	1.00E+14	0	0
R80 ¹⁵⁵	A2C2H*+C2H2=A3-	4.67E+06	1.787	3262
R81 ⁹²	A2-+C4H2=A3-	3.30E+33	-5.7	25334
R82 ⁹²	A2-+C4H4=A3+H	3.30E+33	-5.7	25334
R83 ¹⁵⁵	INDENYL+C5H5=A3+2H	5.00E+12	0	8000
R84 ⁷⁵	A2-+H=A2	1.00E+14	0	0
R85 ⁹²	A2C2H*+H=A2R5	5.00E+13	0	0
R86 ⁹²	INDENE=INDENYL+H	1.10E+15	0	77096
R87 ⁹²	A3-+O2=>CO+HCO+A2R5	2.00E+11	0	7352
R88 ^{92,b}	INDENYL+H2CCCH=A2R5+H2	9.50E+12	0	0
R89 ⁹²	A2-+C2H2=A2R5+H	1.90E+31	-5.26	20863
R90 ⁹²	A2C2H+H=A2R5+H	4.60E+37	-7.03	22949
R91 ⁹²	A2R5-+H=A2R5	1.00E+14	0	0
R92 ⁹²	A2R5+O=A2R5-+OH	2.00E+13	0	14704
R93 ⁹²	A2R5+O=>A2-+HCCO	2.00E+13	0	14704
R94 ⁹²	A2R5+H=A2R5-+H2	2.50E+14	0	15896
R95 ⁹²	A2R5+OH=A2-+CH2CO	1.00E+13	0	9935
R96 ⁹²	A2+O=>INDENYL+CO+H	3.60E+14	0	43899
R97 ⁹²	A2+O=A2-+OH	2.00E+13	0	14704
R98 ⁹²	A2+H=A2-+H2	2.50E+14	0	15896

R99 ⁹²	A2+OH=A2-+H2O	2.10E+13	0	45701
R100 ⁹²	A2+CH3=A2-+CH4	2.00E+12	0	14962
R101 ⁹²	C6H5+H2CCCH=>INDENE	3.86E+11	0	1361
R102 ⁹²	A2-+O=>INDENYL+CO	1.00E+14	0	0
R103 ⁹²	A2-+HO2=>INDENYL+CO+OH	1.00E+13	0	0
R104 ⁹²	A3+C2H=A3C2H+H	5.00E+13	0	0
R105 ⁹²	A3-+C2H2=A3C2H+H	1.20E+26	-3.44	30004
R106 ^{154,c}	DIMERSI82+H=C6H5CH2C6H5+CH3	6.70E+13	0	6468
R-106 ^{131,d}	Reverse	1.20E+12	0	15900
R107 ⁷⁶	C6H5CH2C6H5=FLUORENE+H2	1.00E+08	0	32000

^ak = ATn exp(-Ea/RT): rate constant (units: mol, s, cm³, cal)

^bA-factor x (1/10)

^cRate constant same as C₉H₁₂+H=MXYLENE+CH₃

^dk same as ϕ C₂H₅+CH₃=MCPHC2H5+H

7.4. Discussion of the Modeling Results

This section discusses the modeling results of the fuel, oxygen and the major intermediates for the experimental datasets at nominal reflected shock pressure of 50 atm and for three different equivalence ratios ($\phi = 0.51, 0.95$ and 1.86). The experimental and modeling profiles for the fuel lean and fuel rich oxidation datasets at a nominal pressure of 20 atm could be found in the appendix. The experimental data is shown by open and closed symbols and the modeling results are shown by straight or dashed or dotted lines.

7.4.1. Interpretation of Modeling of the Fuel Decay and Formation of Methane, Ethane and Major Single Ringed Aromatic Hydrocarbons

The experimental and modeling profiles of the fuel, O₂, CO and CO₂, for three different equivalence ratios ($\phi = 0.51, 0.95$ and 1.86) and for a nominal reflected shock pressure of 50 atm,

are presented in Fig 85 (a –f). The modeling profiles show good agreement with the decay of the fuel. The modeling profiles show increased fuel consumption at lower temperatures when compared to experiments. The experimental and modeling profiles for the decay of the oxygen and the formation of CO and CO₂ are shown in Fig 85 (b, d and f). The modeling predictions show fairly good agreement for the decay of the oxygen and the formation of CO and CO₂ for all the three experimental datasets.

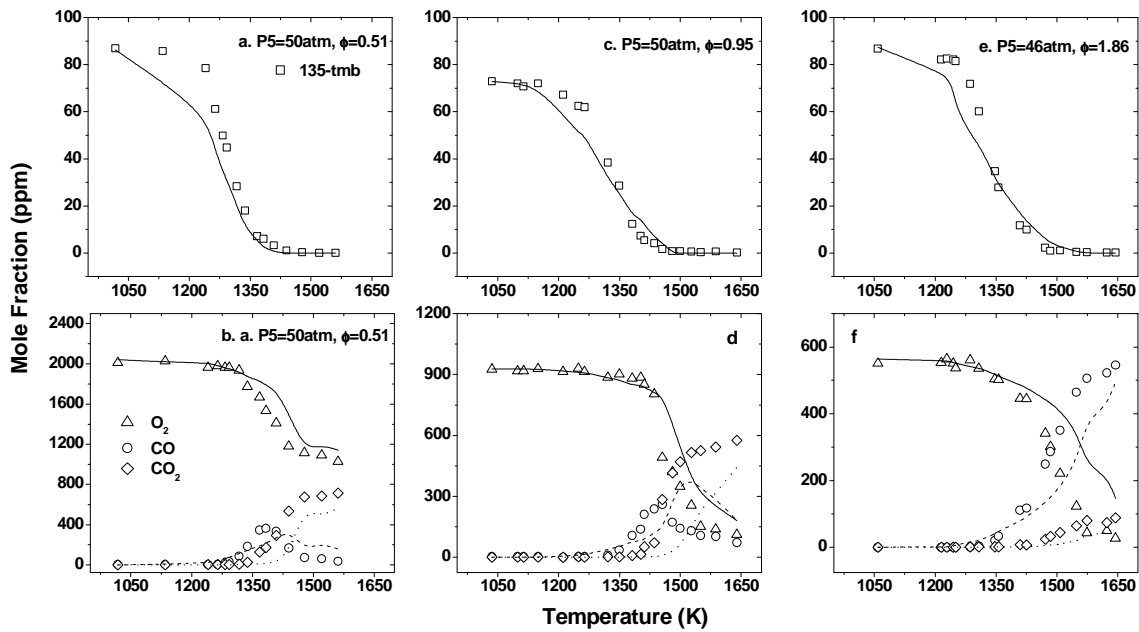


Fig 85. Experimental and modeling profiles for the decay of the fuel and oxidizer, (a-b)-average $P_5 = 49.7$ atm, $\phi = 0.51$, reaction time = 1.26-2.8 ms, (c-d)- average $P_5 = 50.2$ atm, $\phi = 0.95$, reaction time=1.13-1.697 ms, (e-f)-average $P_5 = 45.65$, $\phi=1.86$, reaction time=1.11-2.11 ms, [\square , -]-1,3,5-trimethylbenzene, [Δ , -]-O₂, [\circ , ---]-CO, [\diamond , ...]-CO₂, [Symbols]-Experiments, [Lines]-Modeling Results

The results of the simulation are shown against the experimental data in Fig. 86, Fig. 87 and Fig. 88, for major intermediates such as methane, ethane, benzene, toluene, m-xylene, 1-ethyl-3,5-dimethylbenzene (DIMETB), 1-ethenyl-3,5-dimethyl benzene (DIMSTYR), 3,5-dimethylbenzaldehyde (DIMP HHCO) and $C_{18}H_{22}$ for the datasets at a nominal pressure of 50 atm and for three different equivalence ratios ($\phi \approx 0.5$, 1 and 2). The modeling results show peak concentrations of these intermediates at the correct experimental temperatures which indicate that the hypothesized pathways and the estimated kinetics for the consumption of the fuel and formation of the intermediates are accurate.

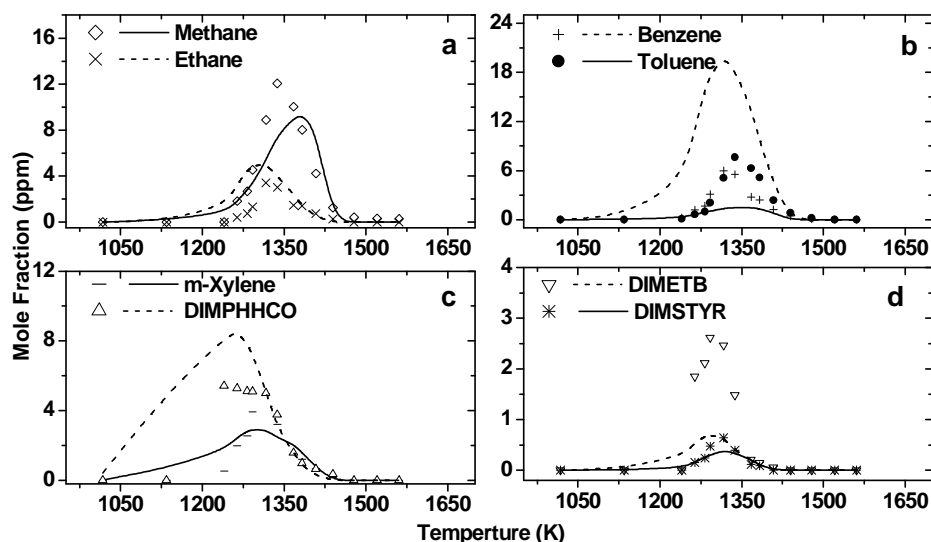


Fig 86. Experimental and modeling profiles of the major intermediates formed in the oxidation of 1,3,5-trimethylbenzene, [Symbols]- average $P_5 = 49.7$ atm, $\phi = 0.51$, reaction time = 1.26-2.8 ms, [Lines]-Modeling profiles

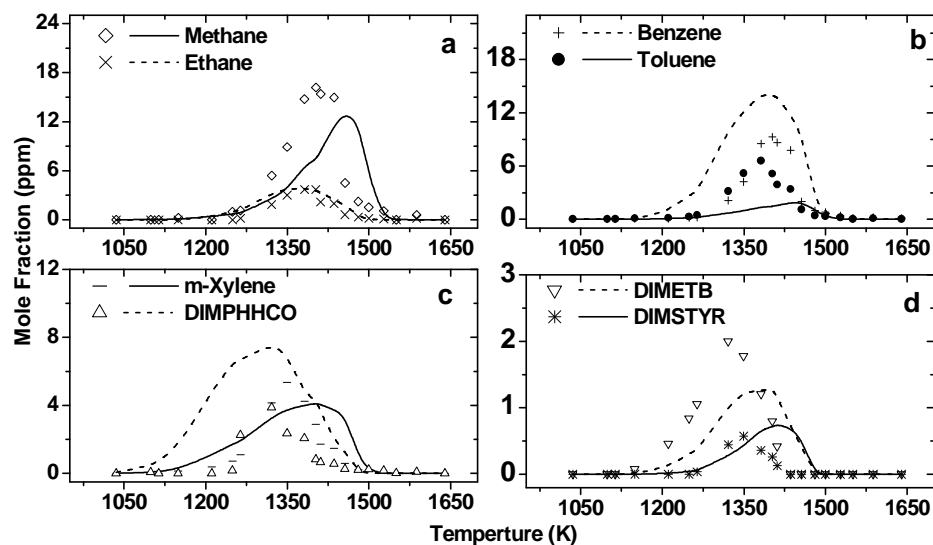


Fig 87. Experimental and modeling profiles of the major intermediates formed in the oxidation of 1,3,5-trimethylbenzene, [Symbols]- average $P_5 = 50.2$ atm, $\phi = 0.95$, reaction time=1.13-1.697 ms, [Lines]-Modeling profiles

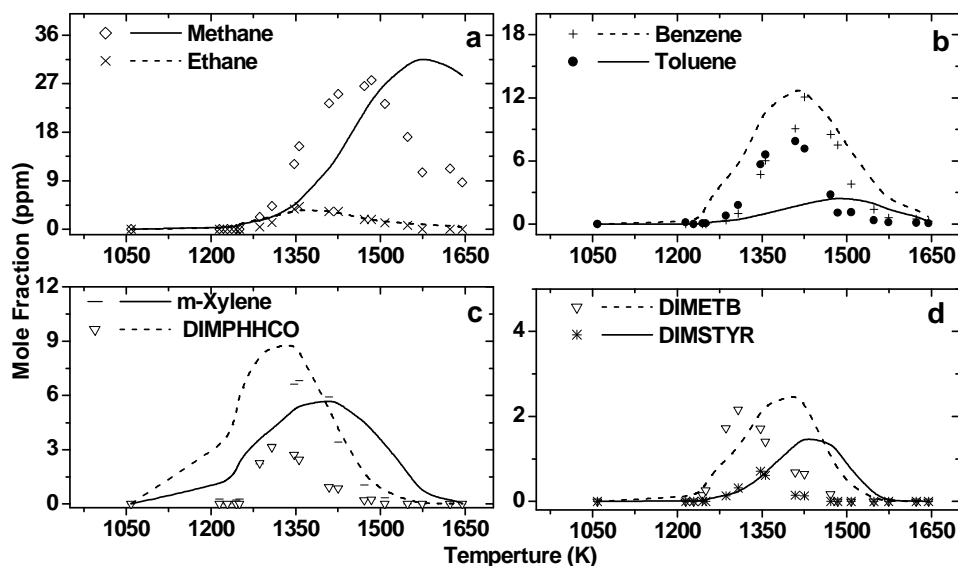


Fig 88. Experimental and modeling profiles of the major intermediates formed in the oxidation of 1,3,5-trimethylbenzene, [Symbols]- average $P_5 = 45.65$, $\phi = 1.86$, reaction time=1.11-2.11 ms, [Lines]-Modeling profiles

Reaction path analysis of the fuel and the major intermediates was performed for a temperature of 1381 K, reaction time of 1.58 ms, and pressure of 46 atm and at fuel lean conditions to validate our hypothesized mechanism and the results are shown in Fig. 89. The direction of the arrow indicates the contribution of that specific pathway to the formation of the species shown below the arrow. For example, the formation of 1-ethyl-3,5-dimethylbenzene is shown by pathway VIII in Fig. 89. It is formed from the recombination reaction of 1,3,5-trimethylbenzyl and methyl radicals. The number 100 % beside VIII indicates that this pathway is the only contributor to the formation of 1-ethyl-3,5-dimethylbenzene. A few interesting aspects could be observed from Fig. 89 and these points (1) and (2) are discussed in greater detail in the following sections.

- (1) Less than 70 % of toluene (V and VIIa), m-xylene (IV and X) and 3,5-dimethylbenzaldehyde (IIIa and IIIb) is formed from the pathways shown in the figure implying that there are other pathways (not shown in Fig. 89) which contribute to the formation of these species.
- (2) Pathway V shows that 0% of benzene is formed from toluene. About 91 % of benzene is produced from dimethylphenoxy radical (VIIb).

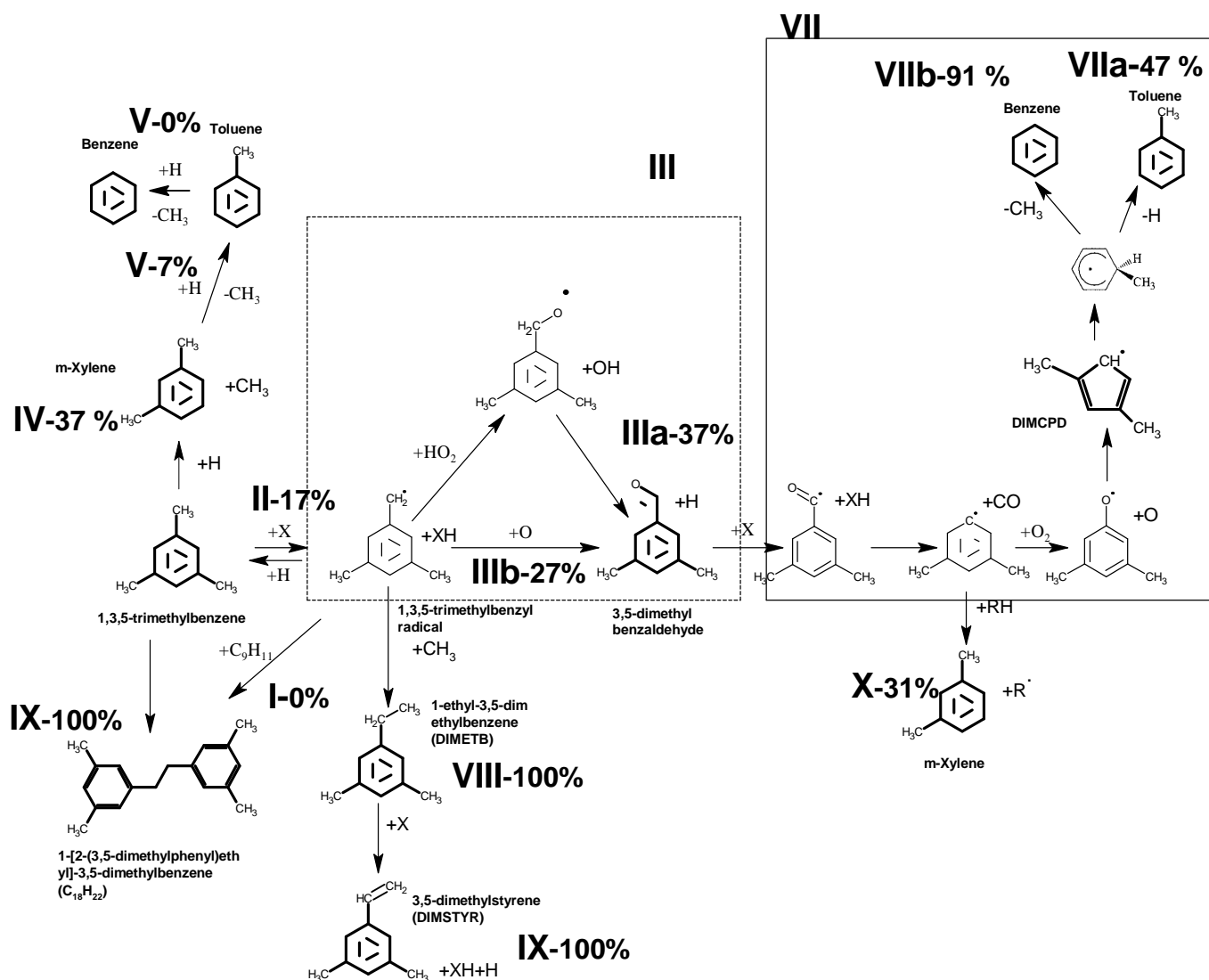


Fig 89. Reaction path analysis of the fuel, $P_5 = 46 \text{ atm}$, $T_5 = 1381 \text{ K}$, reaction time = 1.58 ms, $\phi = 0.51$

7.4.1.1. Importance of $C_9H_{11}+O_2$, $C_9H_{11}+HO_2$ and $C_9H_{11}+O$ Reactions in the Formation of Intermediates

It was previously mentioned in Section 7.3.1, that additional pathways have been included in the model apart from those proposed in Fig. 89, so as to build a comprehensive kinetic model.

These additional pathways included reactions of C_9H_{11} radical with HO_2 , O_2 and O species and reactions for the formation of lower alkylated single-ring aromatic hydrocarbons like m-xylene and toluene from di-alkylated and tri-alkylated single-ring aromatic intermediates (reactions R22-R25 and R48-R56 in Table 22). The species, m-xylene, 3,5-dimethylbenzaldehyde and toluene are partially formed from the reactions shown in Fig. 89 and are partly formed from these additional pathways.

About 36 % of 3,5-dimethylbenzaldehyde is formed from $C_9H_{11}OO$ radical (XI in Fig. 90). The $C_9H_{11}OO$ radical is formed from the reaction of C_9H_{11} and O_2 .

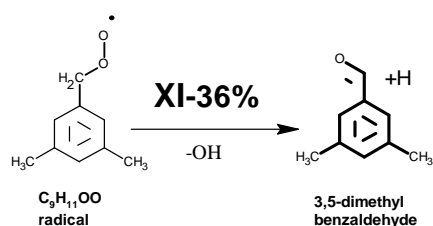


Fig 90. Reaction path analysis of 3,5-dimethylbenzaldehyde, $P_5 = 46$ atm, $T_5 = 1381$ K, reaction time = 1.58 ms

About 20 % of m-xylene is formed from 3,5-dimethylbenzaldehyde by displacement of the formyl side chain by the hydrogen atom (XII in Fig. 91). About 45 % of toluene is formed from 3-methylbenzaldehyde, 3-methylbenzylalcohol radical and 3-methylstyrene by displacement of the non-methyl side chains by a hydrogen atom (see pathways XIII, XIV and XV in Fig. 92).

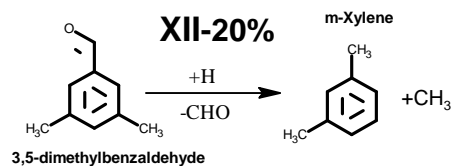


Fig 91. Reaction path analysis of m-xylene, $P_5 = 46 \text{ atm}$, $T_5 = 1381 \text{ K}$, reaction time = 1.58 ms

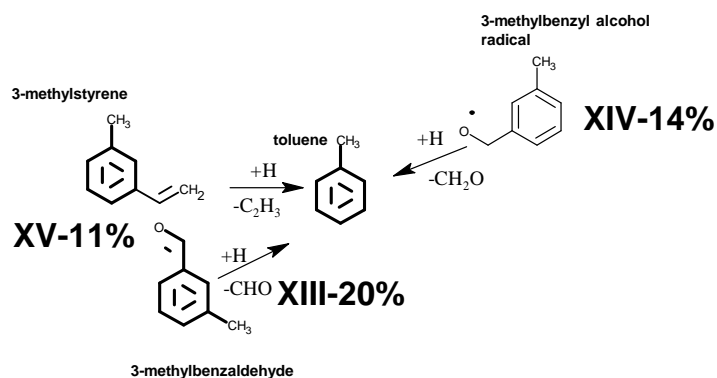


Fig 92. Reaction path analysis of Toluene, $P_5 = 46 \text{ atm}$, $T_5 = 1381 \text{ K}$, reaction time = 1.58 ms

From the pathways shown in figures 90, 91 and 92, we can deduce that the oxidation of C_9H_{11} radical by O_2 , HO_2 and O radicals is important and influences the formation of the stable intermediates such as dimethylbenzaldehyde, and m-xylene. Toluene and m-xylene are formed from dialkylated and trialkylated single -ring aromatics via displacement of the non-methyl side chains by a hydrogen atom.

7.4.1.2. Importance of Dimethylphenoxy Radical Chemistry in the Formation of Benzene

Unlike m-xylene and toluene, benzene is not formed from toluene, styrene, benzaldehyde or benzylalcohol through displacement reactions. About 91 % of benzene is formed from cyclic species, $C_6H_6CH_3$. Hence, this cyclic species is the primary contributor to the formation of benzene.

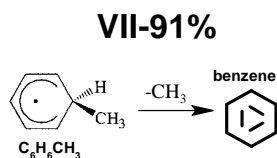


Fig 93. Reaction path analysis of benzene, $P5 = 46 \text{ atm}$, $T5 = 1381 \text{ K}$, reaction time = 1.58 ms

We have previously noticed the importance of the cyclic compound $C_6H_6CH_3$ in the formation of benzene and toluene in our m-xylene oxidation experiments¹³⁴. In m-xylene oxidation, the $C_6H_6CH_3$ radical is produced from dimethylphenoxy radicals and the decay of $C_6H_6CH_3$ species leads to the formation of benzene and toluene (mechanism shown in Fig. 94).

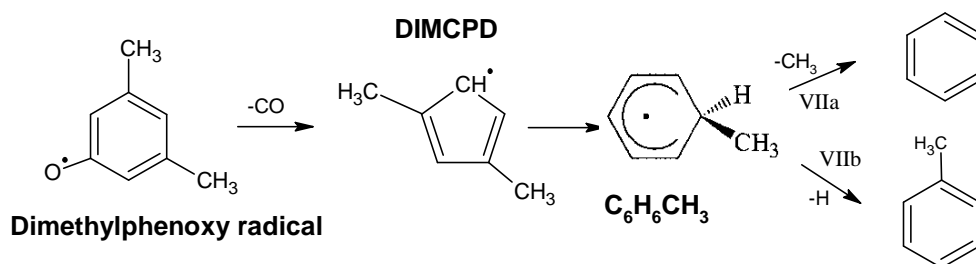


Fig 94. Reaction mechanism of dimethylphenoxy radical

In order to emphasize the importance of this pathway even in the oxidation of 1,3,5-trimethylbenzene, a simple modeling experiment was conducted by removing the reactions for the formation benzene and toluene from $\text{C}_6\text{H}_6\text{CH}_3$ (VIIa and VIIb in Fig. 94). The results of the simulation are shown in Fig. 95 (a-i). The modeling results for the formation of benzene, toluene and oxygen in 1,3,5-trimethylbenzene oxidation experiments by including these reactions are shown by dashed lines and the modeling results after removal of these reactions are shown by straight lines. From Fig. 95, we can observe that removal of these reactions significantly under predicts the consumption of oxygen for the fuel lean and stoichiometric experimental datasets (see Fig. 95 (a, d)) and the formation of benzene for all the experimental datasets (see Fig. 95 (b, e, h)). We can see significantly lower concentrations of benzene being formed, when these reactions are not included. Similarly, the concentrations of toluene are also under predicted when these pathways are not included (see Fig. 95 (c, f, i)). Hence, this modeling experiment reveals the importance of including the dimethylphenoxy radical chemistry in the modeling of not only m-xylene oxidation but also in the oxidation of 1,3,5-trimethylbenzene. In the case of 1,3,5-trimethylbenzene the dimethylphenoxy radicals are formed from the oxidation of dimethylphenyl radical (XVI and XVII in Fig. 96).

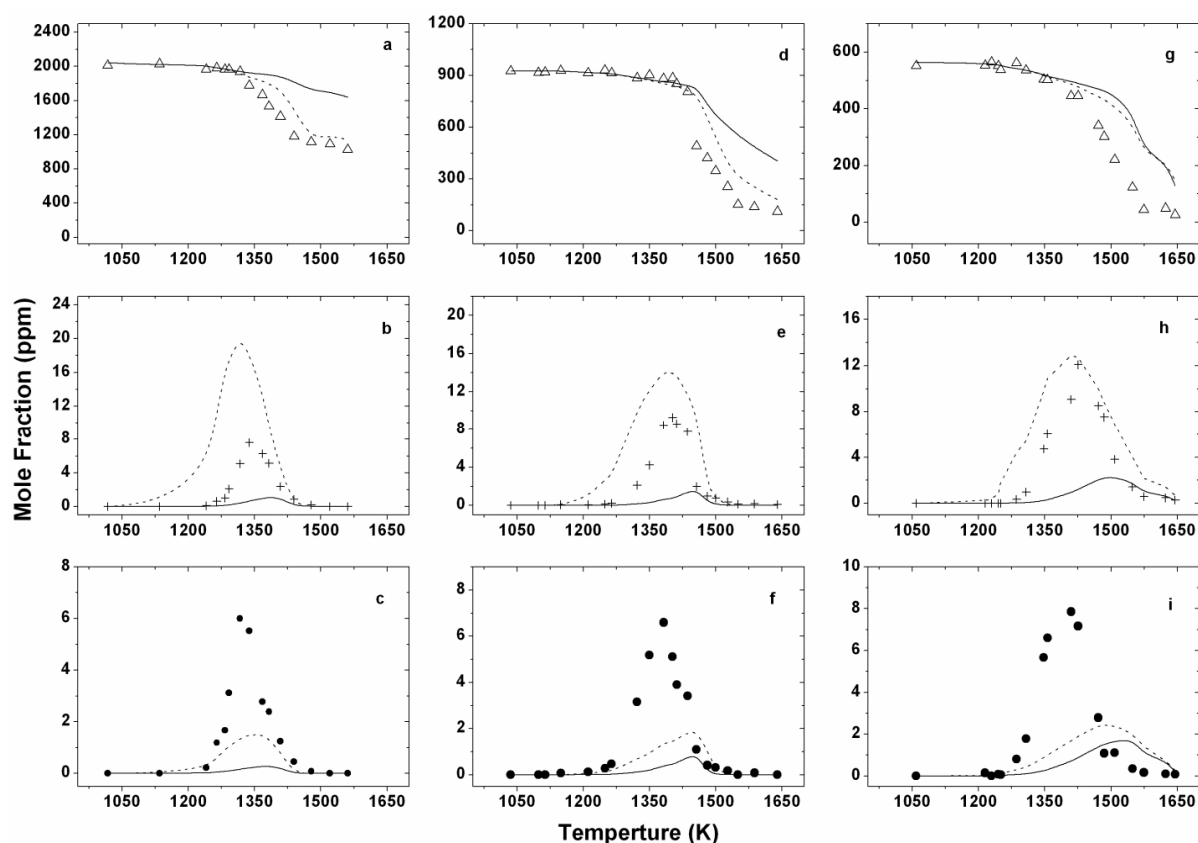


Fig 95. Experimental and modeling profiles of $[\Delta]\text{-O}_2$, $[\oplus]\text{-C}_6\text{H}_6$, $[\square]\text{-C}_6\text{H}_5\text{CH}_3$, in 1,3,5-trimethylbenzene oxidation experiments, (a-c)-average $P_5 = 49.7$ atm, $\phi = 0.51$, reaction time = 1.26-2.8 ms, (d-f)- average $P_5 = 50.2$ atm, $\phi = 0.95$, reaction time=1.13-1.697 ms, (g-i)-average $P_5 = 45.65$, $\phi=1.86$, reaction time=1.11-2.11 ms, [Symbols]-Experiments, [---]-Modeling Results including the chemistry of cyclic C6 species, [-]-Modeling results without including the chemistry of cyclic C6 species

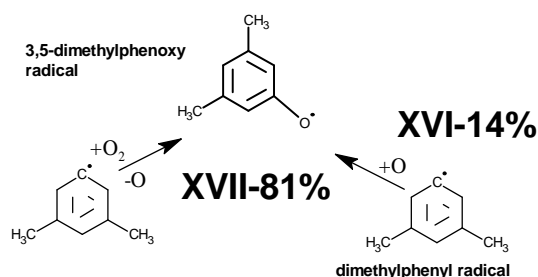


Fig 96. Formation of dimethylphenoxy radical in 1,3,5-trimethylbenzene oxidation, Reaction path analysis at $P_5 = 46$ atm, $T_5 = 1381$ K, reaction time = 1.58 ms

The model shows very low concentrations of toluene being formed, in spite of having reactions for displacement of the non-alkyl side chain by a hydrogen atom, from di-alkylated aromatics like m-xylene, 1-ethyl-3-methylbenzene and 3-methylbenzaldehyde. This implies that an alternative pathway exists for the formation of toluene from 1,3,5-trimethylbenzene.

If we compare the modeling profiles for the formation of toluene and benzene (shown by straight lines), in Fig. 95 (b) and (c), (e) and (f) and in (h) and (i), we can observe the similarity in the peak shapes of these two intermediates, in the absence of the chemistry of the cyclic $C_6H_6CH_3$ species. This observation confirms our hypothesis that an alternative pathway exists for the formation of toluene, which has not been included in the model

Several publications on atmospheric kinetics have observed the formation of alkylated phenols in the oxidation of aromatics¹⁵⁶, such as toluene^{157,158} and trimethylbenzene^{159–161}. Since our experiments are conducted at much higher pressures the mechanism of decay of the trimethylphenol is probably not similar to what is postulated in these publications. However, similar to the decay of dimethylphenoxy radical which results in the formation of benzene and toluene, the trimethylphenoxy radical could result in the formation of minor amounts of m-xylene and major amounts of toluene. The trimethylphenoxy radical could be formed from the oxidation of trimethylphenyl radical. The pathways and kinetics for the formation of m-xylene and toluene from trimethylphenoxy radical is at present not clear to us. Hence, these pathways have not been included into the model. We hypothesize that inclusion of this pathway will result in increased amounts of toluene being formed in the modeling concentrations.

The reaction path analysis of the major intermediates validates our hypothesized mechanism for the oxidation of 1,3,5-trimethylbenzene. Hence, the oxidation of 1,3,5-trimethylbenzene indeed takes place by sequential oxidation and removal of methyl side chains. However, the decreased concentrations of toluene observed in the modeling results, indicate the possibility of having

alternative pathways for the formation of this species which do not fit into our generic description of ‘oxidation of 1,3,5-trimethylbenzene by sequential oxidation and removal of the methyl side chains’.

7.4.2. Interpretation of the Formation of Two Ringed and Three Ringed Aromatic Hydrocarbons

The experimental and modeling profiles of indene, naphthalene, anthracene, 1-(phenylmethyl)-3,5-dimethylbenzene (DIMERS196), 1-[2-(3,5-dimethylphenyl)ethyl]-3,5-dimethylbenzene ($C_{18}H_{22}$) and methyl anthracene are shown in Fig. 97, for three different equivalence ratios ($\phi = 0.51, 0.95$ and 1.86). The model showed the formation of DIMERS196 and $C_{18}H_{22}$ at the right experimental temperatures. The model shows good predictions for the formation of DIMERS196, for all the experimental datasets (see Fig. 97 (a, d, g)). For $C_{18}H_{22}$, the modeling concentrations are slightly under predicted for almost all the experimental datasets but the degree of disagreement decreases as the equivalence ratio is increased, from about 50 % at fuel lean conditions to about 30 % at fuel rich conditions (Fig. 97 (a, g)).

Displaced profiles for the formation of indene and naphthalene could be observed in the fuel lean dataset (see Fig. 97 (b)). However, for the stoichiometric and fuel rich dataset significantly low concentrations of indene and naphthalene could be observed (see Fig. 97 (e, h)). The model was successful in capturing the formation of anthracene and methyl anthracene at lower temperatures and increased amounts of anthracene and methylantracene are observed at higher temperatures for all the experimental datasets. The modeling results showed negligible concentrations of fluorene and ethenylantracene being formed for the fuel rich dataset (the profiles are not shown).

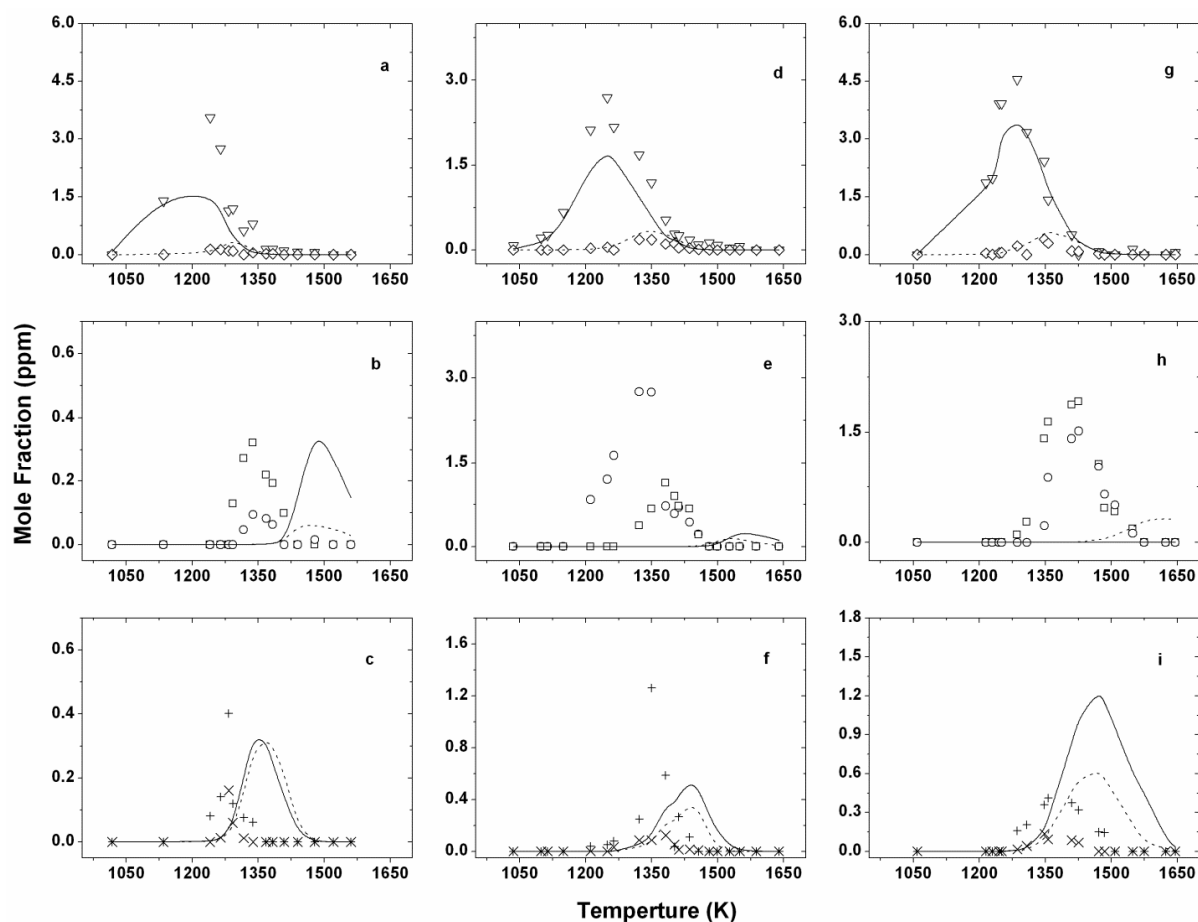


Fig 97. Experimental and modeling profiles of [\square , -]- $C_{18}H_{22}$, [\diamond ,--]-DIMERS196, [\square ,-]-Indene, [\circ ,--]- Naphthalene, [$+$,-]-Anthracene, [x ,--]-Methylantracene, (a-c)-average $P_5 = 49.7$ atm, $\phi = 0.51$, reaction time = 1.26-2.8 ms, (d-f)- average $P_5 = 50.2$ atm, $\phi = 0.95$, reaction time=1.13-1.697 ms, (g-i)-average $P_5 = 45.65$, $\phi=1.86$, reaction time=1.11-2.11 ms, [Symbols]-Experiments, [Lines]-Modeling Results

Reaction path analysis of $C_{18}H_{22}$ revealed that this species is formed from the recombination of 1,3,5-trimethylbenzene and 1,3,5-trimethylbenzyl radical followed by removal of a hydrogen atom (see pathway X in Fig. 89). The species, DIMERS196 (100 %) is formed from recombination of 1,3,5-trimethylbenzyl radical with benzene followed by removal of hydrogen atom (shown in Fig. 98).

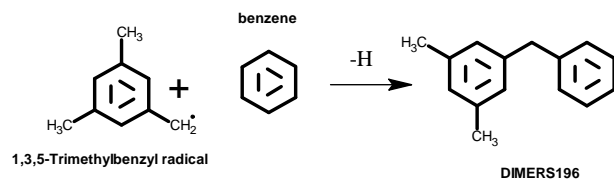


Fig 98. Reaction path analysis of DIMER196 $P5 = 46 \text{ atm}$, $T5 = 1381 \text{ K}$, reaction time = 1.58 ms

Anthracene and methylantracene are confirmed to be formed from DIMERS196 through the sequence of steps shown in Fig. 99, which are similar to the mechanism proposed by Fusetti et al.¹⁶² The authors studied the thermal cracking of methylated monoaromatics which included 1,2,4-trimethylbenzene and proposed a generic pathway for the formation of methylantracene from trimethylbenzenes. This generic pathway has been modified by including the isomerization step so that methylantracene could be formed from DIMERS196 (reaction path analysis was not performed for the formation of anthracene and methylantracene, since only this reaction sequence is present in the model for the formation of these species). Displacement of the methyl side chain from anthracene by hydrogen atom produces anthracene.

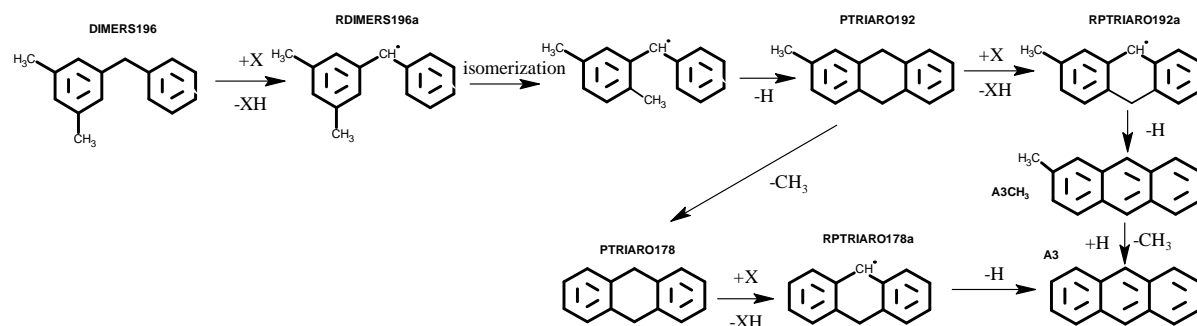


Fig 99. Mechanism for the formation of anthracene and methylantracene from DIMERS196, which is similar to the mechanism proposed by Fusetti et al.¹⁶²

Reaction path analysis was not performed for indene and naphthalene because of the very low modeling concentrations and displaced profiles for the formation of these intermediates, as of result of which the analysis might not give accurate information for the formation of these species. But the absence of formation of indene and naphthalene in the modeling profiles could be due to the lower concentration of toluene being formed in the simulation results. The importance of the presence of intermediates of toluene oxidation, such as benzyl radical, cyclopentadienyl radical and fulvenallene in the formation of indene and naphthalene has been mentioned previously in many publications.^{77,79,81,82,163–165} Improved predictions for the formation of toluene can also result in improved modeling profiles for indene and naphthalene.

7.5. Concluding Remarks

The oxidation of 1,3,5-trimethylbenzene has been studied at nominal reflected shock pressures of 25 and 50 atm, for a temperature range of 1018-1640 K at fuel lean, stoichiometric and fuel rich conditions. Species profiles of small hydrocarbons, mono-aromatic and multi-ringed

aromatic species were obtained as a function of temperature. The 1,3,5-trimethylbenzene oxidation model was developed to predict the decay of the fuel and the formation of aliphatic and single ringed aromatic hydrocarbons, as measured from our experiments. The model shows satisfactory predictions for the formation of most of the major intermediates. Through reaction path analysis it was identified that the pathways involving oxidation of the 1,3,5-trimethylbenzyl and dimethylphenyl radical play an important role in the formation of the major intermediates such as 3,5-dimethylbenzaldehyde, benzene and toluene. Polycyclic aromatic hydrocarbon species such as anthracene and methylantracene were formed through a sequence of steps, following the reaction of 1,3,5-trimethylbenzyl radical with benzene. The mechanism for the oxidation of 1,3,5-trimethylbenzene does not fit into our simple hypothesis of oxidation by simultaneous oxidation and abstraction of the methyl side chains and additional pathway have to be included so that the predictions of the modeling results could be improved.

8. MODELING OF 1,3,5-TRIMETHYLBENZENE AND M-XYLENE PYROLYSIS EXPERIMENTS AND THE FORMATION OF POLYCYCLIC AROMATIC SPECIES IN M-XYLENE OXIDATION EXPERIMENTS

The 1,3,5-trimethylbenzene oxidation model was developed in stages. In the first stage, the m-xylene oxidation model was developed because m-xylene was one of the major intermediates of 1,3,5-trimethylbenzene oxidation and the models available in literature did not succeed in simulating our high pressure m-xylene oxidation experimental data (see Chapter 6, section 6.3). The m-xylene oxidation model was developed and validated against the stable species profiles obtained from our experiments, up to single ringed aromatic hydrocarbons. Since m-xylene is not one of the proposed surrogate fuel components and only aided in the building the 1,3,5-trimethylbenzene oxidation model, the kinetics for the formation of polycyclic aromatic hydrocarbons, which were observed in m-xylene oxidation experiments were not included in the m-xylene oxidation model, at this stage.

In the second stage, the 1,3,5-trimethylbenzene oxidation model was developed using the m-xylene oxidation model as the base mechanism. The 1,3,5-trimethylbenzene oxidation model was validated against our high pressure 1,3,5-trimethylbenzene oxidation experimental data and it showed satisfactory predictions for the formation of intermediates ranging from CO and CO₂, methane up to the three ringed compounds (more details are present in Section 7.3 and 7.4 of Chapter 7).

In the third stage the 1,3,5-trimethylbenzene oxidation model was used to simulate the 1,3,5-trimethylbenzene pyrolysis experiments, m-xylene pyrolysis experiments and the polycyclic aromatic species observed in the m-xylene oxidation experiments. Since the 1,3,5-trimethylbenzene oxidation model also consists of 1,3,5-trimethylbenzene and m-xylene pyrolysis kinetics, it can be used to simulate all the sets of experimental datasets mentioned in the previous two sentences. The

experimental conditions of the 1,3,5-trimethylbenzene and m-xylene pyrolysis experiments are shown in Table 26 and the experimental conditions of the m-xylene oxidation experiments were shown in Table 12.

Table 26. 1,3,5-Trimethylbenzene and m-xylene pyrolysis experimental conditions

Fuel	Average Shock Pressure /atm	Concentration /ppm	Temperature Range /K	Φ	Reaction Time /ms
1,3,5-Trimethylbenzene	47.96	51.39	1085-1663	∞	1.19 - 2.40
m-Xylene	54.47	54.43	1061-1579	∞	1.28 – 1.91

The experimental and modeling profiles for the decay of 1,3,5-trimethylbenzene and m-xylene in 1,3,5-trimethylbenzene and m-xylene pyrolysis experiments are shown in Fig 100 (a-b). The model shows good predictions for the decay of 1,3,5-trimethylbenzene (Fig 100 (a)) and m-xylene (Fig 100 (b)).

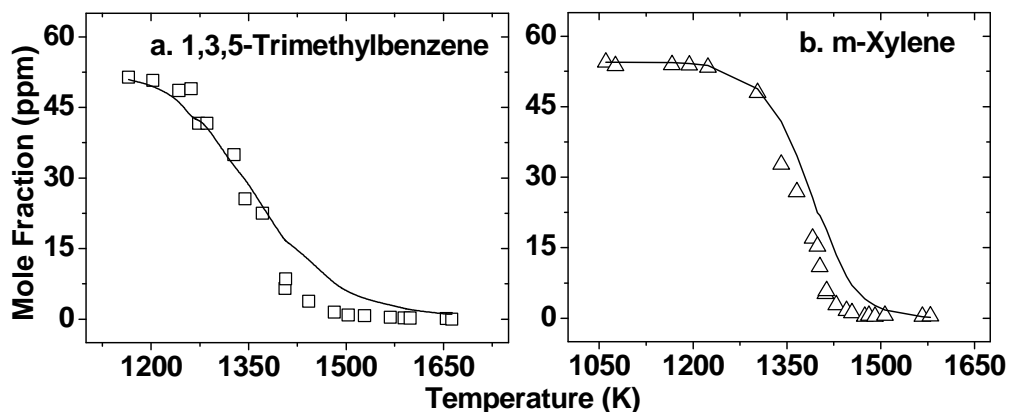


Fig 100. Experimental and modeling profiles of 1,3,5-trimethylbenzene (a) and m-xylene decay (b) in the pyrolysis experiments, (a) [\square]-P5avg = 48 atm, reaction time = 1.19-2.40 ms, (b) [\triangle]-P5avg = 54 atm, reaction time = 1.28-1.91 ms, [Symbol]-Experimental results, [Lines]- Modeling results

In the case of 1,3,5-trimethylbenzene pyrolysis experiments, the agreement of the modeling profiles and experimental profiles for the formation of few of the major intermediates such as m-xylene and $C_{18}H_{22}$ could be considered to be satisfactory (see Fig 101 (a)). The model shows the formation of m-xylene at the correct experimental temperatures and the deviation in the peak concentration in the modeling results when compared to the experiments is about 25 %. The modeling results show a slightly displaced profile for the formation of $C_{18}H_{22}$ and the deviation in the peak concentration of the modeling results when compared to the experiments is about 36 %. For m-xylene pyrolysis experiments, the modeling profiles and the experimental profiles for toluene match well (see Fig 101 (b)). The modeling results show a slightly displaced profile for the formation of toluene and the deviation in the peak concentration of the modeling results when compared to the experiments is about 21 %.

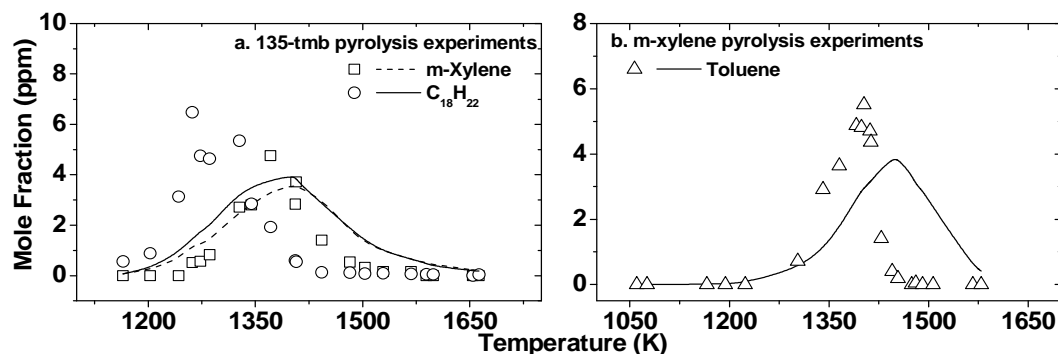


Fig 101. Experimental and modeling profiles of (a) m-xylene[□,---] and $C_{18}H_{22}$ [○, -] formed in 1,3,5-trimethylbenzene pyrolysis experiments, $P_{5avg} = 48$ atm, reaction time = 1.19-2.40 ms (b) toluene[△, -] formed in m-xylene pyrolysis experiments, $P_{5avg} = 54$ atm, reaction time = 1.28-1.91 ms, [Symbol]-Experimental results, [Lines]- Modeling results

The 1,3,5-trimethylbenzene oxidation model also shows under predicted or displaced profiles for the formation of most of the other intermediates observed in 1,3,5-trimethylbenzene and m-xylene pyrolysis experiments such as benzene, toluene, 1-ethyl-3,5-dimethylbenzene, methane and $C_{16}H_{18}$ and the experimental and modeling profiles of these intermediates are shown in Fig 102 (a-e). For example, the model shows almost no benzene and toluene being formed in 1,3,5-trimethylbenzene pyrolysis experiments. Modeling profile of benzene (in Fig 102 (a)) shows a maximum concentration of about 0.018 ppm of benzene being formed at a temperature of 1503 K, whereas the experiments show maximum peak concentration of 8 ppm at 1503 K. The modeling profile of toluene (in Fig 102 (b)) shows a maximum concentration of 0.185 ppm of toluene being formed at 1407 K, whereas the experiments show the maximum peak concentration of 4.86 ppm at 1407 K. The modeling profile of 1-ethyl-3,5-dimethylbenzene shows maximum peak concentration of 4.07 ppm at 1482 K, whereas the experiments show a maximum peak concentration of 0.93 ppm at 1327 K (shown in Fig 102 (c)).

Similarly the modeling profile of one of the major intermediates of m-xylene pyrolysis, $C_{16}H_{18}$ (shown in Fig 102 (f)) shows a maximum concentration of 0.0165 ppm of $C_{16}H_{18}$ being formed at 1340 K whereas the experiments show a maximum concentration of 2 ppm being formed at 1302 K. The modeling profiles of benzene and methane, formed in the m-xylene pyrolysis experiments are shown in Fig 102 (b) and (c). The modeling profiles show steady formation of benzene (3.07 ppm at 1579 K) and methane (31.11 ppm at 1566 K), whereas the experiments show that at these temperatures of 1579 K and 1566 K, all the benzene and methane has reacted and only about 0.18 ppm of benzene and 2.79 ppm of methane is still remaining.

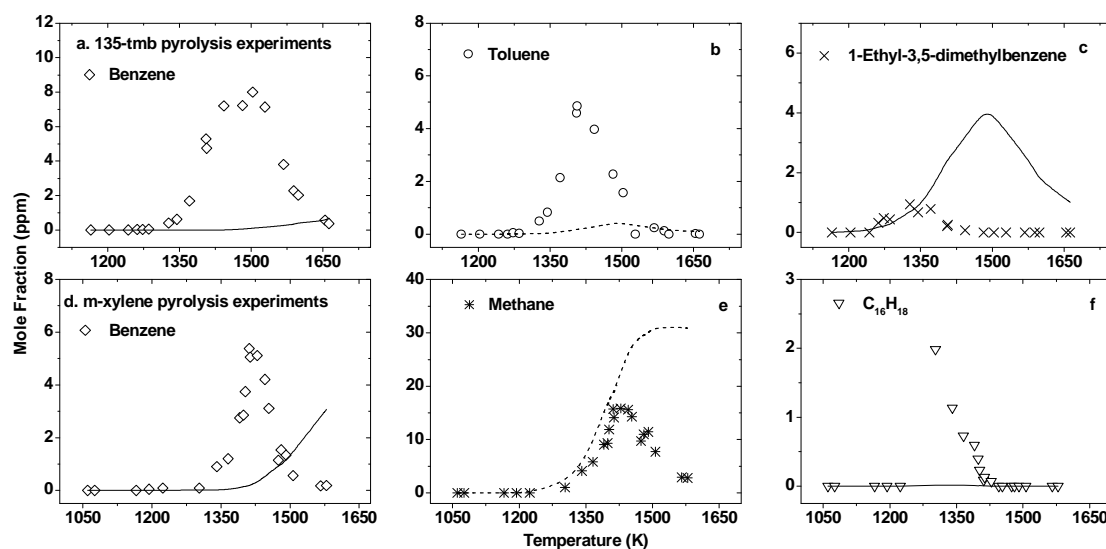


Fig 102. Experimental and modeling profiles of (a) [\diamond ,---]-benzene, (b) [\circ ,---]-toluene, (c) [\times ,]-1-Ethyl-3,5-dimethylbenzene formed in 1,3,5-trimethylbenzene pyrolysis experiments, $P_{5avg} = 48$ atm, reaction time = 1.19-2.40 ms (d) [\diamond ,---]-benzene, (e) [\circ ,---]-methane, (f) [\square ,]-benzene-1,1'-(1,2-ethanediyl)bis[4-meth ($C_{16}H_{18}$), formed in m-xylene pyrolysis experiments, $P_{5avg} = 54$ atm, reaction time = 1.28-1.91 ms, [Symbol]-Experimental results, [Lines]- Modeling results

The experimental and modeling profiles for the formation of acetylene, diacetylene and triacetylene in 1,3,5-trimethylbenzene and m-xylene pyrolysis experiments are shown in Fig. 103 (a) and (b). The model under predicts the formation of acetylenic types of species in both 1,3,5-trimethylbenzene and m-xylene pyrolysis experiments. From Fig. 103 (a) it can be observed that the 1,3,5-trimethylbenzene pyrolysis model shows about 22 ppm of acetylene being formed at the highest temperature of 1662 K, whereas the experiments show 157 ppm of acetylene being formed at 1662 K. The experimental vs. modeling concentrations of diacetylene and triacetylene in 1,3,5-trimethylbenzene pyrolysis experiments are 32 ppm vs. 1.02 ppm and 11 ppm vs. 0.0047 ppm respectively. Similarly the model also under predicts the formation of acetylene, diacetylene and triacetylene in m-xylene pyrolysis experiments and the profiles are shown in Fig. 103 (b).

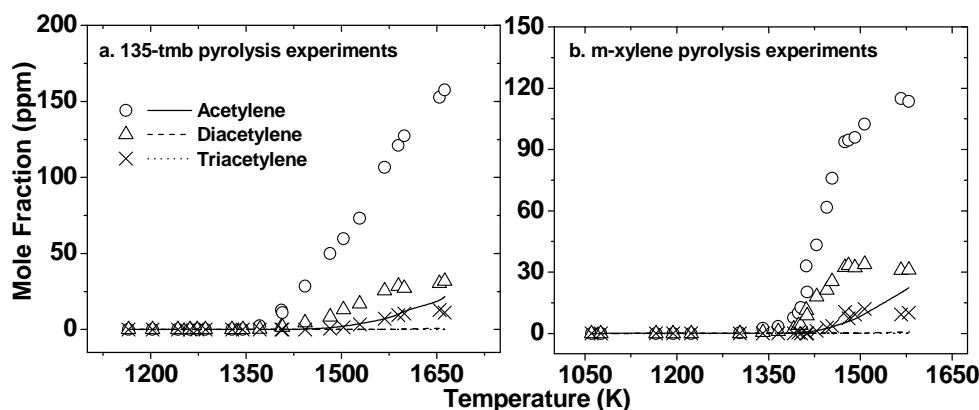


Fig 103. Modeling profiles of (a) [o,-]-acetylene, [Δ ,---]-diacetylene, [\times ,...]-triacetylenec, (a)-1,3,5-Trimethylbenzene pyrolysis experiments, $P_{5avg} = 48$ atm, reaction time = 1.19-2.40 ms, (b)- m-Xylene pyrolysis experiments, $P_{5avg} = 54$ atm, reaction time = 1.28-1.91 ms

In addition to this, the 1,3,5-trimethylbenzene oxidation model has been used to predict the formation of major polycyclic aromatic hydrocarbon intermediates formed during the oxidation of m-xylene. The modeling profiles show negligible amounts of major polycyclic aromatic hydrocarbon intermediates such as indene, naphthalene, anthracene and methylantracene being formed when compared to the experimental results (figures are not shown).

The disagreement between the modeling results and the experimental results merits some comments. It is known from the discussion in the previous paragraphs that the model shows good agreement in predicting the decay of 1,3,5-trimethylbenzene and m-xylene in the pyrolysis experiments (shown in Fig 100 (a) and (b)); however, the model fails to capture the formation of the major intermediates in the 1,3,5-trimethylbenzene and m-xylene pyrolysis experiments, such as benzene, toluene, 1-ethyl-3,5-dimethylbenzene, methane, acetylene, diacetylene, triacetylene and $C_{16}H_{18}$. The experimental and modeling profiles of these intermediates are shown in Fig 102 (a-f) and Fig. 103 (a) and (b). Since the decay of the fuel is captured but not the formation of the intermediates which were mentioned in the previous sentence, there are two possibilities that could describe these modeling results

- (1) The intermediates formed from the fuel decay in the modeling results, which are also referred to as the modeling intermediates, are not necessarily the ones that are observed from our experiments.
- (2) The model does not include steps for the decay of the modeling intermediates that lead to the formation of the intermediates observed in our experiments.

These points are described in greater detail in Sections 8.1 and 8.2.

8.1. Comparison of Major Intermediates Observed in 1,3,5-Trimethylbenzene and m-Xylene Experiments and Modeling results

8.1.1. 1,3,5-Trimethylbenzene Pyrolysis

In order to test the case 1, all the species (both stable and radical species) in the 1,3,5-trimethylbenzene pyrolysis modeling results, which showed concentrations greater than 1 ppm have been identified. As per our proposed hypothesis, a few of these species were indeed different from the intermediates that were observed from our experiments.

The major intermediates formed in the 1,3,5-trimethylbenzene pyrolysis experiments were methane, acetylene, diacetylene, triacetylene, benzene, toluene, m-xylene and $C_{18}H_{22}$. The modeling results of 1,3,5-trimethylmethylbenzene pyrolysis showed m-xylene, 1-ethyl-3,5-dimethylbenzene, methane, acetylene, benzene, toluene and $C_{18}H_{22}$ being formed and these species were also observed in the 1,3,5-trimethylbenzene pyrolysis experiments. Other than these species, the modeling results also predicted the formation of 1,3,5-trimethylbenzyl radical (C_9H_{11}), fulvenallene (C_7H_6) and p-xylylene (CH_2PCH_2), and their profiles are shown in Fig 104 (a - e). Fulvenallene and p-xylylene were not detected in our experiments but the modeling results show that 5.18 ppm of p-xylylene and 2.81 ppm of fulvenallene persist in the modeling results at the highest temperature of 1662 K. From the modeling results of C_9H_{11} , shown in Fig 103 (a), we can observe that about 20 ppm of C_9H_{11} radical remains unreacted at the highest temperature of 1663 K. Even though the C_9H_{11} radical cannot be quantified in our experiments, we can infer from the modeling results that substantial concentrations of C_9H_{11} radical are present at the highest temperature of 1663 K.

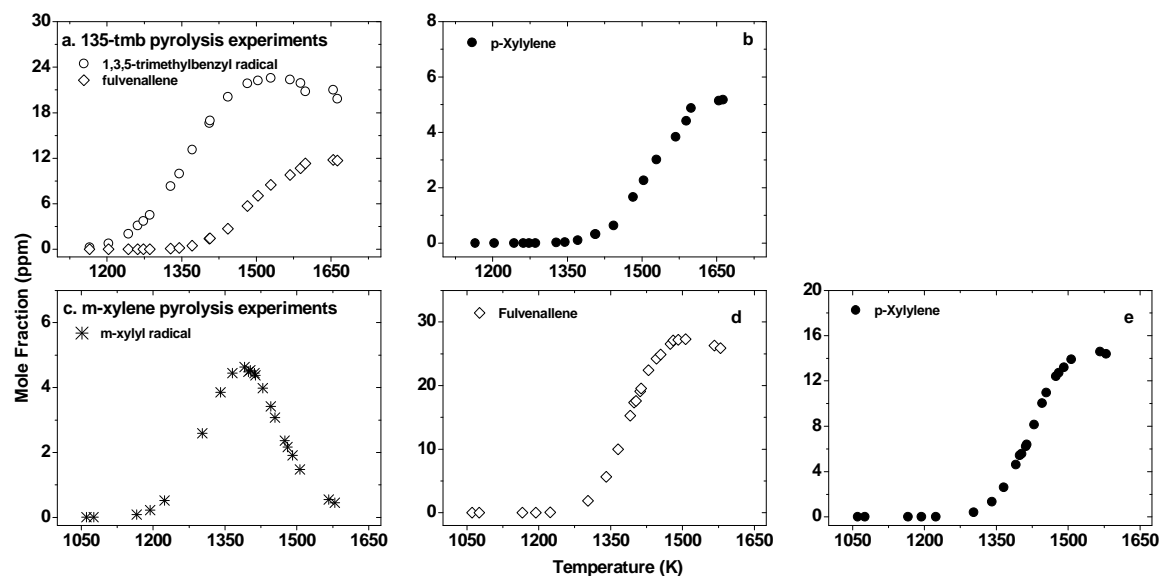


Fig 104. Modeling profiles of (a) [o]-1,3,5-trimethylbenzyl radical, [◇]-fulvenallene, [●]-p-xylylene, [□]-m-xylyl radical, formed in 1,3,5-trimethylbenzene and m-xylene pyrolysis modeling results, [Symbol]- Modeling results, (a – b)-Modeling results for 1,3,5-trimethylbenzene pyrolysis experiments, $P_{5avg} = 48$ atm, reaction time = 1.19-2.40 ms, (d-e)-Modeling results for m-xylene pyrolysis experiments, $P_{5avg} = 54$ atm, reaction time = 1.28-1.91 ms

8.1.2. m-Xylene Pyrolysis

The major intermediates formed in the m-xylene pyrolysis experiments were methane, acetylene, diacetylene, benzene, toluene, styrene and $C_{18}H_{22}$. The modeling results showed toluene, ethane, benzene and $C_{16}H_{18}$ being formed, and these species were also observed in the experiments. Other stable intermediates which were observed in the modeling results but not in the experiments are p-xylylene and fulvenallene. The modeling profiles of these intermediates are shown in Fig 103 (d) and (e) and these profiles show 14 ppm of p-xylylene and 26 ppm of fulvenallene at the highest temperature of 1579 K. The modeling results also showed maximum concentrations of 4 ppm of m-xylyl radical being formed at a temperature of 1391 K (Fig. 103 (c)). Since m-xylyl decays to p-

xylylene and fulvenallene, we can observe only 0.45 ppm of m-xylene remaining in the modeling profiles at the highest temperature of 1579 K.

The modeling results of 1,3,5-trimethylbenzene and m-xylene show a few different stable intermediates (fulvenallene and p-xylylene) being formed when compared to the experiments. The modeling results of 1,3,5-trimethylbenzene pyrolysis experiments also show substantial concentrations of C_9H_{11} radical being formed.

8.2. The Decay Pathways of C_9H_{11} Radical, Fulvenallene and p-Xylylene

Since at present the pyrolysis steps for consumption of C_9H_{11} radical are not known, these steps were not included in the kinetic model and this leads to the build-up of C_9H_{11} radical in the modeling results. The m-xylyl radical consumption routes are included in the model. The m-xylyl radical decays to fulvenallene and p-xylylene. Hence, we observe the presence of small amount of m-xylyl radical (0.4 ppm) and considerable amounts of fulvenallene (25 ppm) and p-xylylene (14 ppm), at the highest temperature of 1579 K in the m-xylene pyrolysis modeling results. In spite of including the steps for the decay of fulvenallene to cyclopentadienyl radical, acetylene and ethynylcyclopentadiene, we can still observe the presence of fulvenallene in the modeling results at the highest temperature of 1579 K. This observation suggests that there could other intermediates being formed in the decomposition of fulvenallene. The model includes the steps which are important for the decay of fulvenallene¹¹⁷ Since the kinetics of this intermediate are still under investigation by other researchers^{116,163,166–169}, additional steps have yet to be included in the model, for the consumption of fulvenallene. The steps for pyrolysis of p-xylylene remain to be included in the model based on recent theoretical and experimental studies conducted on p-xylylene¹⁷⁰ and xylene isomers¹⁷¹.

Based on the discussions presented in Sections 8.1 and 8.2, it can be concluded that including additional, but currently still under investigation, steps for decay of the fulvenallene, p-xylylene, m-xylyl and C_9H_{11} radical will result in improved predictions for the formation and consumption of the major intermediates formed in 1,3,5-trimethylbenzene pyrolysis experiments and m-xylene oxidation and pyrolysis experiments.

9. CONCLUSIONS

In the present work an experimental (A), thermochemical and kinetic database (B) have been developed for the combustion of aromatic surrogate fuel components of jet fuels, n-propylbenzene and 1,3,5-trimethylbenzene. Experiments were also conducted on m-xylene and kinetic model was developed for m-xylene oxidation so that it could help in the development of 1,3,5-trimethylbenzene oxidation model.

(A) The experiments on n-propylbenzene, 1,3,5-trimethylbenzene and m-xylene were conducted in the High Pressure Single Pulse Shock Tube at University of Illinois at Chicago. The experiments were performed for two different nominal reflected shock pressures of 25 and 50 atm and for fuel lean ($\phi = 0.5$), stoichiometric ($\phi = 1$) and fuel rich conditions ($\phi = 2$). The stable intermediates species measured from the combustion of n-propylbenzene, 1,3,5-trimethylbenzene and m-xylene were analyzed using gas-chromatography/mass spectrometry techniques, which included species such as CO, CO₂, n-alkanes, alkenes, single ringed, two ringed and polycyclic aromatic hydrocarbons (PAH). Almost similar major PAH species were formed from the experiments of n-propylbenzene, m-xylene and 1,3,5-trimethylbenzene, which included indene, naphthalene and anthracene. However, the maximum peak concentrations of these species varied with the fuel, which indicates that the formation of these species is dictated by the fuel structure. For example, for n-propylbenzene experiments, bibenzyl and indene were the major two ringed species that were formed. For the m-xylene and 1,3,5-trimethylbenzene, the dimers of the m-xylyl and 1,3,5-trimethylbenzyl radicals, indene, naphthalene and anthracene were the major two ringed and three ringed compound that were formed. This species distribution obtained from n-propylbenzene, 1,3,5-trimethylbenzene and m-xylene experiments was crucial in the development of the mechanism and kinetic model for each individual fuel decay.

(B) Kinetic models were developed for the oxidation of n-propylbenzene, m-xylene and 1,3,5-trimethylbenzene. Development of these models helped in understanding the decay of these fuels.

- a. **n-Propylbenzene:** The oxidation of this species depended on the temperature and the concentration of the oxidizer. At low temperatures (around 1060 K) the species decayed by hydrogen abstraction reactions forming styrene as the major intermediate. At higher temperatures (around 1250 K), the species decayed by the homolysis pathway of the n-propyl side chain thereby forming benzyl and ethyl radical. The concentration of the oxidizer influenced the formation of the single ringed aromatic hydrocarbon intermediates such as benzaldehyde and two ringed and three ringed aromatics such as bibenzyl, indene and anthracene. At fuel lean conditions greater peak concentrations of benzaldehyde were attained when compared to the experiments at fuel rich conditions. The maximum peak concentrations of the polycyclic aromatic hydrocarbon intermediates increased as the equivalence ratio were increased. A direct pathway from the fuel decay was found to be responsible for the formation of indene, which was the major polycyclic aromatic hydrocarbon measured in the fuel lean and stoichiometric oxidation experiments. The oxidation model was also validated against the flow reactor data from different laboratories so as to extend the operating range of this model.

The pyrolysis of the fuel was seen to be primarily dependent on the homolysis pathway; hence benzyl radicals were the major unstable intermediate species. Benzyl radical and the species formed from the decomposition of the benzyl radical such as the cyclopentadienyl radical and propargyl radicals influenced the formation of

polycyclic aromatic hydrocarbons such as indene, naphthalene, anthracene and acenaphthylene.

- b. m-Xylene:** The oxidation model of m-xylene was developed to predict the formation of species with carbons numbers ranging from C1 to C8, which also included the major single ringed aromatic hydrocarbons (toluene and benzene) observed from the experiments. The oxidation chemistry of the fuel was dictated by the formation and consumption of the dimethylphenoxy radicals. Toluene was primarily formed from m-xylene by displacement of the methyl group by a hydrogen atom and minor amounts of toluene was formed from dimethylphenoxy radical. Major amounts of benzene was formed from dimethylcyclopentadienyl radical by internal rearrangement and subsequent loss of the methyl group, which was in turn formed from dimethylphenoxy radical by CO elimination. The importance of the including the pathways for the formation of benzene and toluene from dimethylphenoxy radical was further confirmed in the 1,3,5-trimethylbenzene oxidation model development. In addition to developing kinetics for the formation of benzene and toluene from dimethylphenoxy radical, the toluene oxidation subset of kinetics was also updated for a few major reactions such as benzyl+HO₂ and benzyl+O₂. The m-xylene oxidation model has not only been validated against our high pressure experimental data but also validated against the flow reactor, jet stirred reactor data and shock tube ignition delay data for different experimental regimes of low pressure (1 atm), intermediate pressure (10 -25 atm) and high pressure (25-50 atm) regimes, so as to develop a comprehensive model for the oxidation of m-xylene.
- c. 1,3,5-Trimethylbenzene:** The 1,3,5-Trimethylbenzene oxidation model included the subset of kinetics for m-xylene and toluene oxidation. The mechanism was

developed based on the product distribution obtained from the experiments and the kinetic data for most of the reactions in the mechanism were estimated from analogous reactions of toluene. The model predicted the fuel decay, oxygen decay and the formation of major intermediates such as CO, CO₂ and m-xylene adequately well. However, the over-prediction or under-prediction of other major intermediates such as toluene has highlighted the specific kinetics in the model which need to be included. A number of pathways such as for formation of the trimethylphenoxy radical have to be included so as to improve the predictions of toluene. Among the polycyclic aromatic hydrocarbons a direct route was identified for the formation of anthracene from the fuel. However, the formation of indene and naphthalene was under predicted and it is possible that the prediction of these species could be improved if the formation of toluene is predicted accurately by the model.

In the present work, the combustion of aromatic surrogate fuel components was studied both experimentally and theoretically. Hence, an experimental, thermochemical and kinetic validation database are now available for these aromatic surrogate fuel components of jet fuel.

10. FUTURE WORK

The oxidation model for n-propylbenzene, which also consists of pyrolysis kinetics shows excellent predictions not only for our experimental data but also for the data obtained from other laboratories. Therefore the oxidation model of n-propylbenzene can be considered complete and no further work is needed in the development of n-propylbenzene kinetics.

The oxidation model for 1,3,5-trimethylbenzene which includes 1,3,5-trimethylbenzene and m-xylene oxidation and pyrolysis kinetics has to be further improved. One of the challenges associated with improving the 1,3,5-trimethylbenzene oxidation model is that experimental measurements of the rate constants for the formation and decay of most of the intermediates observed in our experiments are not available. This is not surprising since the species distribution in 1,3,5-trimethylbenzene oxidation and pyrolysis experiments was obtained for the first time in the present work and such measurements do not exist in the literature. Most of the models available in the literature for m-xylene are validated only against the oxidation experiments and the pyrolysis of these species has not been studied. Specifically the pyrolysis kinetics are not complete for 1,3,5-trimethylbenzene and m-xylene and further research is required in this area. Both experimental measurements and theoretical calculations are required for further development of the m-xylene and 1,3,5-trimethylbenzene oxidation and pyrolysis kinetics. The pathways for the formation of different polycyclic aromatic hydrocarbons has to be further investigated, since in our present study we have identified that a few of the PAH species could be formed from the fuel via unconventional channels, which depended on the fuel structure and the type of intermediates formed from the fuel decay.

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APPENDICES

n-Propylbenzene and 1,3,5-Trimethylbenzene Oxidation Experiments

Oxidation experiments were conducted on 1,3,5-trimethylbenzene (60 %) and n-propylbenzene (40 %) mixture for an equivalence ratio of 1.4 and at an average pressure of 22 atm, in the High Pressure Single Pulse Shock Tube. These experiments were conducted to examine the differences in reactivity of 1,3,5-trimethylbenzene and n-propylbenzene in the mixture when compared to oxidation of pure 1,3,5-trimethylbenzene and n-propylbenzene. The decay of 1,3,5-trimethylbenzene and n-propylbenzene are shown in Figure 1 as a function of temperature. From the figure it can be observed that n-propylbenzene decays at lower temperatures when compared to 1,3,5-trimethylbenzene. For instance, at a temperature of 1193 K, about 98 % of n-propylbenzene has been consumed whereas only 45 % of 1,3,5-trimethylbenzene was consumed at the same temperature.

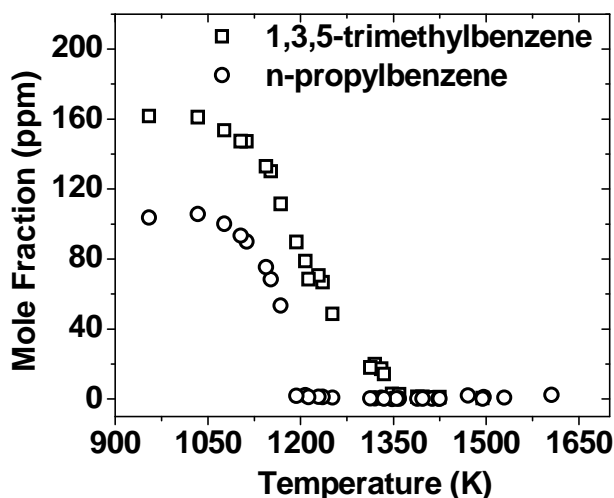


Figure 1. Decay of 1,3,5-trimethylbenzene (1,3,5-tmb) and n-propylbenzene (npb) in 1,3,5-trimethylbenzene (60 %) and n-propylbenzene (40 %) mixture experiments, average $P_5 = 22$ atm, average reaction time = 2.16 ms, $\Phi = 1.4$

The decay of 1,3,5-trimethylbenzene in the presence and absence of n-propylbenzene (100 % 1,3,5-trimethylbenzene) is compared in Figure 2. In the latter case, 1,3,5-trimethylbenzene (100 %) oxidation experiments were conducted at an average pressure of 24 atm, average reaction time of 1.77 ms and an equivalence ratio of 1.3. From the figure it can be observed that 1,3,5-trimethylbenzene decays at lower temperatures in the presence of n-propylbenzene. For example, at

a temperature of approximately 1250 K, almost 70 % of 1,3,5-trimethylbenzene has been consumed in the presence of n-propylbenzene, whereas only about 22 % of 1,3,5-trimethylbenzene has decayed in the absence of n-propylbenzene. The decay of 1,3,5-trimethylbenzene at lower temperatures in the mixture could be the result of cross-reactions between 1,3,5-trimethylbenzene and the radicals formed from the oxidation of n-propylbenzene. Since n-propylbenzene decays at lower temperatures, when compared to 1,3,5-trimethylbenzene, the radicals formed in the oxidation of n-propylbenzene react with 1,3,5-trimethylbenzene and promote the consumption of 1,3,5-trimethylbenzene in the presence of n-propylbenzene.

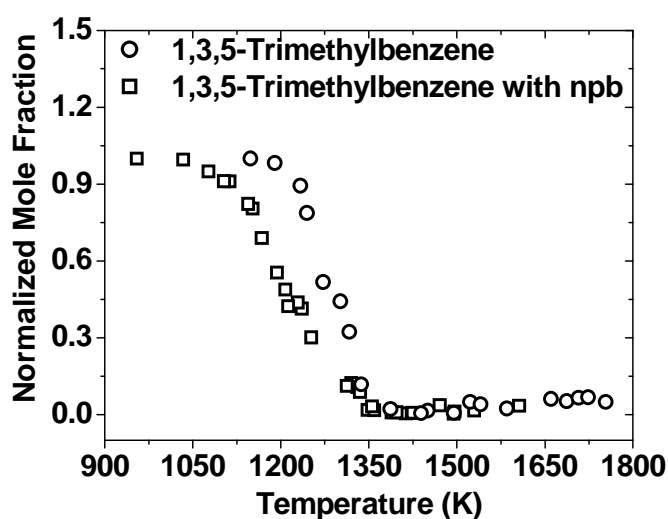


Figure 2. Decay of 1,3,5-Trimethylbenzene in the presence of n-propylbenzene (□) and in the absence of n-propylbenzene (○). Experiments of 1,3,5-Trimethylbenzene (60 %) and n-propylbenzene (40 %) were conducted at average $P_5=22$ atm, average reaction time=2.16 ms, $\Phi = 1.4$. Experiments of 1,3,5-trimethylbenzene were conducted at average $P_5=24$ atm, average reaction time = 1.77 ms, $\phi = 1.3$

The decay of n-propylbenzene in the presence and absence of 1,3,5-trimethylbenzene (100 % 1,3,5-trimethylbenzene) is compared in Figure 3. In the latter case, n-propylbenzene (100 %) oxidation experiments were conducted at an average pressure of 18 atm, average reaction time of 2.29 ms and an equivalence ratio of 0.55. From the figure it can be observed that the decay of n-propylbenzene is similar in the presence and absence of 1,3,5-trimethylbenzene. In spite of difference in the equivalence ratio, it can be observed that the decay of n-propylbenzene is not influenced by the presence of 1,3,5-trimethylbenzene.

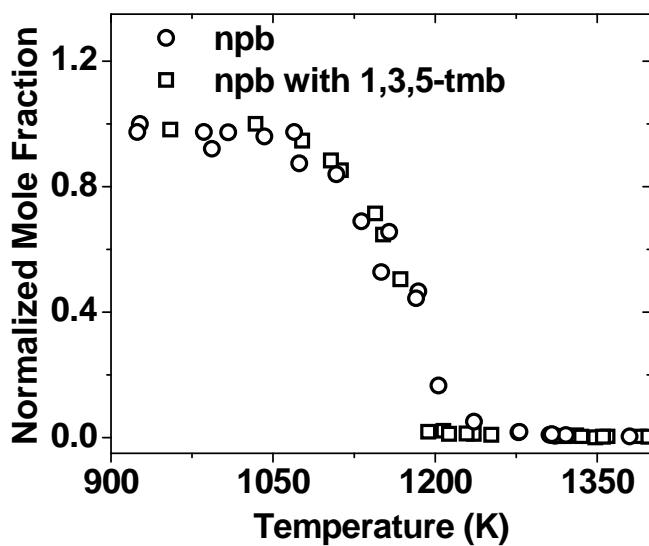


Figure 3. Decay of n-propylbenzene in the presence of 1,3,5-trimethylbenzene (\square) and in the absence of 1,3,5-trimethylbenzene (\circ). Experiments of 1,3,5-Trimethylbenzene (60 %) and n-propylbenzene (40 %) were conducted at average $P_5=22$ atm, average reaction time=2.16 ms, $\Phi = 1.4$. Experiments of n-propylbenzene were conducted at average $P_5=18$ atm, average reaction time = 2.29 ms, $\phi = 0.55$

From the discussion presented in the above paragraphs, it can be concluded that the decay of 1,3,5-trimethylbenzene is influenced by the presence of n-propylbenzene but not vice-versa. This experimental study reveals that when a mixture of fuels is oxidized, the reactivity of the fuels that decay at higher temperatures could be enhanced due to the presence of the fuels that decay at lower temperatures.

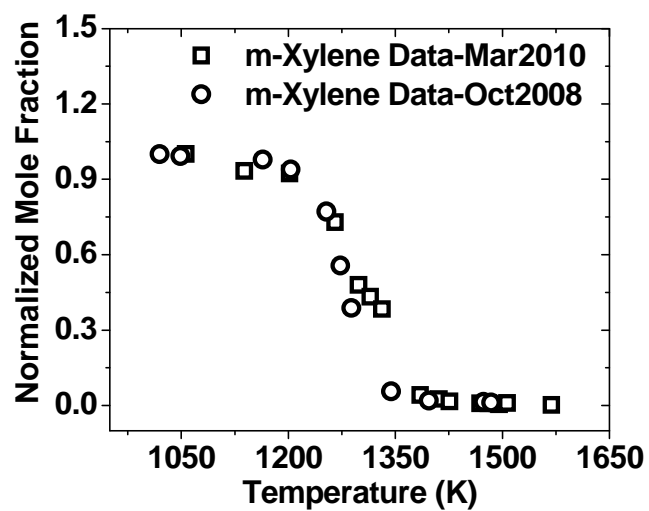


Figure 4. Reproducibility of the High Pressure Shock Tube experiments is shown by comparing the m-xylene decay obtained from two different experimental datasets. The experiments were performed in March 2010 and in October 2008.

Constant GC Injection Pressure of 16 psi

The scatter in data and over prediction of CO₂ at higher reflected shock temperatures in the experiments could be due to inaccurate GC analysis. In order to test this hypothesis, calibration mixture of different concentrations of CO₂ were prepared using Scotty Analyzed Gases Mix14 (mole% of species- C₂H₂ .979%, CO₂ .999%, CO 1.0%, C₂H₆ .997%, C₂H₄ 1%, CH₄ .998%, balance of nitrogen in 14lit vessel at 240 psig). For a fixed concentration of CO₂ the GC injection pressure was varied from 33psi to 6psi. A Plot-Q column eluting into FID was used to identify CO₂. A nickel catalyst (Methaniser) was placed in between the Plot-Q column and FID to convert CO₂ eluting from the column to CH₄, thereby permitting CO₂ to be detected on the FID. All the sample lines to the GC, including the pressure gauge were heated.

Filename	Pinj/psi	Area	Area/Pinj	Molefraction/ ppm	Area/Pinj %Error
141008ag	29.71	206506048	6950725.3	1856	reference
141008ah	21.8	147053155	6745557.6	1856	2.95%
151008ab	13.17	96699318	7342393.2	1856	-5.23%
151008ac	28.74	191143667	6650788.7	1733.22	reference
151008ad	11.07	81379460	7351351.4	1733.22	-10.53%
151008ae	33.04	121207797	3668516.9	1051.715	reference
151008af	25.45	97748645	3840811.2	1051.715	-4.70%
151008ag	19.34	75961626	3927695.2	1051.715	-7.06%
201008ad	28.88	178936951	6195877.8	1732.64	reference
201008ae	28.53	179634975	6296353.8	1732.64	-1.62%
211008ab	23.13	147833511	6391418.5	1732.64	-3.16%
211008ac	16.21	107915247	6657325.5	1732.64	-7.45%
211008ad	6.72	46776256	6960752.4	1732.64	-12.34%

The highest injection pressure chosen was ~30psi, the pressure at which the post shock samples were analyzed. The area/pinj of the highest injection pressure was taken as the reference value to calculate the percentage error at subsequent pressures for each concentration. It can be seen that the percentage error in area/pinj increases as the difference in the injection pressure increases. This trend is reproducible for different concentrations and the response is sensitive to the concentration as seen in Figure 5. The %error is minimal if the injection pressures are close (as seen in the **bolded** rows).

In order to test if this error could be caused by faulty reading of the pressure gauge (range: 0-20psi) another gauge (of range: 0-200psi) was connected in series. No discernible difference was seen in the readings.

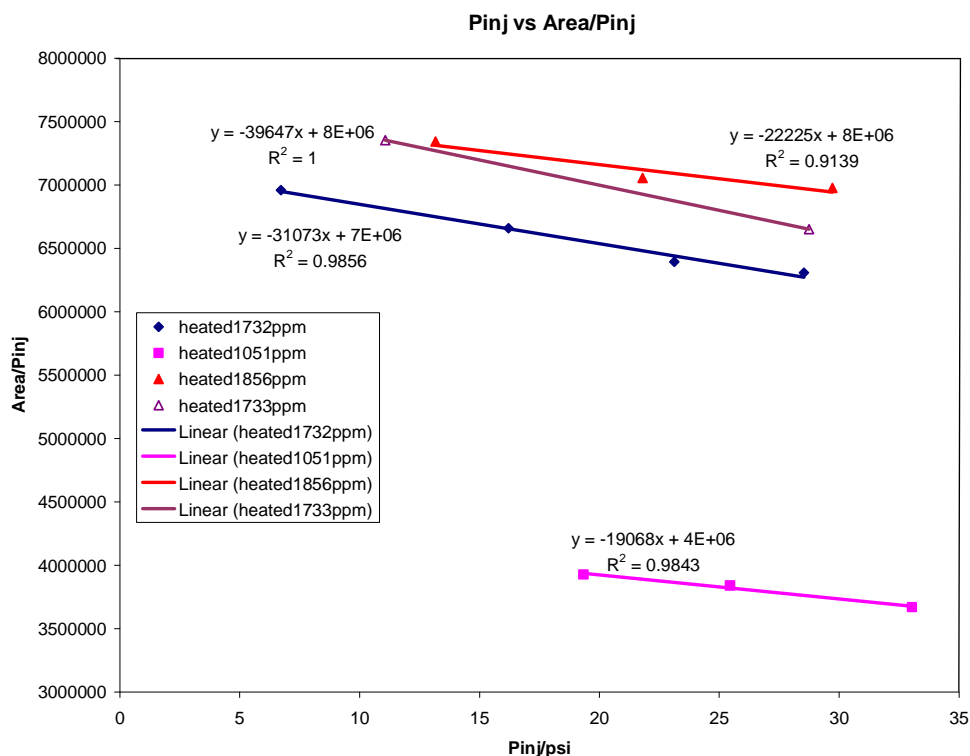


Figure 5

In order to test if the heating of the sample lines has caused this discrepancy in the measurement, experiments were done with sample lines unheated (at room temperature). The same trend was seen, the % error in area/pinj increased with the difference in the injection pressure, Figure 6. The **bolded** rows again show reproducibility of constant pressure injections.

Filename	Pinj	Area	Area/psi	Molefraction/ ppm	Area/Pinj %Error
161008ab	31.7	158682686	5005763	1231.83	reference
161008ac	26.8	129811710	4843720.5	1231.83	3.24%
161008ad	19.5	101796354	5220325.8	1231.83	-4.29%
161008ae	8.45	46426313	5494238.2	1231.83	-0.62%
161008af	8.94	49421332	5528113.2	1231.83	reference
181008ab	16.17	76711645	4744072	1177.74	-2.6%
181008ac	16.18	78792659	4869756.4	1177.74	reference

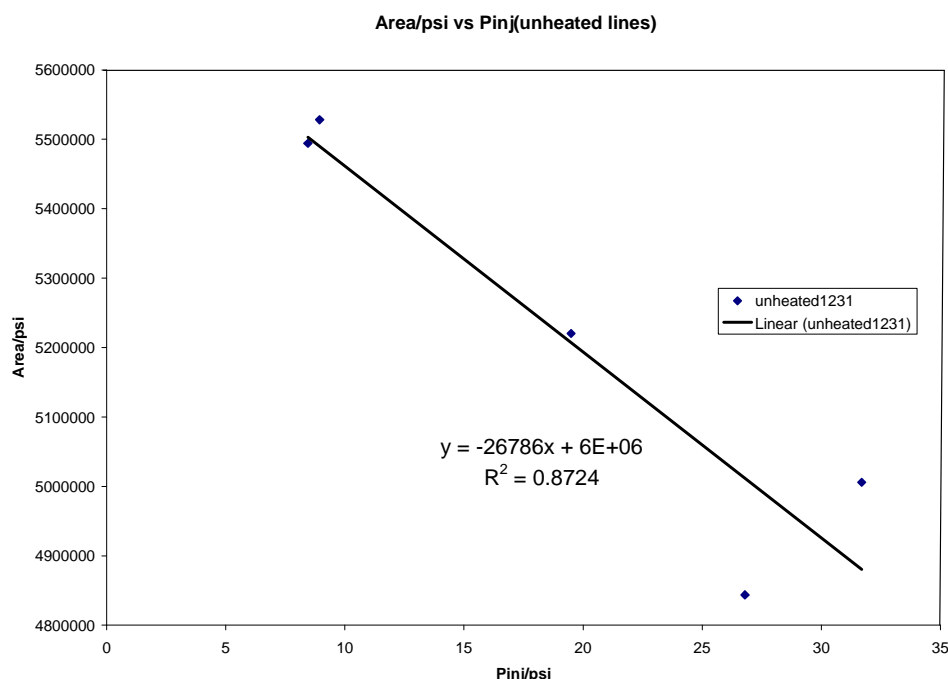


Figure 6

The above results conclude that constant pressure GC injection could minimize the errors in calibration and quantification of the stable species. To confirm this, shock tube experiments were done on the CO₂ reagent mixture at low and high reflected shock temperatures ($T_5 = 1095.51\text{K}$ and $T_5 = 1473.84\text{K}$) at a pressure of 23atm.

Shock Tube Experiments:

Reagent mixtures consisting of CO₂ (Bone Dry 99.8%, Matheson tri-gas), 1996.59 ppm, krypton (Research grade, 99.999%, Specialty gases of America) and balance argon (Ultra High Purity, Air gas) were prepared in 50-liter vessel. The deviation in the CO₂ quantification in the preshock and the postshock sample was 4.50% which is within the experimental error. For almost constant injection pressures the peak areas of CO₂ in the post shock samples differed by 0.36%, confirming the hypothesis that constant GC injection pressure minimizes the error.

Shock	P5/atm	T5/K	Filename	Pinj/psi	Area	CO ₂ (Area/Pinj)
Preshock			271008ag	17.10	146171693	8548052
sample						
11	22.91	1095.51	271008ah	17.10	152746694	8932555
12	22.91	1473.84	271008ak	17.06	152944791	8965111

Conclusions:

As a result of the above investigations the following conclusions and recommendations have been formulated.

- 1) Error in quantification of stable species can be minimized by constant GC injection pressures.
- 2) The GC injection pressure will be fixed in all subsequent analyses by the use of a high flow (3600 psig), high-sensitivity (0.2%) diaphragm-sensing pressure reducing (0-25psig) regulator (KHF1DRA828A20000, Chicago Fluid System Technologies) placed in between the sample vessel outlet and the inlet valve of the sample injection rig of the GC/MS. This regulator can be heated to at least 200°C to be consistent with the heating of the sample gas transfer lines
- 3) The regulator and the sample lines to the GC/MS should be heated to a constant and consistent temperature by the use of heating tapes, to get reproducible results. The temperature should be measured and a standard value should be adopted as a standard laboratory operating procedure.

Included for each experimental set presented in appendix

- Experimental conditions (temperatures-K, pressures-atm, and reaction times-ms)
- Mole fraction of the major products ppm

n-Propylbenzene Oxidation Datasets

Experimental data for n-propylbenzene oxidation, average P5 = 51 atm, $\Phi = 0.55$

Shock No.	4	25	17	23	30	32	38	42	44	46
T5 /K	958.71	1017.1	1052.8	1114.3	1181	1273.2	1347.6	1408.9	1477.9	1558.2
P5 /atm	50.55	53.28	56.33	55.11	51.83	54.54	48.91	49.52	47.84	45.11
Reaction Time /ms	1.64	1.57	1.63	1.68	1.78	1.9	1.71	1.58	1.5	1.27
n-Propylbenzene	90.51	84.1	79.41	53.07	17.6	1.61	0.8	0	0	0
O2	1975.9	1940.6	1883.9	1846.3	1699.5	1616.1	1327.9	1058.3	1069.3	1059.6
CO	0	0.6	1.09	8.35	69.46	333.52	418.56	180.95	37.49	29.23
CO2	0	3.56	3.29	5.13	11.21	56.03	255.17	552.37	771.8	780.69
Methane	0	0.37	0.6	1.74	4.17	10.41	3.22	0.37	0.4	0.25
Ethene	0	0	3.04	14.91	35.22	29.25	4.44	0.74	0	0.25
Ethane	0	0	0.25	1.08	1.8	1.77	0.34	0.09	0	0.08
Acetylene	0	0	0.1	0.28	4.8	26.6	6.08	0.56	0	0
Propene	0	0	0.22	1.06	1.43	0.7	0.16	0	0	0
1,2-Propadiene	0	0	0	0	0.25	0.51	0.19	0	0	0
Propyne	0	0	0	0	0.53	1.73	0.58	0	0	0
1,3-Butadiene	0	0	0	0.05	0.33	0.71	0.13	0	0	0
Vinylacetylene	0	0	0	0.18	1.26	2.74	0.44	0	0	0
Diacetylene	0	0	0	0	0.07	0.21	0.12	0	0	0
Benzene	0	0.07	0.16	1.26	5.24	7.96	1.21	0.17	0.06	0.09
Toluene	0	0.07	0.23	1.22	4.23	2.65	0.36	0.1	0	0
Phenylacetylene	0	0	0	0.07	0.87	1.26	0.48	0.1	0.04	0
Styrene	0	0.6	3.71	11.8	19.52	4.66	0.67	0.27	0.2	0.25
1-Propenylbenzene	0	0.02	0.06	0.16	0.18	0.02	0.01	0	0	0
Cyclopentadiene	0	0	0.05	0.16	1.39	1.7	0.31	0	0	0
Ethylbenzene	0	0	0.7	3.28	4.61	0.49	0	0	0	0
Bibenzyl	0	0.18	0.91	1.83	1.89	0.39	0	0	0	0
Benzaldehyde	0	0.43	0.42	3.49	9.72	4.02	0.58	0.28	0.08	0.07
Benzofuran	0	0.44	0.74	1.79	2.18	1.71	0.88	0.26	0.06	0.06
Phenol	0	0.15	0.29	2.84	2.35	0.99	0.39	0.16	0.04	0.08
Indene	0	0.06	0.17	2.51	4.87	2.73	1.2	0.17	0.59	0.27
Naphthalene	0	0	0	0.25	0.3	0.31	0.13	0	0	0
2-Ethynylnaphthalene	0	0	0.02	0.04	0.46	0.37	0.03	0	0	0
Biphenylmethane	0	0	0	0	0.24	0.19	0.01	0	0	0
Preshock Carbon	814.55	814.55	814.55	814.55	814.55	814.55	814.55	814.55	814.55	814.55
Postshock Carbon	814.55	777.84	791.34	777.46	796.1	769.78	758.7	747.72	818.54	817.18

Experimental data for n-propylbenzene oxidation, average P5 = 49 atm, Φ = 1.0 (Page 1/2)

Shock No.	5	2	8	11	25	34	28	43	48	45
T5 /K	837.98	869.74	993.35	1027.8	1103.3	1156.6	1220.8	1297	1374.8	1387.4
P5 /atm	47.77	49.86	53.15	46.92	52.28	50.21	52.74	48.74	48.8	48.18
Reaction Time /ms	1.65	1.7	1.7	1.71	1.74	1.95	1.89	1.79	1.77	1.7
n-Propylbenzene	89.44	89.73	88.59	84.22	67.81	28.04	3.87	1	0.43	0.25
O2	1038.4	1038.1	1030.1	1033	1029.8	1018.2	1018.7	968.92	721.54	538.86
CO	0	0	0	0	5.87	19.14	63.31	132.09	336.67	368.49
CO2	1.91	2.89	2.13	2.72	3.03	3.83	9	11.93	78.55	233.42
Methane	0	0	0	0.31	1.41	2.66	5.59	8.38	13.48	8.42
Ethene	0	0	0	1.12	11.73	35.14	53.55	53.9	23.93	11.07
Ethane	0	0	0	0.12	0.92	1.66	2.07	2.56	1.74	0.63
Acetylene	0	0	0	0	0.26	2.55	11.27	21.85	45.93	19.38
Propane	0	0	0	0	0.76	2.1	1.47	1.06	0.41	0.24
1,2-Propadiene	0	0	0	0	0	0.13	0.36	0.74	0.57	0.42
Propyne	0	0	0	0	0	0.25	0.82	1.35	1.33	0.33
1,3-Butadiene	0	0	0	0	0.05	0.14	0.49	0.8	0.48	0.24
Vinylacetylene	0	0	0	0	0.17	0.84	2.56	3.24	1.77	0.76
Diacetylene	0	0	0	0	0	0	0.1	0.42	0.6	0.31
Benzene	0	0	0	0.08	1.02	3.94	9.43	12.79	7.89	3.41
Toluene	0	0	0.23	0.15	1.22	5.55	12.79	15.04	4.03	1.87
Phenylacetylene	0	0.17	0	0.04	0.24	0.77	1.92	2.38	1.06	0.74
Styrene	0	0	0	1.08	10.52	20.25	17.63	9.28	1.78	0.88
1-Propenylbenzene	0	0	0.01	0.04	0.14	0.18	0.12	0	0	0
Cyclopentadiene	0	0	0	0	0.22	0.94	2.59	3.35	1.74	0.82
Methylcyclopentadiene	0	0	0	0	0.12	0.4	0.58	0.45	0.21	0.08
1,3-Hexadiene	0	0	0	0	0	0.31	0.39	0.36	0.13	0.05
Ethylbenzene	0	0	0	0.33	3.13	6.67	4.66	1.12	0.55	0
Bibenzyl	0	0	0.11	0.3	2.23	1.45	0.52	0.03	0	0
Indene	0	0	0	0	2.25	4.73	6.45	3.75	1.06	0.98
Benzaldehyde	0	0	0	0	2.62	6.72	8.75	4.89	1.81	0.59
Benzofuran	0	0	0	0	0.82	1.04	1.59	1.71	1.47	0.38
Phenol	0	0	0	0	0.32	0.92	1.56	1.29	0.17	0.08
Naphthalene	0	0	0	0	0.08	0.48	1.82	1.8	0.53	0
2-Ethynyl-naphthalene	0	0	0	0	0.03	0.05	0.25	0.2	0.14	0
Diphenylmethane	0	0	0	0	0.03	0.05	0.25	0.14	0.04	0
Stilbene	0	0	0	0	0.06	0.07	0.24	0.17	0.07	0
Fluorene	0	0	0	0	0.03	0.04	0.17	0.18	0.03	0
Anthracene	0	0	0	0.04	0.1	0.21	0.23	0.15	0.01	0
Preshock Carbon	807.56	807.56	807.56	807.56	807.56	807.56	807.56	807.56	807.56	807.56
Postshock Carbon	806.87	811.82	802.75	781.69	860.84	796.66	808.5	770.02	751.53	750.75

Experimental data for n-propylbenzene oxidation, average P5 = 49 atm, $\Phi = 1.0$ (Page 2/2)

Shock No.	56	54	52	58	60
T5 /K	1412.7	1448.1	1488.2	1509.4	1635.4
P5 /atm	48.79	50.59	44.71	43.74	43.9
Reaction Time /ms	1.52	1.51	1.48	1.39	1.21
n-Propylbenzene	0	0	0	0	0
O2	235.49	176.58	130.31	89.05	86.27
CO	277.28	159.36	123.47	120.76	108.52
CO2	502.19	628.9	676.41	680.92	708.75
Methane	0.9	0.39	0.52	0.31	0.53
Ethene	1.89	0.65	0.07	0.37	0.57
Ethane	0.11	0.11	0.03	0.1	0.12
Acetylene	6.83	0.95	0.58	0.3	0.21
Propane	0	0	0	0	0
1,2-Propadiene	0.14	0	0	0	0
Propyne	0.16	0	0	0	0
1,3-Butadiene	0.07	0	0	0	0
Vinylacetylene	0.15	0	0	0	0
Diacetylene	0.05	0	0	0	0
Benzene	0.44	0.18	0.09	0.06	0
Toluene	0.39	0	0	0	0
phenace	0.19	0.18	0.26	0.11	0
Styrene	0.32	0.21	0.18	0	0
1-Propenylbenzene	0	0	0	0	0
Cyclopentadiene	0.19	0.17	0.11	0.07	0
Methylcyclopentadiene	0.02	0	0	0	0
1,3-Hexadiene	0	0	0	0	0
Ethylbenzene	0	0	0	0	0
Bibenzyl	0	0	0	0	0
Indene	0	0	0	0	0
Benzaldehyde	0	0	0.18	0	0
Benzofuran	0.06	0	0	0	0
Phenol	0.04	0	0	0	0
Naphthalene	0	0	0	0	0
2-Ethynylnapthalene	0	0	0	0	0
Diphenylmethane	0	0	0	0	0
Stilbene	0	0	0	0	0
Fluorene	0	0	0	0	0
Anthracene	0	0	0	0	0
Preshock Carbon	807.56	807.56	807.56	807.56	807.56
Postshock Carbon	811.33	797.09	807.65	805.18	819.62

Experimental data for n-propylbenzene oxidation, average P5 = 52 atm, $\Phi = 1.9$ (Page 1/2)

Shock No.	2	5	13	69	16	66	22	63	60	19	57
T5 /K	847.38	923.38	1009.7	1040.5	1133.8	1107	1172.7	1227.6	1263.2	1286.4	1374.3
P5 /atm	47.62	46.22	54.19	54.36	54.02	60.31	53.06	54.05	55.27	57.89	44.69
Reaction Time /ms	1.5	1.52	1.61	1.59	1.85	1.72	1.78	1.95	1.95	1.9	1.79
n-Propylbenzene	89.99	88.78	87.14	86.44	42.34	55.98	19.79	5.28	2.49	1.89	0.99
O2	575.09	556.67	573	548.84	554.67	525.17	530.89	508.05	510.72	503.05	433.22
CO	0	0	5.54	3.32	21.48	5.73	24.59	34.38	39.05	57.41	107.41
CO2	0	0	2.54	2.38	3.13	2.22	3.77	3.13	4.24	2.72	12.15
Methane	0	0	0	0.31	2.2	1.77	3.06	4.42	5.62	7.05	15.11
Ethene	0	0	0	1.8	28.8	18.7	49.99	63.88	67.99	65.76	55.51
Ethane	0	0	0	0.2	1.61	1.29	1.89	2.19	2.62	2.92	2.34
Acetylene	0	0	0	0	0.92	0.63	2.92	8.49	12.12	16.36	57.18
Propene	0	0	0	0.08	1.26	0.93	1.65	1.73	1.26	1.34	0.65
1,2-Propadiene	0	0	0	0	0	0.08	0.13	0.27	0.43	0.52	1.15
Propyne	0	0	0	0	0	0	0.32	0.49	0.72	0.97	2.88
1,3-Butadiene	0	0	0	0	0.06	0	0.17	0.07	0.35	0.41	0.52
Vinyl Acetylene	0	0	0	0	0.35	0	0.8	1.45	1.79	2.04	2.53
Diacetylene	0	0	0	0	0	0	0	0.07	0.15	0.21	2.28
Benzene	0	0	0.09	0.19	3.76	2.1	7.1	10.63	12.56	14.17	19.92
Toluene	0	0.18	0.2	0.32	6.68	3.21	14.76	24.62	30.38	29.57	20.85
Ethylbenzene	0	0.09	0.09	0.4	7.13	4.76	9.01	7	4.39	2.48	0.63
p-Xylene	0	0	0.01	0.03	0.22	0.18	0.34	0.38	0.35	0.31	0.1
Styrene	0	0	0.33	1.26	12.88	9.38	16.38	14.91	12.85	10.73	3.78
Cyclopentadiene	0	0	0	0	0.62	0.3	1.55	2.68	3.25	3.6	2.92
1,3-hexadiene	0	0	0.03	0.03	0.24	0.24	0.43	0.62	0.71	0.63	0.46
Methylcyclopentadiene	0	0	0	0	0.4	0.23	0.68	0.72	0.63	0.56	0.32
Benzaldehyde	0	0	0	0.24	2.58	1.68	3.48	3.69	3.67	3.3	1.11
1-Propenyl benzene	0	0	0	0	0.17	0.11	0.13	0.09	0.07	0.06	0.01
Bibenzyl	0	0	0	0	4.46	3.93	3.28	1.97	1.52	1.02	0.27
Benzylalcohol	0	0	0	0	0.15	0.06	0.35	0.55	0.63	0.77	1
Phenol	0	0	0	0	0.35	0.26	0.67	0.57	0.47	0.33	0.14
Phenylacetylene	0	0	0	0	0.18	0.15	0.41	0.84	1.01	1.38	1.77
2-Propenylbenzene	0	0	0	0	0	0	0	0.08	0.28	0.31	1.01
2-Ethynylnaphthalene	0	0	0	0	0.2	0.09	0.31	0.53	0.73	0.41	0
Biphenylmethane	0	0	0	0	0.14	0.04	0.24	0.46	0.5	0.43	0.17
Benzofuran	0	0	0.02	0	0.51	0.36	0.51	0.36	0.29	0.21	0.06
Indene	0	0	0	0	0.28	0.08	0.51	0.8	0.9	1.02	1.04
Naphthalene	0	0	0	0	0	0	0	0.08	0.28	0.31	1.01
Fluorene	0	0	0	0	0	0	0.06	0.14	0.2	0.41	0.35
Stilbene	0	0	0	0	0.45	0.15	0.45	0.33	0.27	0.08	0.01
1,2-Diphenylethyne	0	0	0	0	0	0	0.07	0.04	0.03	0.08	0.09
Anthracene	0	0	0	0	0	0	0.12	0.19	0.26	0.39	0.3
Preshock Carbon	809.89	809.89	809.89	809.89	809.89	809.89	809.89	809.89	809.89	809.89	809.89
Postshock Carbon	809.89	800.98	798.11	806.86	817.68	789.97	800.31	787.62	807.09	789.97	800.71

Experimental data for n-propylbenzene oxidation, average P5 = 52 atm, $\Phi = 1.9$ (Page 2/2)

Shock No.	54	34	48	51	45	37
T5 /K	1419.1	1448.7	1471.4	1500	1527.1	1639.9
P5 /atm	50.09	52.15	47.09	47.77	50.15	49.68
Reaction Time /ms	1.34	1.59	1.53	1.4	1.32	1.26
n-Propylbenzene	0.86	0.66	0.78	0.67	0.56	0
O2	260.64	115.63	86.63	41.48	26.19	8.02
CO	343.48	500.67	510.48	552.94	557.44	659.68
CO2	51.47	85.48	91.05	103.25	135.72	119.77
Methane	22.39	16.45	14.57	9.85	4.79	1.85
Ethene	18.92	6.14	4.13	2.12	0.74	0.5
Ethane	1.34	0.59	0.55	0.26	0.12	0.07
Acetylene	119.03	86.78	71.63	53.66	26.56	11.92
Propene	0.3	0.1	0.16	0.1	0	0
1,2-Propadiene	0.86	0.43	0.38	0.24	0	0
Propyne	2.68	1.18	0.96	0.73	0	0
1,3-Butadiene	0.05	0.07	0.09	0.02	0	0
Vinyl Acetylene	0.92	0.29	0.2	0.1	0	0
Diacetylene	3.92	2.51	1.65	1.4	0.44	0
Benzene	7.53	1.71	1.06	0.35	0.18	0.17
Toluene	3.5	0.81	0.48	0.23	0.14	0.14
Ethylbenzene	0.12	0.04	0	0.02	0	0.05
p-Xylene	0.06	0	0	0	0	0
Styrene	0.51	0.05	0.1	0.07	0.1	0.1
Cyclopentadiene	0.8	0.19	0.12	0.03	0	0
1,3-hexadiene	0.18	0.01	0	0	0	0
Methylcyclopentadiene	0.09	0	0	0	0	0
Benzaldehyde	0.18	0.06	0.04	0.02	0.02	0.03
1-Propenyl benzene	0	0.01	0	0	0	0
Bibenzyl	0	0	0	0	0	0
Benzylalcohol	0.42	0	0	0	0	0
Phenol	0	0	0	0	0	0
Phenylacetylene	0	0.22	0.11	0	0	0
2-Propenylbenzene	0.47	0.05	0	0	0	0
2-Ethynyl naphthalene	0	0	0	0	0	0
Biphenylmethane	0	0	0	0	0	0
Benzofuran	0	0	0	0	0	0
Indene	0.29	0.01	0	0	0	0
Naphthalene	0.47	0.05	0	0	0	0
Fluorene	0.01	0	0	0	0	0
Stilbene	0	0	0	0	0	0
1,2-Diphenylethyne	0	0	0	0	0	0
Anthracene	0.1	0	0	0	0	0
Preshock Carbon	809.89	809.89	809.89	809.89	809.89	809.89
Postshock Carbon	831.5	833.18	800.21	798.18	762.54	809.62

Experimental data for n-propylbenzene oxidation, average P5 = 28 atm, $\Phi = 0.54$
(Page 1/2)

Shock No.	18	6	4	12	10	14	20	16	40	22
T5 /K	906.87	989.31	1044.6	1135.7	1175.5	1245.1	1264.5	1300	1340.6	1368.5
P5 /atm	28.56	28.05	28.84	27.67	27.82	27.81	26.99	27.6	28.15	27.5
Reaction Time /ms	1.76	1.84	1.87	1.98	1.9	1.78	2.05	1.91	1.89	1.83
n-Propylbenzene	85.94	83.81	76.95	34.83	12.26	2.02	0.93	0.52	0	0
O2	1891.7	1900.7	1864.8	1812.7	1793.6	1785.1	1784.4	1451	1284.6	1131.5
CO	0	0	2.32	25.42	57.05	149.77	195.73	369.43	345.65	254.34
CO2	0	0	2.57	3.49	5.35	13.09	18.85	160.39	312.76	443.12
Methane	0	0	0	2.12	4	6.93	8.28	5.81	1.9	0.52
Ethene	0	0	3.31	27.59	42.33	46.04	42.26	15.35	4.52	1.58
Ethane	0	0	0.34	1.71	2.06	2.31	2.31	0.96	0.36	0.13
Acetylene	0	0	0.48	1.35	5.72	18.46	25.46	16.5	3.7	1.27
Propane	0	0	0.31	1.34	1.69	1.25	0.94	0.36	0.12	0
1,2-Propadiene	0	0	0	0.13	0.28	0.61	0.69	0.35	0.12	0
Propyne	0	0	0	0.13	0.45	1.09	1.25	0.57	0.28	0
1,3-Butadiene	0	0	0	0.13	0.35	0.85	0.96	0.4	0.12	0.05
Vinylacetylene	0	0	0	0.52	1.4	2.72	2.86	0.96	0.27	0.1
Diacetylene	0	0	0	0.12	0.21	0.25	0.31	0.14	0.05	0
Benzene	0	0.02	0.25	2.98	6.11	11.03	10.64	4.14	1.22	0.37
Toluene	0	0	0.25	3.73	6.84	8.65	7.23	2.05	0.67	0.29
Phenylacetylene	0	0	0.2	0.33	0.79	1.5	1.23	0.51	0	0
Styrene	0	0.62	4.03	20.11	21.43	11.89	8.97	1.91	0.84	0.35
1-propenylbenzene	0.02	0.03	0.08	0.22	0.17	0.06	0.04	0.01	0	0
cyclopentadiene	0	0	0	0.77	1.61	3.08	2.76	1.05	0.36	0.14
methylcyclopentadiene	0	0	0	0.33	0.44	0.55	0.43	0.13	0	0
1,3-hexadiene	0	0	0	0.23	0.24	0.32	0.21	0.08	0.01	0
ethylbenzene	0	0	0.95	5.37	5.18	2.41	1.65	0.52	0	0
bibenzyl	0	0	1.51	2.18	0.82	0.31	0.3	0	0	0
Benzaldehyde	0	0.2	0.86	3.71	7.13	5.76	4.46	0.96	0	0
Benzofuran	0	0.16	0.78	1.04	1.15	1.24	1.04	0.75	0.06	0
Phenol	0	0.05	0.47	0.79	0.89	1.19	1.49	0.51	0.02	0
Indene	0	0.12	0.52	3.53	5.58	5.15	3.15	0.64	0.61	0
Naphthalene	0	0	0	0.03	0.18	0.23	0.32	0.16	0.13	0.12
2-Ethynyl-naphthalene	0	0	0	0.03	0.14	0.09	0.07	0.01	0	0
Diphenylmethane	0	0	0	0.04	0.08	0.1	0.11	0.01	0	0
Preshock Carbon	765.63	765.63	765.63	765.63	765.63	765.63	765.63	765.63	765.63	765.63
Postshock Carbon	773.62	763.8	792.89	772.53	735.97	727.55	706.54	707.04	708.73	713.45

Experimental data for n-propylbenzene oxidation, average P5 = 28 atm, $\Phi = 0.54$
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Shock No.	24	27	29	38	37	33
T5 /K	1406.7	1432.6	1450.2	1491.1	1527.9	1550.5
P5 /atm	26.89	25.69	23.9	26.59	29.5	28.22
Reaction Time /ms	1.76	1.67	1.7	1.57	1.44	1.4
n-Propylbenzene	0	0	0	0	0	0
O2	1075.4	1065.1	1030.5	993.44	1000.3	953.2
CO	178.86	140.49	124.67	70.83	48.12	51.19
CO2	536.5	570.7	595.91	656.57	684.43	698.08
Methane	0.32	0	0	0	0	0
Ethene	0.37	0.3	0.19	0	0	0
Ethane	0.12	0.05	0.07	0	0	0
Acetylene	0.54	0.4	0.13	0	0	0
Propane	0	0	0	0	0	0
1,2-Propadiene	0	0	0	0	0	0
Propyne	0	0	0	0	0	0
1,3-Butadiene	0	0	0	0	0	0
Vinylacetylene	0	0	0	0	0	0
Diacetylene	0	0	0	0	0	0
Benzene	0.06	0.04	0	0.1	0.04	0.03
Toluene	0	0	0	0	0	0
Phenylacetylene	0	0	0	0	0.04	0
Styrene	0.16	0	0	0	0	0
1-propenylbenzene	0	0	0	0	0	0
cyclopentadiene	0.06	0.04	0	0.1	0.05	0.07
methylcyclopentadiene	0	0	0	0	0	0
1,3-hexadiene	0	0	0	0	0	0
ethylbenzene	0	0	0	0	0	0
bibenzyl	0	0	0	0	0	0
Benzaldehyde	0	0	0	0	0	0
Benzofuran	0	0	0	0	0	0
Phenol	0	0	0	0	0	0
Indene	0	0	0	0	0	0
Naphthalene	0.05	0	0	0	0	0
2-Ethynyl-naphthalene	0	0	0	0	0	0
Diphenylmethane	0	0	0	0	0	0
Preshock Carbon	765.63	765.63	765.63	765.63	765.63	765.63
Postshock Carbon	720.12	713.16	721.33	728.52	733.37	749.81

Experimental data for n-propylbenzene oxidation, average P5 = 24 atm, $\Phi = 1.9$

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Shock No.	60	57	3	12	9	63	33	27	24	18	54
T5 /K	905.26	940.86	950.76	992.06	996.02	1028	1113.3	1159.6	1223.8	1310.1	1330.2
P5 /atm	18.96	21.84	28.66	23.12	28.21	17.53	27.59	27.52	25.63	23.86	21.39
Reaction Time /ms	1.63	1.71	1.68	1.8	1.77	2.93	1.74	1.91	1.8	1.66	1.75
n-Propylbenzene	88.34	89.08	89.29	87.02	87.39	87.51	52.78	31.73	6.37	1.13	0.73
O2	563.37	553.59	550.13	558.23	558.39	553.14	550.01	525.95	517.28	509.65	512.85
CO2	0	0	0	0	0	2.34	0	0	0	0	0
CO	0	0	0	0	0	0.99	3.09	9.34	16.41	30.95	34.7
Methane	0	0	0	0	0	0	1.46	2.13	2.96	5.29	6.54
Ethene	0	0	0	0.42	0	0.37	20.71	39.63	63.63	69.37	68.68
Ethane	0	0	0	0.09	0	0.08	1.18	1.54	1.75	2.94	3.2
Acetylene	0	0	0	0	0	0	0.84	1.95	5.79	11.84	16.8
Propane	0	0	0	0	0	0	1.04	1.49	1.34	1.13	1.09
1,2-Propadiene	0	0	0	0	0	0	0	0.18	0.18	0.45	0.52
Propyne	0	0	0	0	0	0	0	0.33	0.33	0.87	1.46
1,3-Butadiene	0	0	0	0	0	0	0.04	0.09	0.17	0.28	0.38
Benzene	0	0	0.03	0.08	0.11	0	2.14	4.41	7.89	11.13	13.11
Toluene	0.17	0.2	0.18	0.22	0.21	0.21	5	12.97	29.18	40.79	41.11
Ethylbenzene	0	0	0	0.16	0.18	0.15	5.37	8.44	8.61	3.22	1.55
Styrene	0	0	0.11	0.46	0.41	0.39	8.59	13.36	13.58	10.15	8.49
Cyclopentadiene	0	0	0	0	0	0	0.36	0.89	1.92	2.33	2.51
Methylcyclopentadiene	0	0	0	0	0	0	0.24	0.41	0.47	0.32	0.31
Benzaldehyde	0	0	0.03	0.08	0.09	0.00	1.08	1.95	2.49	2.29	1.85
Benzylalcohol	0	0	0	0	0	0.00	0.07	0.14	0.32	0.51	0.59
Bibenzyl	0	0	0	0	0	0.00	5.53	6.42	4.91	2.48	1.71
Vinyl Acetylene	0	0	0	0	0	0.00	0.19	0.46	0.95	1.19	1.45
Diacetylene	0	0	0	0	0	0.00	0	0	0	0.23	0.54
1,2-Butadiene	0	0	0	0	0	0.00	0.05	0.06	0.09	0.08	0.07
2-Butyne	0	0	0	0	0	0.00	0.01	0.02	0.03	0.05	0.05
Phenyl Acetylene	0	0	0	0	0	0.00	0	0.16	0.35	0.44	0.67
1-Propenylbenzene	0	0	0	0	0	0.00	0.08	0.11	0.09	0.06	0.04
2-Propenylbenzene	0	0	0	0	0	0.00	0.08	0.11	0.09	0.06	0.04
2-Ethynynaphthalene	0	0	0	0	0	0.00	0.11	0.26	0.5	0.62	0.48
Diphenylmethane	0	0	0	0	0	0.00	0.05	0.18	0.36	0.41	0.35
Phenol	0	0	0	0	0	0.00	0.1	0.24	0.26	0.21	0.12
Benzofuran	0	0	0.01	0.01	0.01	0.00	0.28	0.35	0.37	0.22	0.11
Indene	0	0	0	0	0	0.00	0.09	0.2	0.45	0.65	0.73
Naphthalene	0	0	0	0	0	0.00	0	0	0.25	0.16	0.5
Fluorene	0	0	0	0	0	0.00	0	0.03	0.07	0.24	0.32
Diphenylethylene	0	0	0	0	0	0.00	0.13	0.14	0.13	0.08	0.07
Stilbene	0	0	0	0	0	0.00	0.14	0.6	0.31	0.13	0.13
Anthracene	0	0	0	0	0	0.00	0.03	0.07	0.09	0.24	0.35
Preshock Carbon	803.64	803.64	803.64	803.64	803.64	803.64	803.64	803.64	803.64	803.64	803.64
Postshock Carbon	796.26	803.07	806.22	791.78	794	797.57	787.44	818.91	791.45	791.93	785.97

Experimental data for n-propylbenzene oxidation, average P5 = 24 atm, $\Phi = 1.9$

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Shock No.	51	15	42	45	39
T5 /K	1390	1434.6	1512.3	1582.1	1669.3
P5 /atm	21.34	24.34	25.61	24.75	28.59
Reaction Time /ms	1.67	1.7	1.56	1.36	1.51
n-Propylbenzene	0.53	0.5	0.41	0.33	0.3
O2	472.3	294.62	84.86	45.7	0
CO2	5.6	40.37	75.58	106.21	109.24
CO	88.21	291.95	538.2	629.79	656.09
Methane	12.84	17.79	11.01	5.28	1.88
Ethene	59.39	22.41	3.9	0.98	0.39
Ethane	2.66	1.6	0.54	0.18	0.06
Acetylene	59.55	125.4	83.9	44.42	19.58
Propane	0.55	0.33	0.26	0.1	0
1,2-Propadiene	1.35	0.93	0.33	0.14	0
Propyne	3.5	2.65	0.95	0.33	0
1,3-Butadiene	0.56	0.16	0.04	0.03	0
Benzene	18.61	8.01	0.99	0.24	0.19
Toluene	26.21	4.26	0.4	0.14	0.1
Ethylbenzene	0.92	0.19	0	0.03	0
Styrene	3.63	0.52	0.08	0.06	0.07
Cyclopentadiene	2.11	0.86	0	0	0
Methylcyclopentadiene	0.24	0.11	0	0	0
Benzaldehyde	0.9	0.17	0.02	0	0.09
Benzylalcohol	0.72	0.88	0	0	0
Bibenzyl	0.29	0.47	0	0	0
Vinyl Acetylene	2.27	0.78	0.19	0.06	0
Diacetylene	4.48	3.76	3.15	1.2	0.21
1,2-Butadiene	0.05	0.05	0.02	0.04	0
2-Butyne	0.1	0.11	0.03	0	0
Phenyl Acetylene	1.08	0.28	0	0	0
1-Propenylbenzene	0.02	0	0	0	0
2-Propenylbenzene	0.02	0	0	0	0
2-Ethynyl naphthalene	0	0	0	0	0
Diphenylmethane	0	0	0	0	0
Phenol	0.02	0	0	0	0
Benzofuran	0.04	0.01	0	0	0
Indene	0.88	0.37	0	0	0
Naphthalene	0.79	0.03	0	0	0
Fluorene	0.3	0.01	0	0	0
Diphenylethylene	0.02	0	0	0	0
Stilbene	0.03	0	0	0	0
Anthracene	0.25	0.05	0	0	0
Preshock Carbon	803.6	803.64	803.64	803.64	803.64
Postshock Carbon	791.6	793.21	833.1	845.67	813.78

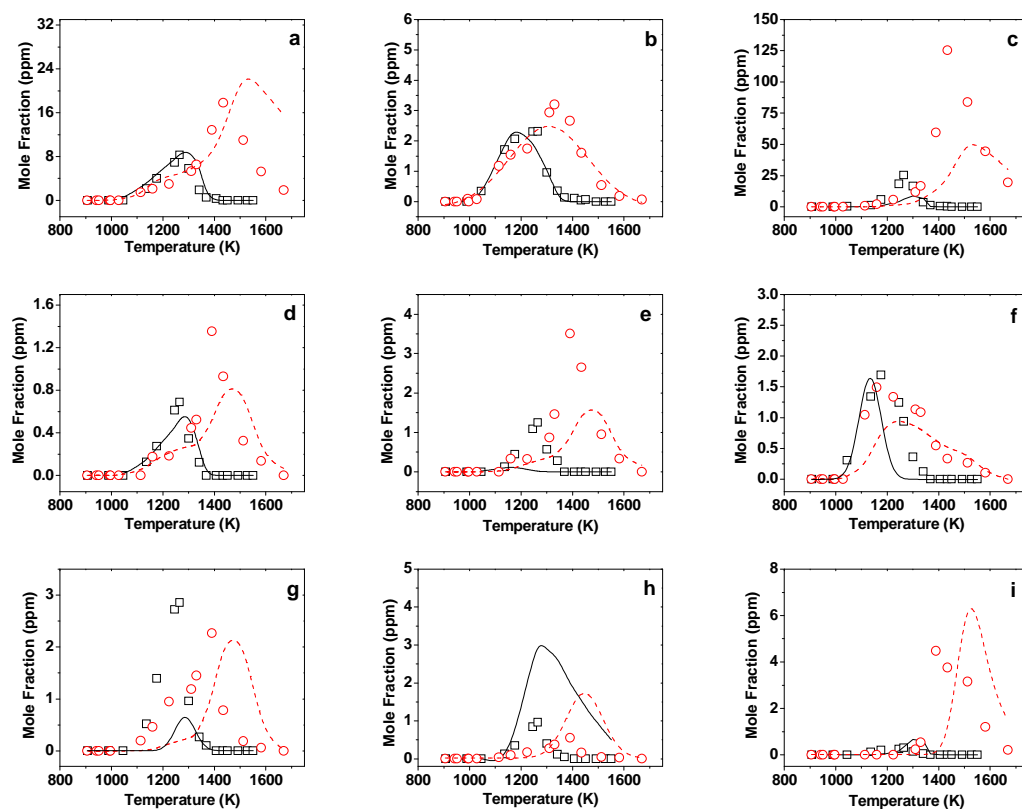


Figure 7. Comparison between experimental mole fraction profiles and model predictions of stable intermediates formed from n-propylbenzene oxidation experiments. $[\square, -]$ - average $P5 = 28$ atm, $\Phi = 0.54$, $[o, --]$ – average $P5 = 24$ atm, $\Phi = 1.9$, a) Methane b) Ethane c) Acetylene d) Allene e) Propyne, f) Propene g) Vinylacetylene h) 1,3-Butadiene i) Diacetylene

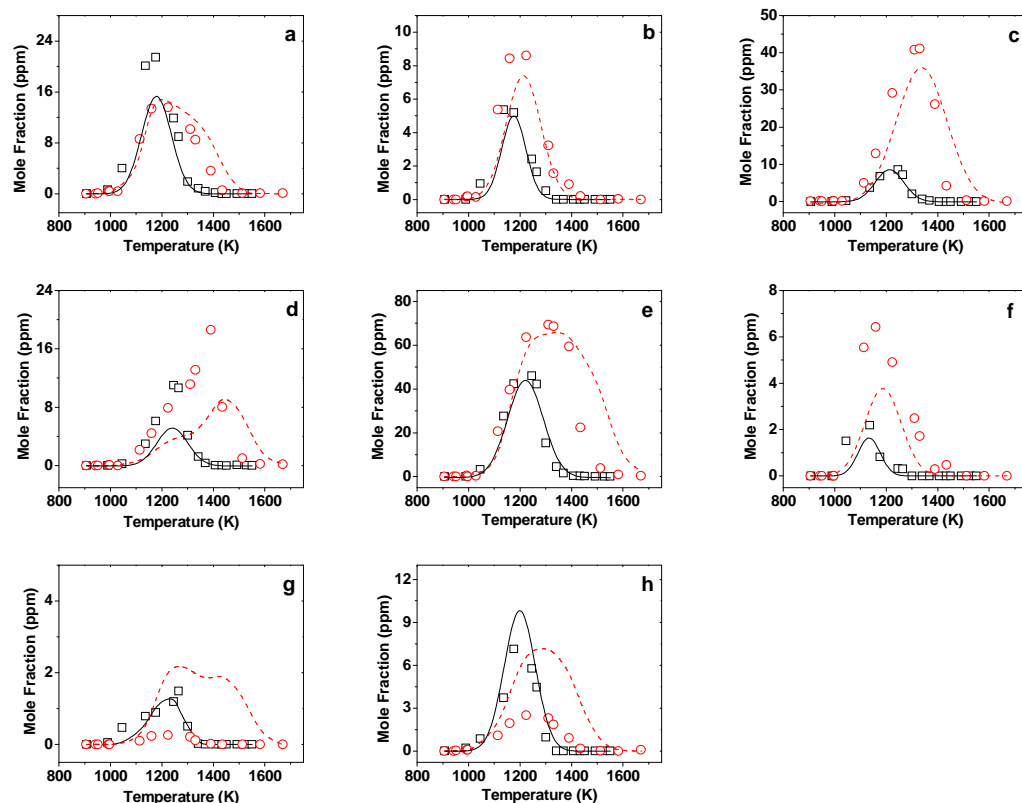


Figure 8. Comparison between experimental mole fraction profiles and model predictions [-] of stable intermediates formed from n-propylbenzene oxidation experiments. [□] - average P5 = 28 atm, $\Phi = 0.54$, [○] - average P5 = 24 atm, $\Phi = 1.9$, a) Styrene b) Ethylbenzene, c) Toluene d) Benzene e) Ethene f) Bibenzyl g) Phenol h) Benzaldehyde

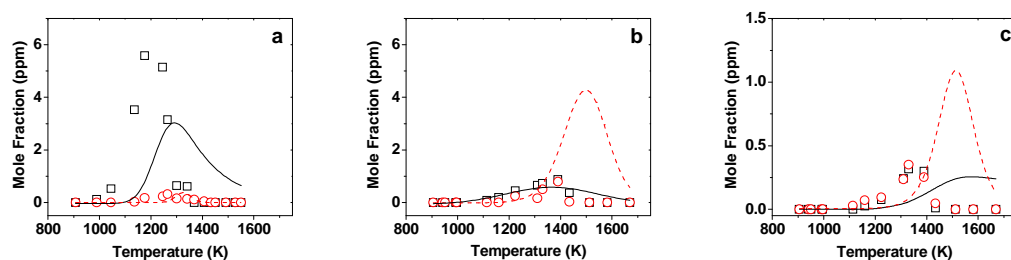


Figure 9. Comparison between experimental mole fraction profiles and model predictions [-] of stable intermediates formed from n-propylbenzene oxidation experiments. a) average P5 = 28 atm, $\Phi = 0.54$, [□] - Indene, [○] - Naphthalene, b) average P5 = 24 atm, $\Phi = 1.9$, [□] - Indene, [○] - Naphthalene, c) average P5 = 24 atm, $\Phi = 1.9$, [□] - Fluorene, [○] - Anthracene

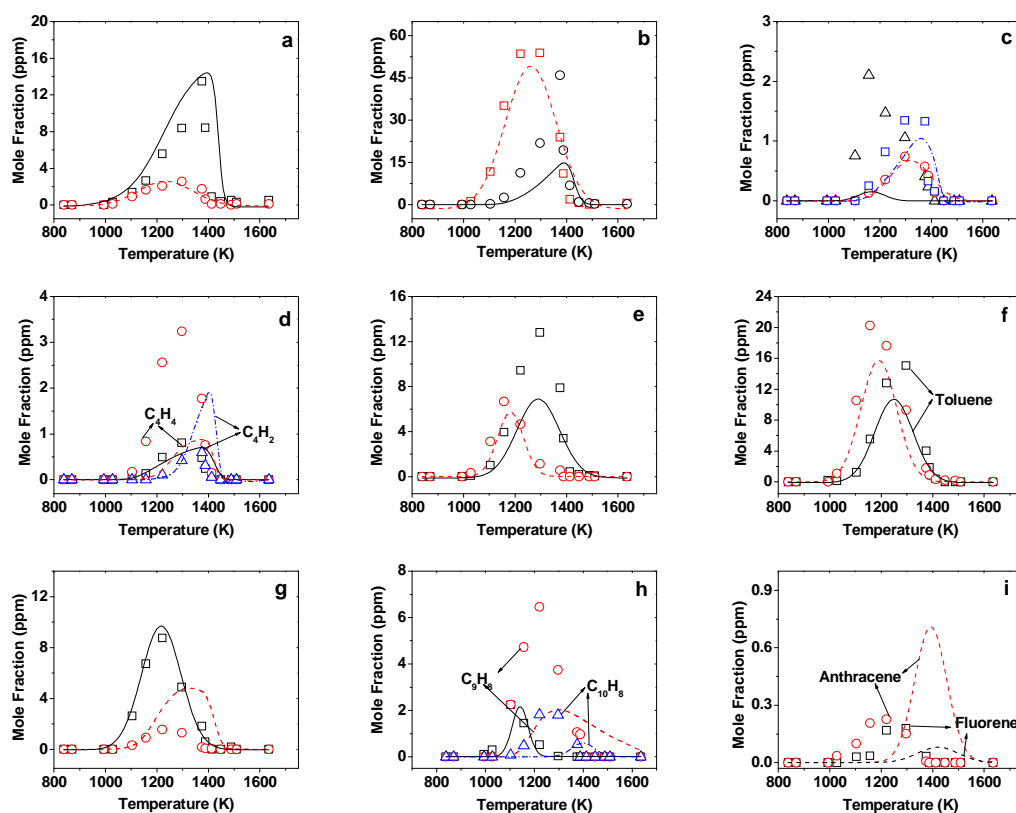


Figure 10. Comparison between experimental mole fraction profiles and model predictions [-] of stable intermediates formed from n-propylbenzene oxidation experiments, symbols - experiments, average $P5 = 49$ atm, $\Phi = 1.0$, a) \square - Methane, \circ - Ethane, b) \square - Ethene, \circ - Acetylene, c) Δ - Propene, \square - Propyne, \circ - Allene, d) Δ - Diacetylene, \square - 1,3-Butadiene, \circ - Vinylacetylene e) \square - Benzene, \circ - Ethylbenzene, f) \square - Toluene, \circ - Styrene, g) \square - Benzaldehyde, \circ - Phenol, h) \square - Bibenzyl, \circ - Indene, Δ - Naphthalene i) \square - Fluorene, \circ - Anthracene

n-Propylbenzene Pyrolysis Dataset

Experimental data for n-propylbenzene pyrolysis, average P5 = 54 atm, $\Phi = \infty$ (Page 1/3)

Shock	9	22	19	16	25	28	39
T5 (K)	1027.04	1052.16	1113.02	1137.13	1158.81	1173.3	1225.2
P5 (atm)	53.57	53.97	58.81	60.40	58.24	52.67	55.95
Reaction Time (s)	1.61E-03	1.70E-03	1.73E-03	2.07E-03	1.80E-03	1.89E-03	2.04E-03
n-Propylbenzene	83.00	81.84	67.11	37.43	26.15	19.91	3.02
Methane	0.00	0.51	0.97	1.61	1.90	2.01	2.65
Ethene	0.00	1.71	14.22	35.45	45.46	49.50	68.71
Ethane	0.00	0.22	0.71	0.93	1.01	1.11	1.26
Acetylene	0.00	0.07	0.25	0.51	0.64	0.92	1.77
Propane	0.00	0.10	0.59	0.92	1.07	1.12	1.19
1,2-Propadiene	0.00	0.00	0.00	0.00	0.00	0.00	0.16
Propyne	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1,3-Butadiene	0.00	0.00	0.00	0.00	0.04	0.04	0.08
Vinylacetylene	0.00	0.00	0.00	0.00	0.00	0.03	0.05
Diacetylene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Benzene	0.06	0.19	1.28	2.63	3.18	3.45	4.17
Toluene	0.05	0.25	2.74	9.47	13.46	15.87	26.98
Phenylacetylene	0.00	0.00	0.00	0.00	0.00	0.00	0.63
Styrene	0.00	1.38	7.03	13.84	15.07	15.58	15.65
Ethylbenzene	0.22	0.79	4.89	8.71	9.67	9.94	8.78
Triacetylene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Bibenzyl	0.00	0.00	3.86	8.41	8.90	9.84	9.38
Biphenylmethane	0.00	0.00	0.23	0.77	1.01	1.19	1.65
Indene	0.00	0.00	0.00	0.00	0.00	0.00	0.08
Naphthalene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1-Methylnaphthalene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1-ethynyl-naphthalene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Fluorene	0.00	0.00	0.00	0.00	0.00	0.05	0.31
2-Methylfluorene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1-Methylfluorene	0.00	0.00	0.00	0.00	0.00	0.00	0.07
Methylfluorenes	0.00	0.00	0.00	0.00	0.00	0.00	0.07
Phenanthrene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Anthracene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Phenanthrene+anthracene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Diphenylethyne	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2-Methylantracene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2-Phenylnaphthalene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
m-Terphenyl	0.00	0.00	0.00	0.00	0.00	0.00	0.00
p-Terphenyl	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Acenaphthylene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cyclopentadiene	0.00	0.02	0.02	0.03	0.04	0.00	0.11
Preshock Carbon	756.45	756.45	756.45	756.45	756.45	756.45	756.45
Postshock Carbon	749.43	761.62	816.31	804.71	782.95	776.45	744.78

Experimental data for n-propylbenzene pyrolysis, average P5 = 54 atm, $\Phi = \infty$ (Page 2/3)

Shock	31	36	42	54	57	51	63
T5 (K)	1256.24	1272.81	1326.57	1375.47	1407.19	1413.52	1429.03
P5 (atm)	56.32	57.73	56.62	52.16	56.47	56.03	51.29
Reaction Time (s)	1.89E-03	1.85E-03	1.87E-03	1.92E-03	1.59E-03	1.53E-03	1.38E-03
n-Propylbenzene	1.32	1.13	0.31	0.35	0.41	0.35	0.40
Methane	3.21	3.75	6.24	8.73	17.85	19.38	20.96
Ethene	71.71	73.08	71.99	70.66	59.30	55.43	48.84
Ethane	1.43	1.57	1.99	1.65	0.74	0.58	0.38
Acetylene	2.65	2.52	5.27	8.72	42.65	52.58	75.19
Propane	1.30	1.46	1.12	1.02	0.41	0.44	0.22
1,2-Propadiene	0.16	0.20	0.24	0.55	0.97	0.97	0.98
Propyne	0.16	0.24	0.48	0.99	2.60	2.40	2.62
1,3-Butadiene	0.06	0.06	0.13	0.21	0.26	0.23	0.17
Vinylacetylene	0.00	0.04	0.11	0.21	0.62	0.62	0.56
Diacetylene	0.00	0.00	0.31	1.19	9.19	12.06	18.17
Benzene	4.17	4.27	5.18	6.43	11.93	12.38	12.11
Toluene	30.15	31.58	34.98	33.58	14.73	11.34	6.38
Phenylacetylene	0.64	0.88	1.48	1.71	3.65	4.27	3.78
Styrene	15.26	14.86	12.59	10.32	5.76	2.90	2.55
Ethylbenzene	6.95	5.83	2.53	0.36	0.48	0.42	0.20
Triacetylene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Bibenzyl	7.80	7.44	2.39	0.47	0.68	0.60	0.24
Biphenylmethane	1.51	1.58	1.21	0.57	0.10	0.10	0.04
Indene	0.22	0.39	0.45	0.70	0.77	0.80	0.64
Naphthalene	0.00	0.00	0.14	0.31	1.50	1.34	1.19
1-Methylnaphthalene	0.00	0.00	0.04	0.15	0.12	0.10	0.06
1-Ethynyl-naphthalene	0.00	0.00	0.07	0.23	0.32	0.25	0.22
Fluorene	0.35	0.50	0.95	0.96	0.80	0.70	0.41
2-Methylfluorene	0.00	0.00	0.00	0.03	0.05	0.05	0.06
1-Methylfluorene	0.11	0.13	0.18	0.19	0.15	0.14	0.14
Methylfluorenes	0.11	0.13	0.18	0.22	0.20	0.20	0.20
Phenanthrene	0.00	0.00	0.12	0.26	1.01	0.64	0.54
Anthracene	0.00	0.00	0.15	0.63	0.97	0.73	0.52
Phenanthrene+anthracene	0.00	0.00	0.27	0.88	1.98	1.37	1.07
Diphenylethyne	0.00	0.00	0.06	0.10	0.25	0.14	0.09
2-Methylantracene	0.00	0.00	0.00	0.04	0.06	0.12	0.11
2-Phenylnaphthalene	0.00	0.00	0.00	0.06	0.34	0.39	0.43
m-Terphenyl	0.00	0.00	0.00	0.05	0.07	0.33	0.13
p-Terphenyl	0.00	0.00	0.00	0.04	0.13	0.19	0.21
Acenaphthylene	0.00	0.00	0.21	0.30	0.78	0.96	1.03
Cyclopentadiene	0.12	0.14	0.23	0.24	0.24	0.22	0.20
Preshock Carbon	756.45	756.45	756.45	756.45	756.45	756.45	756.45
Postshock Carbon	721.56	722.16	650.05	612.94	612.17	586.68	583.53

Experimental data for n-propylbenzene pyrolysis, average P5 = 54 atm, $\Phi = \infty$ (Page 3/3)

Shock	60	66	72	69	78
T5 (K)	1464.20	1485.27	1523.49	1567.61	1678.05
P5 (atm)	52.53	51.14	48.94	49.20	49.58645
Reaction Time (s)	1.47E-03	1.39E-03	1.33E-03	1.32E-03	1.19E-03
n-Propylbenzene	0.00	0.00	0.00	0.00	0.00
Methane	18.20	11.17	5.39	1.74	1.20
Ethene	18.32	6.66	2.32	1.27	2.01
Ethane	0.16	0.13	0.10	0.07	0.15
Acetylene	170.31	206.17	238.15	239.33	243.60
Propane	0.07	0.10	0.09	0.09	0.15
1,2-Propadiene	0.53	0.41	0.19	0.25	0.14
Propyne	1.18	0.85	0.63	0.41	0.22
1,3-Butadiene	0.05	0.04	0.05	0.05	0.05
Vinylacetylene	0.28	0.00	0.00	0.00	0.00
Diacetylene	37.16	44.52	51.81	57.60	59.86
Benzene	5.48	1.84	0.49	0.16	0.17
Toluene	0.69	0.22	0.10	0.04	0.17
Phenylacetylene	2.08	0.76	0.19	0.19	0.00
Styrene	0.40	0.20	0.13	0.10	0.21
Ethylbenzene	0.00	0.00	0.00	0.00	0.00
Triacetylene	0.90	2.64	6.79	8.82	12.78
Bibenzyl	0.16	0.15	0.00	0.00	0.00
Biphenylmethane	0.00	0.00	0.00	0.00	0.00
Indene	0.36	0.13	0.00	0.00	0.00
Naphthalene	0.51	0.19	0.00	0.00	0.00
1-Methylnaphthalene	0.04	0.00	0.00	0.00	0.00
1-ethynyl-naphthalene	0.05	0.00	0.00	0.00	0.00
Fluorene	0.02	0.04	0.00	0.00	0.00
2-Methylfluorene	0.07	0.05	0.02	0.00	0.00
1-Methylfluorene	0.07	0.05	0.00	0.00	0.00
Methylfluorenes	0.15	0.10	0.02	0.00	0.00
Phenanthrene	0.08	0.01	0.00	0.00	0.00
Anthracene	0.06	0.03	0.00	0.00	0.00
Phenanthrene+anthracene	0.14	0.04	0.00	0.00	0.00
Diphenylethyne	0.04	0.01	0.00	0.00	0.00
2-Methylantracene	0.10	0.09	0.04	0.01	0.00
2-Phenylnaphthalene	0.23	0.07	0.00	0.00	0.00
m-Terphenyl	0.19	0.05	0.00	0.00	0.00
p-Terphenyl	0.19	0.14	0.01	0.00	0.00
Acenaphthylene	0.85	0.23	0.01	0.00	0.00
Cyclopentadiene	0.15	0.06	0.00	0.00	0.00
Preshock Carbon	756.45	756.45	756.45	756.45	756.45
Postshock Carbon	640.62	666.90	743.84	771.05	814.47

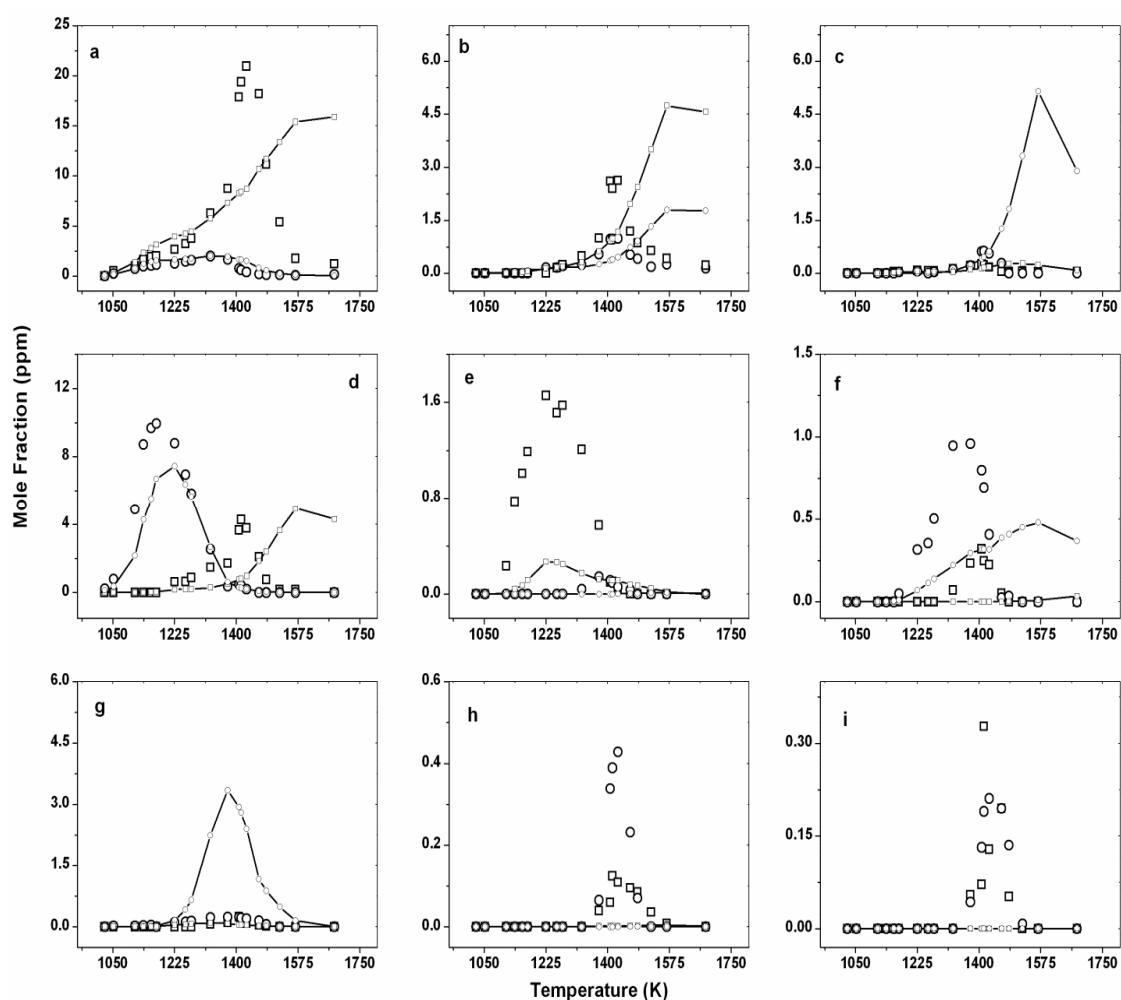


Figure 11. Experimental and modeling profiles of the minor intermediates of the n-propylbenzene pyrolysis experiments, average P5 = 50 atm, [□]-Experimental data, [-□]-Modeling Results (Mod2) (a) [□] – Methane, [○]-Ethene, (b) [□] – Allene, [○]- Propyne, (c) [□] –1,3-Butadiene, [○]-Vinylacetylene, (d) [□] – Phenylacetylene, [○]-Ethylbenzene, (e) [□] –Biphenylmethane, [○]- Methylanthracene, (f) [□] – Ethynynaphthalene, [○]-Fluorene, (g) [□] –1,3-Cyclopentadiene, [○]-Diphenylethyne, (h) [□] – Methylantracene, [○]- Phenylanthracene, (i) [□] –m-terphenyl, [○]-p-terphenyl

m-Xylene Oxidation Datasets

Experimental data for m-xylene oxidation, $\Phi = 0.53$, average P5 = 53 bar (Page 1/2)

Shock No.	2	4	6	10	19	52	21	12	25
T5/K	1056.38	1138.31	1201.88	1265.68	1298.82	1314.95	1331.29	1384.78	1411.27
P5/bar	51.61	54.77	57.03	52.65	49.91	50.08	49.3	57.87	52.71
Rxn Time/s	1.64E-03	1.76E-03	1.90E-03	1.90E-03	1.90E-03	1.97E-03	1.87E-03	1.75E-03	1.61E-03
m-C ₈ H ₁₀	87.96	82.18	81.17	64.25	42.25	38.11	33.72	3.67	2.22
O ₂	1666.41	1614.89	1585.6	1591.41	1602.71	1583.86	1606.06	1143.81	1074.53
CO	0	0	0	9.42	33.38	43.15	57.76	315.93	197.44
CO ₂	0	0	0	0	0	0	0	274.6	425.87
CH ₄	0	0	0.38	1.41	3.31	4.47	5.36	1.14	0.38
C ₂ H ₄	0	0	0	0.27	1.13	1.96	2.32	0.42	0.22
C ₂ H ₆	0	0	0	0.53	0.95	1.31	1.52	0.28	0.19
C ₂ H ₂	0	0	0	0.36	1.66	2.59	5.7	1.43	0.51
1,2-Propadiene	0	0	0	0.11	0.36	0.47	0.47	0.1	0
Propyne	0	0	0	0.33	0.65	0.81	1.12	0.28	0
1,3-Butadiene	0	0	0	0.08	0.27	0.34	0.36	0.06	0
Vinylacetylene	0	0	0	0	0.6	0.76	1.25	0.2	0
Benzene	0	0	0.1	1.53	4.72	5.82	6.88	0.74	0.22
Toluene	0	0	0.22	2.25	4.6	3.52	5.66	0.38	0.17
Phenylacetylene	0	0	0.35	0.72	1.02	1.31	1.3	0.3	0.09
Styrene	0	0	0	0.41	1.44	2.11	2.55	0.37	0.13
p-Xylene	0.11	0.09	0.1	0.16	0.26	0.23	0.27	0.05	0
m-Ethylmethylbenzene	0	0	0.14	1.33	1.41	1.3	1.2	0	0
1,3-Cyclopentadiene	0	0	0.03	0.43	1.22	1.56	1.94	0.27	0.14
5-Methylcyclopentadiene	0	0	0.03	0.13	0.26	0.33	0.29	0.03	0
1,3-Hexadiene	0	0	0.04	0.59	0.88	0.98	0.85	0.05	0.03
1,3,5-Cycloheptatriene	0	0	0.07	0.21	0.29	0.22	0.2	0.05	0
Benzaldehyde	0	0	0	0.24	0.37	0.45	0.52	0.29	0.05
m-Methylstyrene	0	0	0	0.14	0.28	0.42	0.52	0.21	0
Ethylbenzene	0	0	0	0.09	0.23	0.25	0.24	0.05	0
Preshock Carbon	657.44	657.44	657.44	657.44	657.44	657.44	657.44	657.44	657.44
Postshock Carbon	704.57	658.16	687.84	672.9	619.79	621.05	633.52	678.03	658.2

Experimental data for m-xylene oxidation, $\Phi = 0.53$, average P5 = 53 bar (Page 2/2)

Shock No.	23	43	45	37	35	33
T5/K	1425.98	1469.00	1480.82	1495.54	1506.75	1569.05
P5/bar	54.50	52.50	55.96	52.44	49.05	52.64
Rxn Time/s	1.60E-03	1.50E-03	1.42E-03	1.35E-03	1.42E-03	1.28E-03
m-C ₈ H ₁₀	1.48	0.83	0.82	0.51	0.90	0.27
O ₂	989.66	906.46	878.35	885.25	872.76	957.65
CO	122.32	62.24	29.23	36.54	25.89	17.07
CO ₂	511.45	587.99	613.46	610.00	619.61	659.87
CH ₄	0.30	0.00	0.00	0.00	0.00	0.00
C ₂ H ₄	0.13	0.00	0.03	0.00	0.00	0.00
C ₂ H ₆	0.11	0.00	0.00	0.00	0.00	0.00
C ₂ H ₂	0.34	0.00	0.50	0.00	0.00	0.00
1,2-Propadiene	0.00	0.00	0.00	0.00	0.00	0.00
Propyne	0.00	0.00	0.00	0.00	0.00	0.00
1,3-Butadiene	0.00	0.00	0.00	0.00	0.00	0.00
Vinylacetylene	0.00	0.00	0.00	0.00	0.00	0.00
Benzene	0.20	0.04	0.10	0.00	0.00	0.00
Toluene	0.10	0.00	0.00	0.00	0.00	0.00
Phenylacetylene	0.00	0.00	0.00	0.00	0.00	0.00
Styrene	0.00	0.00	0.00	0.00	0.00	0.00
p-Xylene	0.00	0.00	0.00	0.00	0.00	0.00
m-Ethylmethylbenzene	0.00	0.00	0.00	0.00	0.00	0.00
1,3-Cyclopentadiene	0.15	0.11	0.16	0.16	0.12	0.18
5-Methylcyclopentadiene	0.00	0.00	0.00	0.00	0.00	0.00
1,3-Hexadiene	0.00	0.00	0.00	0.00	0.00	0.00
1,3,5-Cycloheptatriene	0.00	0.00	0.00	0.00	0.00	0.00
Benzaldehyde	0.00	0.00	0.00	0.00	0.00	0.00
m-Methylstyrene	0.00	0.00	0.00	0.00	0.00	0.00
Ethylbenzene	0.00	0.00	0.00	0.00	0.00	0.00
Preshock Carbon	657.44	657.44	657.44	657.44	657.44	657.44
Postshock Carbon	657.38	657.63	651.70	651.42	653.33	679.96

Experimental data for m-xylene oxidation, $\Phi = 1.19$, average P5 = 51 bar (Page 1/2)

Shock No.	2	6	8	10	18	44	14	30	42
T5/K	1079.77	1112.17	1188.55	1256.38	1326.58	1352.24	1375.95	1400.25	1431.93
P5/bar	50.58	49.23	48.41	49.29	52.74	59.63	52.65	48.72	53.17
Rxn Time/s	1.84E-03	1.81E-03	2.00E-03	2.10E-03	1.80E-03	1.80E-03	1.92E-03	1.67E-03	1.63E-03
m-C ₈ H ₁₀	61.51	60.43	59.68	52.24	31.44	19.93	14.99	9.36	1.05
O ₂	540.91	540.2	539.13	536.69	509.96	507.47	512.16	211.17	132.67
CO	0	0	2.1	2.67	19.68	3.44	58.01	217.37	208.4
CO ₂	0	0	0	0.77	4.09	7.74	9.1	119.37	221.89
CH ₄	0	0	0	0.79	3.44	5.69	6.72	3.27	0.85
C ₂ H ₄	0	0	0	0	1.05	2.47	3.02	1.15	0.37
C ₂ H ₆	0	0	0	0	1.12	1.54	1.51	0.33	0.14
C ₂ H ₂	0	0	0	0	3.58	7.56	13.25	8.18	1.79
1,2-Propadiene	0	0	0	0	0.28	0.55	0.57	0.19	0
Propyne	0	0	0	0	0.66	0.95	1.17	0.31	0
1,3-Butadiene	0	0	0	0	0.13	0.25	0.28	0.08	0.27
Vinylacetylene	0	0	0	0	0.44	0.82	1.11	0.89	0.28
Diacetylene	0	0	0	0	0.26	0.58	0.97	0.42	0.17
Benzene	0	0	0.06	0.21	2.85	5.31	5.71	1.3	0.28
Toluene	0.02	0.05	0.13	0.47	3.25	4.97	4.21	0.7	0.19
Styrene	0	0	0	0.13	2.48	3.19	3.55	0.63	0.25
Triacetylene	0	0	0	0.16	0.61	0.62	0.36	0	0
Phenylacetylene	0	0	0	0.1	0.23	0.66	0.58	0.1	0
p-Xylene	0.06	0.06	0.07	0.1	0.21	0.21	0.18	0.03	0
m-Ethylmethylbenzene	0	0	0	0.35	0.4	0.32	0.27	0.12	0
3-Methylbenzaldehyde	0	0	0	0	0.33	0.45	0.46	0.87	0.22
1,3-Cyclopentadiene	0	0	0.04	0.09	0.64	1	1.06	1.05	0.18
5-Methylcyclopentadiene	0	0	0	0.04	0.1	0.13	0.12	0.11	0.05
1,3-Hexadiene	0	0	0.03	0.11	0.32	0.37	0.3	0.21	0
1,3,5-Cycloheptatriene	0	0	0	0.01	0.07	0.04	0.06	0.04	0
Ethylbenzene	0	0	0	0	0.09	0.16	0.14	0	0
Preshock Carbon	492.07	492.07	492.07	492.07	492.07	492.07	492.07	492.07	492.07
Postshock Carbon	497.49	495.18	513.42	510.6	507.68	486.67	470.73	505.25	466.31

Experimental data for m-xylene oxidation, $\Phi = 1.19$, average P5 = 51 bar (Page 2/2)

Shock No.	34	32	40
T5/K	1441.2	1472.99	1514.23
P5/bar	47.85	51.26	51.67
Rxn Time/s	1.60E-03	1.56E-03	1.35E-03
m-C₈H₁₀	0.52	0.49	0.32
O₂	127.25	83.68	45.19
CO	202.55	139.03	126.6
CO₂	232.1	302.54	329.78
CH₄	0.59	0.34	0.26
C₂H₄	0.25	0	0
C₂H₆	0.07	0	0
C₂H₂	1.53	0.57	0.42
1,2-Propadiene	0	0	0
Propyne	0	0	0
1,3-Butadiene	0	0	0
Vinylacetylene	0	0	0
Diacetylene	0.1	0.05	0
Benzene	0.17	0.08	0.07
Toluene	0	0	0
Styrene	0.15	0	0
Triacetylene	0	0	0
Phenylacetylene	0	0	0
p-Xylene	0	0	0
m-Ethylmethylbenzene	0	0	0
3-Methylbenzaldehyde	0.11	0	0
1,3-Cyclopentadiene	0.07	0	0
4-Methylcyclopentadiene	0	0	0
1,3-Hexadiene	0	0	0
1,3,5-Cycloheptatriene	0	0	0
Ethylbenzene	0	0	0
Preshock Carbon	492.07	492.07	492.07
Postshock Carbon	451.55	451.29	460.45

Experimental data for m-xylene oxidation, $\Phi = 2.35$, average P5 = 50 bar, (Page 1/2)

Shock No.	6	8	16	12	25	14	20	31	47
T5/K	1130.51	1159.93	1205.49	1231.8	1261.47	1290.08	1335.53	1375.11	1385.69
P5/bar	56.72	51.57	50.42	51.65	47.92	56.01	58.73	44.5	47.78
Rxn Time/s	1.69E-03	1.92E-03	1.90E-03	1.88E-03	1.91E-03	1.89E-03	1.81E-03	1.84E-03	1.72E-03
m-C8H10	92.82	92.21	92.03	91.52	84.25	71.25	54.07	40.49	15.11
O ₂	414.15	412.8	409.86	406.82	394.41	389.38	386.45	378.92	339.83
CO	0	0	0	0	0	1.43	16.76	36.08	73.81
CO ₂	0	0	1.65	0	0	0	3.25	4	7.41
CH ₄	0	0	0.37	0.38	1.48	1.43	3.31	8.67	17.48
C ₂ H ₄	0	0	0	0	0.31	0.37	1.47	3.25	7.34
C ₂ H ₆	0	0	0	0	0.05	0.25	1.49	2.41	1.94
C ₂ H ₂	0	0	0	0	0.36	0.37	4.02	8.9	36.2
1,2-Propadiene	0	0	0	0	0.08	0.08	0.35	0.55	1.08
Propyne	0	0	0	0	0.12	0.2	0.79	1.2	2.67
1,3-Butadiene	0	0	0	0	0.08	0.04	0.18	0.28	0.44
Vinylacetylene	0	0	0	0	0.05	0	0.5	0.82	1.82
Diacetylene	0	0	0	0	0	0	0.34	0.83	3.98
Benzene	0	0	0.07	0	0.44	0.55	3.55	5.88	9.91
Toluene	0	0	0.22	0.28	1.09	1.36	5.25	7.12	6.5
Styrene	0	0	0	0	0	0.47	3.86	6.08	6.42
Triacetylene	0	0	0	0	0	0	0.61	0.49	0.17
Phenylacetylene	0	0	0	0	0	0	0.32	0.63	1.56
p-Xylene	0.14	0.13	0.12	0.17	0.22	0.24	0.49	0.56	0.25
m-Ethylmethylbenzene	0	0	0.13	0.17	0.62	0.72	0.96	0.72	0.26
1,3-Cyclopentadiene	0	0	0.04	0.07	0.12	0.16	0.72	1	1.02
5-Methylcyclopentadiene	0	0	0	0.02	0.16	0.15	0.11	0.11	0.1
1,3-Hexadiene	0	0	0	0.03	0.43	0.5	0.36	0.3	0.26
1,3,5-Cycloheptatriene	0	0	0	0.02	0.04	0.05	0.05	0.03	0.02
Ethylbenzene	0	0	0	0	0	0.03	0.21	0.26	0.19
Preshock Carbon	742.56	742.56	742.56	742.56	742.56	742.56	742.56	742.56	742.56
Postshock Carbon	744.65	747.01	763.6	767.63	758.95	691.15	748.19	716.14	656.93

Experimental data for m-xylene oxidation, $\Phi = 2.35$, average P5 = 50 bar, (Page 2/2)

Shock No.	35	41	33	45	43
T5/K	1450.86	1473.59	1489.04	1522.39	1583.26
P5/bar	44.64	46.14	47.97	45.86	50.68
Rxn Time/s	1.52E-03	1.42E-03	1.44E-03	1.47E-03	1.38E-03
m-C ₈ H ₁₀	1.45	1.75	0.85	0.76	0.56
O ₂	209.24	87.09	63.73	32.05	0
CO	309.23	435.71	451.06	505.86	543.65
CO ₂	37.2	57.21	62.19	74.93	79.07
CH ₄	17.42	11.44	9.94	5.14	2.85
C ₂ H ₄	4.69	1.76	1.4	0.54	0.4
C ₂ H ₆	0.75	0.23	0.25	0	0
C ₂ H ₂	80.57	72.09	58.46	42.67	31.86
1,2-Propadiene	0.72	0.47	0.39	0.23	16.82
Propyne	1.58	1.08	0.77	0.41	0.25
1,3-Butadiene	0.12	0.71	0.06	0.08	0.16
Vinylacetylene	0.57	0.24	0.13	0.07	0.04
Diacetylene	6.46	4.82	3.01	1.41	0.52
Benzene	2.63	0.53	0.36	0.08	0
Toluene	0.58	0.11	0.12	0	0
Styrene	0.7	0.27	0.14	0	0
Triacetylene	0	0	0	0	0
Phenylacetylene	0	0	0	0	0
p-Xylene	0	0	0	0	0
m-Ethylmethylbenzene	0	0	0	0	0
1,3-Cyclopentadiene	0.38	0	0	0	0
5-Methylcyclopentadiene	0.03	0	0	0	0
1,3-Hexadiene	0.04	0	0	0	0
1,3,5-Cycloheptatriene	0	0	0	0	0
Ethylbenzene	0	0	0	0	0
Preshock Carbon	742.56	742.56	742.56	742.56	742.56
Postshock Carbon	644.14	710.11	672.71	688.98	748.67

Experimental data for m-xylene oxidation, $\Phi = 0.55$, average P5 = 27 bar (Page 1/2)

Shock No.	6	8	10	12	22	24	16	14	28
T5/K	1024.86	1054.33	1127.17	1172.89	1233.61	1274.04	1326.59	1342.84	1378.26
P5/bar	28.55	27.36	27.18	25.84	25.84	27.41	28.54	27.69	26.05
Rxn Time/s	1.73E-03	1.81E-03	1.90E-03	1.90E-03	1.91E-03	2.01E-03	1.96E-03	1.86E-03	1.83E-03
m-C8H10	102.29	100.58	99.43	92.05	100.4	81.07	47.99	22.32	16.54
O ₂	89.45	90.07	90.8	87.81	83.2	70.42	42.87	19.93	13.17
CO	1733.72	1711.05	1726.07	1689	1702.98	1706.97	1653.19	1671.21	1560.74
CO ₂	0	0	0	0	0	6.29	38.71	132.43	218.16
CH ₄	6.27	1.85	2.09	2.51	2.84	3.59	8.53	24.07	63.01
C ₂ H ₄	0	0	0	0	0	1.19	2.85	7.07	7.24
C ₂ H ₆	0	0	0	0	0.16	0.42	1.42	4.29	3.72
C ₂ H ₂	0	0	0	0	0.13	0.47	1.53	1.97	1.5
Acetylene	0	0	0	0	0	0.35	2.81	11.13	16.09
1,2-Propadiene	0	0	0	0	0	0.05	0.39	0.71	0.57
Propyne	0	0	0	0	0	0.35	0.88	1.33	1.53
1,3-Butadiene	0	0	0	0	0.02	0.06	0.25	0.54	0.46
Vinylacetylene	0	0	0	0	0	0.12	0.68	1.48	2
Diacetylene	0	0	0	0	0	0	0.11	0.2	0.57
Benzene	0	0	0	0.06	0.13	1.23	5	9.31	7.33
Toluene	0	0	0	0.15	0.33	2.02	5.18	6.09	4.45
Phenylacetylene	0	0	0	0	0.57	1	1.66	1.47	1.73
Styrene	0	0	0	0	0.11	0.66	2.68	3.33	3.1
Triacetylene	0	0	0	0	0	0.58	0.75	0.46	0.26
p-Xylene	0.06	0.07	0.07	0.09	0.09	0.18	0.27	0.19	0.1
Benzaldehyde	0	0	0	0	0.09	0.19	0.77	1.32	0
4-methylbenzaldehyde	0	0	0	0	0.75	3.4	5.05	5.42	4.58
m-Ethylmethylbenzene	0	0	0	0.13	0.21	0.79	0.98	1.37	0.4
1,3-Cyclopentadiene	0	0	0	0.02	0.1	0.32	1.06	1.99	1.89
5-Methylcyclopentadiene	0	0	0	0.03	0.06	0.11	0.17	0.24	0.33
1,3-Hexadiene	0	0	0	0.05	0.1	0.38	0.61	0.48	0.41
1,3,5-Cycloheptatriene	0	0	0	0.02	0.04	0.1	0.1	0.05	0.04
Ethylbenzene	0	0	0	0	0.01	0.07	0.22	0.23	0.15
Preshock Carbon	727.04	727.04	727.04	727.04	727.04	727.04	727.04	727.04	727.04
Postshock Carbon	722.3	723	729.06	740.2	768.87	767.5	700.02	682.74	671.27

Experimental data for m-xylene oxidation, $\Phi = 0.55$, average P5 = 27 bar (Page 2/2)

Shock No.	46	31	34	37	40
T5/K	1411.79	1447.94	1470.19	1484.23	1560.72
P5/bar	26.4	30.24	28.01	27.32	28.12
Rxn Time/s	1.65E-03	1.57E-03	1.52E-03	1.56E-03	1.37E-03
m-C8H10	4.48	1.36	1.51	1.41	0.78
O ₂	2.75	0.25	0.54	0.56	0
CO	1189.41	999.75	1021.97	1023.43	996.13
CO ₂	284.65	115.98	113.66	101.99	69.47
CH ₄	318.85	534.3	552.03	568.64	649.14
C ₂ H ₄	0.93	0	0	0	0
C ₂ H ₆	0.45	0	0	0	0
C ₂ H ₂	0.23	0	0	0	0
Acetylene	2.52	0	0	0	0
1,2-Propadiene	0	0	0	0	0
Propyne	0	0	0	0	0
1,3-Butadiene	0	0	0	0	0
Vinylacetylene	0	0	0	0	0
Diacetylene	0.06	0	0	0	0
Benzene	0.85	0.09	0.1	0.16	0.11
Toluene	0.44	0	0	0	0
Phenylacetylene	0.47	0	0	0	0
Styrene	0.63	0.12	0.1	0.08	0
Triacetylene	0	0	0	0	0
p-Xylene	0	0	0	0	0
Benzaldehyde	0.38	0.21	0	0	0
4-methylbenzaldehyde	0	0	0	0	0
m-Ethylmethylbenzene	0	0	0	0	0
1,3-Cyclopentadiene	0.3	0.13	0	0	0
1-Methylcyclopentadiene	0	0	0	0	0
1,3-Hexadiene	0	0	0	0	0
1,3,5-Cycloheptatriene	0	0	0	0	0
Ethylbenzene	0	0	0	0	0
Preshock Carbon	727.04	727.04	727.04	727.04	727.04
Postshock Carbon	659.44	659.64	672.36	676.7	719.29

Experimental data for m-xylene oxidation, $\Phi = 2.15$, average P5 = 28 bar (Page 1/2)

Shock No.	5	3	10	12	34	18	14	20	32
T5/K	898.18	1051.97	1167.95	1237.34	1346.39	1375.72	1396.9	1416.21	1440.1
P5/bar	23.7	28.71	27.53	25.61	28.58	28.32	29.19	27.57	26.78
Rxn Time/s	1.81E-03	1.77E-03	1.96E-03	1.94E-03	1.90E-03	1.84E-03	1.81E-03	1.78E-03	1.73E-03
m-C8H10	89.84	89.94	87.2	86.46	42.92	24.31	11.03	0.97	0
O ₂	444.36	438.24	436.37	438.09	411.81	376.24	347.14	331.86	282.98
CO	0	0	0	0	36.94	64.37	101.74	130.15	192.2
CO ₂	0	0	0	0	7.69	9.51	14.04	18.24	27.5
CH ₄	0	0	0.28	0.7	6.91	11.04	15.52	16.72	18.05
C ₂ H ₄	0	0	0	0	3.3	6.02	7.84	8.97	8.57
C ₂ H ₆	0	0	0	0	2.66	2.96	2.25	2.11	1.52
C ₂ H ₂	0	0	0	0	7.06	20.06	39.5	56.28	74.72
1,2-Propadiene	0	0	0	0	0.56	0.93	1.25	1.25	1.24
Propyne	0	0	0	0	1.21	2.1	2.91	3.17	2.73
1,3-Butadiene	0	0	0	0	0.31	0.5	0.49	0.46	0.32
Vinylacetylene	0	0	0	0	0.75	1.45	1.71	1.92	1.55
Diacetylene	0	0	0	0	0.93	2.73	4.87	7.37	8.29
Benzene	0	0	0.04	0.15	4.59	7.65	8.66	8.92	6.96
Toluene	0	0	0.15	0.13	6.18	7.53	5.72	5.01	2.65
Phenylacetylene	0.65	0.56	0.54	0.63	3.96	5.54	4.32	3.95	3.13
Styrene	0	0	0	0.3	7.4	9.46	7.31	6.35	1.92
Triacetylene	0	0	0	0	0	0	0	0.05	0.06
p-Xylene	0.1	0.08	0.11	0.18	0.55	0.4	0.19	0.15	0
m-Ethylmethylbenzene	0	0	0	0	0.25	0.15	0	0	0
Ethylbenzene	0	0	0	0.03	0.25	0.26	0.14	0.12	0
1,3-Cyclopentadiene	0	0	0	0.02	0.85	1.19	1.18	0.62	0
5-Methylcyclopentadiene	0	0	0	0.01	0.11	0.12	0.11	0.09	0
1,3-Hexadiene	0	0	0	0.02	0.15	0.11	0.08	0.06	0
1,3,5-Cycloheptatriene	0	0	0	0.03	0.08	0.04	0.03	0.01	0
Preshock Carbon	697.6	697.6	697.6	697.6	697.6	697.6	697.6	697.6	697.6
Postshock Carbon	724.72	724.6	711.25	780.96	703.31	719.37	633.95	619.57	617.08

Experimental data for m-xylene oxidation, $\Phi = 2.15$, average P5 = 28 bar (Page 2/2)

Shock No.	22	26	24	28	30
T5/K	1467.86	1506.46	1536.08	1619.05	1632.49
P5/bar	28.53	27.64	28.81	29.25	27.23
Rxn Time/s	1.52E-03	1.53E-03	1.42E-03	1.30E-03	1.30E-03
m-C8H10	0.73	0	0	0	0
O ₂	147.22	82.48	29.07	21	15.33
CO	354.82	435.82	502	518.11	520.87
CO ₂	51.46	65.88	82.95	90.64	87.78
CH ₄	13.08	9.73	5.77	3.4	2.33
C ₂ H ₄	4.16	2.03	1.07	0.45	0.33
C ₂ H ₆	0.63	0.38	0.21	0.11	0.05
C ₂ H ₂	76.12	56.91	38.14	21.33	16.47
1,2-Propadiene	0.6	0.37	0.25	0	0
Propyne	1.45	0.86	0.54	0	0
1,3-Butadiene	0.1	0.07	0.04	0	0
Vinylacetylene	0.46	0.22	0.08	0	0
Diacetylene	5.41	2.74	1.04	0	0
Benzene	1.64	0.65	0.19	0.17	0.1
Toluene	0.31	0	0	0	0
Phenylacetylene	0.5	0.3	0	0	0
Styrene	0.52	0.26	0.09	0	0.1
Triacetylene	0.1	0.1	0.03	0	0
p-Xylene	0	0	0	0	0
m-Ethylmethylbenzene	0	0	0	0	0
Ethylbenzene	0	0	0	0	0
1,3-Cyclopentadiene	0	0	0	0	0
5-Methylcyclopentadiene	0	0	0	0	0
1,3-Hexadiene	0	0	0	0	0
1,3,5-Cycloheptatriene	0	0	0	0	0
Preshock Carbon	697.6	697.6	697.6	697.6	697.6
Postshock Carbon	653.95	654.81	678.57	656.96	646.12

m-Xylene Pyrolysis Dataset

m-Xylene pyrolysis, Average P5 = 54 atm, $\phi = \infty$ (page 1/3)

Shock	3	1	2	5	6	8	10
T(5) Decomp	1060.58	1075.88	1166.00	1193.97	1223.57	1302.95	1340.81
P5 (atm)	50.12	57.34	63.72	59.31	55.50	54.12	54.56
Reaction Time (s)	0.00	0.00	0.00	0.00	0.00	0.00	0.00
m-xylene-GC2	54.43	53.70	53.89	53.81	53.31	47.93	32.68
Methane	0.00	0.00	0.00	0.00	0.00	1.05	4.10
Ethene	0.00	0.00	0.00	0.00	0.00	0.21	1.44
Ethane	0.00	0.00	0.00	0.00	0.00	0.27	1.27
Acetylene	0.00	0.00	0.00	0.00	0.00	0.32	2.45
1,2-Propadiene	0.00	0.00	0.00	0.00	0.00	0.00	0.28
Propyne	0.00	0.00	0.00	0.00	0.00	0.00	0.53
1,3-Butadiene	0.00	0.00	0.00	0.00	0.00	0.00	0.14
Vinylacetylene	0.00	0.00	0.00	0.00	0.00	0.00	0.12
Diacetylene	0.00	0.00	0.00	0.00	0.00	0.00	0.62
Benzene	0.00	0.00	0.00	0.04	0.08	0.09	0.90
Toluene	0.00	0.00	0.00	0.00	0.00	0.72	2.91
Styrene	0.00	0.00	0.00	0.00	0.00	0.70	5.62
Triacetylene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
p-xylene	0.10	0.09	0.07	0.10	0.09	0.19	0.37
PhenylAcetylene	0.00	0.00	0.00	0.00	0.00	0.00	0.18
Styrene	0.00	0.00	0.00	0.00	0.00	0.00	3.19
Indene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Naphthalene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
diphenylmethane	0.00	0.00	0.00	0.00	0.00	0.00	0.03
Acenaphthalene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,2'-dimethylbiphenyl	0.00	0.00	0.00	0.00	0.00	0.06	0.15
benzene-1,1'-(1-methyl-1,2-ethanediyl)b	0.00	0.00	0.00	0.00	0.00	0.21	0.38
benzene-1-methyl-3,[4-methylphenyl]methyl	0.00	0.00	0.00	0.00	0.00	0.14	0.19
Fluorene	0.00	0.00	0.00	0.00	0.00	0.00	0.21
benzene-1,1'-(1,2-ethanediyl)bis[4-meth	0.00	0.00	0.00	0.00	0.00	1.99	1.14
diphenylethyne	0.00	0.00	0.00	0.00	0.00	0.46	0.33
9H-flourene-2-methy	0.00	0.00	0.00	0.00	0.00	0.00	0.05
anthracene	0.00	0.00	0.00	0.00	0.00	0.00	0.42
phenylnaphthalene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
m-terphenyl	0.00	0.00	0.00	0.00	0.00	0.00	0.00
p-terphenyl	0.00	0.00	0.00	0.00	0.00	0.00	0.00
benzoanthracene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Preshock Carbon	431.04	431.04	431.04	431.04	431.04	431.04	431.04
Postshock Carbon	435.46	429.62	431.09	430.75	427.02	397.30	352.52

m-Xylene pyrolysis, Average P5 = 54 atm, $\phi = \infty$ (page 2/3)

Shock	41	7	24	18	22	25	39	16
T(5) Decomp	1365.66	1391.01	1398.79	1402.58	1411.59	1413.18	1428.68	1445.27
P5 (atm)	58.17	62.02	48.41	56.50	55.09	49.48	49.41	61.34
Reaction Time (s)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
m-xylene-GC2	26.85	17.00	15.33	10.89	5.22	5.80	2.84	1.60
Methane	5.81	9.05	9.33	11.87	15.71	14.09	15.82	15.62
Ethene	1.84	3.49	4.11	5.09	6.58	6.70	6.25	4.48
Ethane	1.50	1.69	1.73	1.56	0.65	1.35	0.47	0.26
Acetylene	3.35	7.71	10.04	12.64	32.95	20.22	43.22	61.62
1,2-Propadiene	0.37	0.48	5.47	0.72	0.82	0.84	0.82	0.60
Propyne	0.66	1.25	1.36	1.62	1.91	2.01	1.90	0.62
1,3-Butadiene	0.19	0.26	0.27	0.29	1.26	0.29	0.13	0.07
Vinylacetylene	0.15	0.26	0.35	0.43	0.49	0.61	0.47	0.23
Diacetylene	0.99	2.15	3.96	3.97	11.38	8.67	18.01	21.31
Benzene	1.21	2.75	2.85	3.75	5.38	5.06	5.11	4.20
Toluene	3.64	4.88	4.82	5.51	4.71	4.36	1.41	0.40
Styrene	7.19	10.66	8.55	10.23	4.98	8.49	3.67	1.66
Triacetylene	0.00	0.00	0.39	0.00	0.00	0.00	1.27	2.80
p-xylene	0.43	0.38	0.39	0.30	0.11	0.23	0.06	0.00
PhenylAcetylene	0.28	1.20	0.99	0.67	1.49	2.04	1.39	0.00
Styrene	3.95	6.81	6.64	0.92	4.29	7.08	3.39	0.00
Indene	0.28	0.66	0.99	0.72	1.49	2.04	1.39	0.46
Naphthalene	0.27	0.37	0.51	0.68	1.35	1.08	1.29	1.01
diphenylmethane	0.03	0.10	0.09	0.14	0.16	0.16	0.12	0.08
Acenaphthalene	0.07	0.12	0.26	0.40	0.80	0.59	0.86	0.96
2,2'-dimethylbiphenyl	0.18	0.25	0.22	0.23	0.17	0.16	0.07	0.00
benzene-1,1'-(1-methyl-1,2-ethanediyl)b	0.35	0.36	0.28	0.23	0.00	0.08	0.00	0.00
benzene-1-methyl-3,[4-methylphenyl]methyl	0.19	0.22	0.17	0.11	0.08	0.08	0.05	0.00
Fluorene	0.24	0.51	0.51	0.53	0.29	0.45	0.25	0.12
benzene-1,1'-(1,2-ethanediyl)bis[4-meth	0.73	0.60	0.40	0.24	0.09	0.14	0.07	0.00
diphenylethyne	0.23	0.21	0.17	0.13	0.17	0.14	0.10	0.13
9H-flourene-2-methy	0.06	0.11	0.15	0.16	0.19	0.13	0.10	0.05
anthracene	0.45	0.62	0.98	1.26	0.98	1.33	0.85	0.54
phenylnaphthalene	0.00	0.00	0.00	0.12	0.30	0.33	0.41	0.89
m-terphenyl	0.04	0.00	0.06	0.09	0.19	0.11	0.21	0.22
p-terphenyl	0.02	0.02	0.04	0.14	0.27	0.11	0.31	0.49
benzoanthracene	0.00	0.00	0.09	0.29	0.13	0.10	0.35	1.03
Preshock Carbon	431.04	431.04	431.04	431.04	431.04	431.04	431.04	431.04
Postshock Carbon	332.63	322.58	323.27	306.32	303.61	292.61	295.97	303.76

m-Xylene pyrolysis, Average P5 = 54 atm, $\phi = \infty$ (page 3/3)

Shock	15	27	37	35	29	31	33
T(5) Decomp	1453.89	1474.58	1480.66	1490.94	1506.73	1566.42	1579.25
P5 (atm)	63.62	52.47	45.36	49.48	50.80	51.04	51.70
Reaction Time (s)	0.00	0.00	0.00	0.00	0.00	0.00	0.00
m-xylene-GC2	1.13	0.39	0.57	0.40	0.59	0.37	0.41
Methane	14.30	9.72	10.96	11.45	7.70	2.91	2.80
Ethene	3.34	1.35	1.81	1.90	1.01	0.44	0.48
Ethane	0.20	0.20	0.18	0.09	0.16	0.24	0.14
Acetylene	75.88	93.77	94.56	95.85	102.40	114.86	113.57
1,2-Propadiene	0.45	0.29	0.39	0.38	0.36	0.00	0.24
Propyne	1.14	0.65	1.01	1.04	0.87	0.88	1.19
1,3-Butadiene	0.06	0.04	0.06	0.05	0.05	0.05	0.05
Vinylacetylene	0.18	0.12	0.12	0.16	0.10	0.09	0.11
Diacetylene	25.44	32.34	33.24	32.16	33.81	30.87	31.03
Benzene	3.11	1.14	1.54	1.34	0.57	0.17	0.19
Toluene	0.19	0.00	0.05	0.00	0.00	0.00	0.00
Styrene	0.63	0.15	0.20	0.23	0.10	0.00	0.00
Triacetylene	3.58	10.44	7.34	9.25	11.92	9.17	10.06
p-xylene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PhenylAcetylene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Styrene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Indene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Naphthalene	0.76	0.23	0.28	0.20	0.00	0.00	0.00
diphenylmethane	0.03	0.00	0.00	0.00	0.00	0.00	0.00
Acenaphthalene	0.85	0.27	0.26	0.23	0.02	0.00	0.00
2,2'-dimethylbiphenyl	0.00	0.00	0.00	0.00	0.00	0.00	0.00
benzene-1,1'-(1-methyl-1,2-ethanediyl)b	0.00	0.00	0.00	0.00	0.00	0.03	0.00
benzene-1-methyl-3,[4-methylphenyl]methyl	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Fluorene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
benzene-1,1'-(1,2-ethanediyl)bis[4-meth	0.00	0.00	0.00	0.00	0.00	0.00	0.00
diphenylethyne	0.06	0.00	0.00	0.00	0.00	0.00	0.00
9H-flourene-2-methy	0.04	0.00	0.00	0.00	0.00	0.00	0.00
anthracene	0.38	0.12	0.11	0.08	0.07	0.00	0.00
phenylnaphthalene	1.11	0.46	0.05	0.00	0.00	0.00	0.00
m-terphenyl	0.22	0.07	0.00	0.00	0.00	0.00	0.00
p-terphenyl	0.57	0.13	0.15	0.10	0.06	0.00	0.00
benzoanthracene	0.82	0.32	0.13	0.00	0.00	0.00	0.00
Preshock Carbon	431.04	431.04	431.04	431.04	431.04	431.04	431.04
Postshock Carbon	329.04	386.12	387.09	390.93	410.96	401.27	404.78

1,3,5-Trimethylbenzene Oxidation Datasets

1,3,5-trimethylbenzene oxidation Average P5 = 20.17 atm, ϕ = 0.46, reaction time = 1.55 – 2.55 ms (page 1/3)

Shock number	2	5	7	15	20	26	28
Temperature (K)	964.05	845.49	1042.41	1161.37	1186.78	1240.95	1268.95
Pressure (atm)	18.21	16.99	19.24	15.85	21.75	22.64	22.43
Rxn Time (s)	3.18E-03	4.05E-03	2.71E-03	2.31E-03	2.22E-03	2.15E-03	2.11E-03
O2	1972.05	1999.6	1946.42	1944.2	1972.85	1939.53	1978.35
CO	0	0	2.71	0	2.94	2.17	2.17
CH4	0	0	0.31	0	0.47	0.98	1.63
CO2	2.48	0	2.44	3.05	7.93	3.19	3.37
C2H4	0	0	0	0	0	0	0
C2H6	0	0	0	0	0	0.29	0.53
C2H2	0	0	0	0	0	0	0
C3H6	0	0	0	0	0	0	0
C3H4-a	0	0	0	0	0	0	0
C3H4-p	0	0	0	0	0	0	0
1-BUTENE	0	0	0	0	0	0	0
1,3-BUTADIENE	0	0	0	0	0	0	0
BENZENE	0	0	0	0.08	0.05	0.22	0.52
TOLUENE	0	0	0	0.19	0.06	0.46	1
ETHYLBENZENE	0	0	0	0	0	0	0
m+p-xylene	0	0	0	0.56	0.18	1.01	1.72
135tmb-GC2	79.79	77.09	77.44	72.81	66.4	70.19	67.92
Vinylacetylene	0	0	0	0	0	0	0
Diacetylene	0	0	0	0	0	0	0
o-Xylene	0	0	0	0	0	0	0
Styrene	0	0	0	0	0	0	0.24
Phenylacetylene	0	0	0	0	0	0	0
1,2,4-Trimethylbenzene	0.39	2.22	0.32	0.42	0.42	0.43	0.39
1-ethenyl-4-methylbenzene	0	0	0	0	0	0	0
1-ethenyl-3-methylbenzene	0	0	0	0	0	0	0.12
1-ethyl-3,5-dimethylbenzene	0	0	0	0.35	0.22	1.04	1.59
Indene	0	0	0	0	0	0	0.05
1-ethenyl-3,5-dimethylbenzene	0	0	0	0	0	0	0.08
3-methylbenzaldehyde	0	0	0.26	0	0	0	0.08
1-methylindene	0	0	0	0	0	0	0.07
methyleneindene	0	0	0	0	0	0	0.09
Ethylbenzaldehyde	0	0	0	0	0	0.73	1.13
3,5-dimethylbenzaldehyde	0	0	0	0	0.18	0.26	0.67
Benzene, 1,2-dimethyl-4-(phenylmethyl)	0	0	0	0	0	0	0.03
2,4-dimethyldiphenylmethane	0	0	0	0.01	0	0.04	0.07
2,3,5-trimethyldiphenylmethane	0	0	0	0	0	0	0.01
3,3'-dimethyldiphenylmethane	0	0	0	0	0	0	0.01
benzene,1,1'-(1,2-ethanediy)bi[3,5-dimethyl	0.03	0.04	0.07	0.42	0.56	1.33	1.63
Phenanthrene	0	0	0	0	0	0.03	0.07
Naphthalene	0	0	0	0	0	0	0
Precarb bal	678.41	678.41	678.41	678.41	678.41	678.41	678.41
Postcarb bal	681.14	702.78	697.75	24.48	690.77	664.06	652.5

1,3,5-trimethylbenzene oxidation Average P5 = 20.17 atm, ϕ = 0.46, reaction time = 1.55 – 2.55 ms (page 2/3)

Shock number	30	34	36	38	40	44	46	48
Temperature (K)	1317.79	1304.76	1349.54	1373.43	1428.22	1393.14	1400.96	1463.68
Pressure (atm)	23.49	20.9	21.38	21.34	22.42	21.91	21.46	21.6
Rxn Time (s)	1.92E-03	2.05E-03	1.87E-03	1.82E-03	1.71E-03	1.79E-03	1.77E-03	1.66E-03
O2	1935.98	1882.58	1839.71	1659.78	1197.73	1424.32	1272.21	1044.58
CO	50.45	7.53	120.63	215.59	251.28	282.14	304.45	194.93
CH4	7.03	3.37	9.36	10.39	1.43	7.01	2.97	0.86
CO2	6.2	4.09	29.97	94.4	437.98	171.96	328.99	497.74
C2H4	2.39	0.58	4.93	6.77	0	4.43	1.45	0
C2H6	2.94	1.37	3.78	2.94	0.4	1.63	0.68	0
C2H2	6.71	1.18	14.41	22.52	2	17.46	6.42	1.01
C3H6	0.29	0.22	0.19	0.17	0	0.13	0	0
C3H4-a	0.45	0.2	0.53	0.67	0	0.41	0	0
C3H4-p	1.17	0.55	1.5	1.82	0	0.65	0	0
1-BUTENE	0	0	0.37	0.49	0.07	0	0	0
1,3-BUTADIENE	0.26	0.12	1.02	0.51	0.07	0.3	0.12	0
BENZENE	4.32	1.39	6.66	8.29	0.89	4.32	1.76	0.45
TOLUENE	5.08	2.3	6.18	5.37	0.6	2.45	0.99	0.26
ETHYLBENZENE	0.18	0.08	0.24	0.25	0.03	0.1	0	0
m-+p-xylene	4.92	3.2	4.6	2.98	0.38	1.32	0.56	0.11
135tmb-GC2	37.38	50.17	20.83	10.29	2.34	5.4	3.5	0.17
Vinylacetylene	0.64	0	1.15	1.48	0.13	0.85	0.3	0
Diacetylene	0.49	0	0.79	1.07	0	0.56	0.18	0
o-Xylene	0.16	0.1	0.3	0.54	0	0.11	0	0
Styrene	1.2	0.59	1.83	1.46	0.22	0.72	0	0
Phenylacetylene	0.55	0.14	0.67	0.51	0	0.32	0	0
1,2,4-Trimethylbenzene	0.37	0.41	0.35	0.15	0	0	0	0
1-ethenyl-4-methylbenzene	0.58	0.26	0.71	0.32	0	0	0	0
1-ethenyl-3-methylbenzene	0.77	0.36	0.81	0.51	0	0.31	0	0
1-ethyl-3,5-dimethylbenzene	2.35	2.26	1.27	0.82	0.13	0.54	0.25	0
Indene	0.54	0.18	0.72	0.62	0	0.26	0.13	0
1-ethenyl-3,5-dimethylbenzene	0.41	0.2	0.33	0.24	0	0	0	0
3-methylbenzaldehyde	0.24	0.19	0.23	0.13	0	0	0	0
1-methylindene	0.08	0.13	0.06	0.03	0	0	0	0
methyleneindene	0.28	0.21	0.21	0	0	0	0	0
Ethylbenzaldehyde	1.99	1.71	1.54	0.76	0	0	0	0
3,5-dimethylbenzaldehyde	1.41	1.13	0.93	0.3	0	0.21	0.13	0
Benzene, 1,2-dimethyl-4-(phenylmethyl)	0.11	0.06	0.11	0.06	0	0.01	0.01	0
2,4-dimethyldiphenylmethane	0.14	0.12	0.13	0.06	0	0.01	0	0
2,3,5-trimethyldiphenylmethane	0.02	0.02	0.02	0	0	0	0.02	0
3,3'-dimethyldiphenylmethane	0.01	0.01	0.01	0	0	0	0	0
benzene,1,1'-(1,2-ethanediy)bi[3,5-dimethyl	0.85	1.04	0.67	0.23	0.04	0.07	0.05	0.03
Phenanthrene	0.12	0.08	0.12	0.03	0	0	0	0
Naphthalene	0.04	0	0.09	0.14	0	0.05	0.02	0
Precarb bal	678.41	678.41	678.41	678.41	678.41	678.41	678.41	678.41
Postcarb bal	625.03	589.61	637.22	668.04	735.75	648.73	718.85	734.14

1,3,5-trimethylbenzene oxidation Average P5 = 20.17 atm, ϕ = 0.46, reaction time = 1.55 – 2.55 ms (page 3/3)

Shock number	50	52
Temperature (K)	1505.46	1515.37
Pressure (atm)	21.03	21.25
Rxn Time (s)	1.64E-03	1.56E-03
O2	989.4	978.49
CO	117.2	86.65
CH4	0.31	0
CO2	617.27	644.49
C2H4	0	0
C2H6	0	0
C2H2	0	0
C3H6	0	0
C3H4-a	0	0
C3H4-p	0	0
1-BUTENE	0	0
1,3-BUTADIENE	0	0
BENZENE	0	0.11
TOLUENE	0	0.06
ETHYLBENZENE	0	0
m-+p-xylene	0	0
135tmb-GC2	0	0.41
Vinylacetylene	0	0
Diacetylene	0	0
o-Xylene	0	0
Styrene	0	0
Phenylacetylene	0	0
1,2,4-Trimethylbenzene	0	0
1-ethenyl-4-methylbenzene	0	0
1-ethenyl-3-methylbenzene	0	0
1-ethyl-3,5-dimethylbenzene	0	0
Indene	0	0
1-ethenyl-3,5-dimethylbenzene	0	0
3-methylbenzaldehyde	0	0
1-methylindene	0	0
methyleneindene	0	0
Ethylbenzaldehyde	0	0
3,5-dimethylbenzaldehyde	0	0
Benzene, 1,2-dimethyl-4-(phenylmethyl)	0	0
2,4-dimethyldiphenylmethane	0	0
2,3,5-trimethyldiphenylmethane	0	0
3,3'-dimethyldiphenylmethane	0	0
benzene,1,1'-(1,2-ethanediyl)bi[3,5-dimethyl	0	0
Phenanthrene	0	0
Naphthalene	0	0
Precarb bal	678.41	678.41
Postcarb bal	734.79	732.19

1,3,5-trimethylbenzene oxidation, average P5 =19.69 atm, ϕ = 1.79, reaction time = 1.40 – 2.47 ms (page 1/3)

Shock number	1	3	4	5	7	11	14
Temperature (K)	1051.3	1133.7	1178.6	1232.9	1151.4	1034.7	1283.2
Pressure (atm)	15.68	17.51	16.68	15.7	15.26	16.61	20.75
Rxn Time (s)	0	0	0	0	0	0	0
O2	550.2	558.2	546.9	553	548.5	549	553.3
CO	0	0	0	0	0	0	0
CH4	0	0	0	0	0	0	0
CO2	0	0	0	0	0	0	0
C2H4	0	0	0	0	0	0	0
C2H6	0	0	0	0	0	0	0
C2H2	0	0	0	0	0	0	0
C3H6	0	0	0	0	0	0	0
C3H4-a	0	0	0	0	0	0	0
C3H4-p	0	0	0	0	0	0	0
1-BUTENE	0	0	0	0	0	0	0
1,3-BUTADIENE	0	0	0	0	0	0	0
BENZENE	0	0	0	0.05	0	0	0.21
TOLUENE	0	0	0	0.1	0	0	0.41
ETHYLBENZENE	0	0	0	0	0	0	0
m-+p-xylene	0	0.17	0.17	0.43	0	0	1.23
135tmb-GC2	80.85	84.6	82.04	81.8	81.96	83.34	75.64
Vinylacetylene	0	0	0	0	0	0	0
Diacetylene	0	0	0	0	0	0	0
o-xylene	0	0	0	0	0	0	0
Styrene	0	0	0.03	0.03	0	0	0.17
Phenylacetylene	0	0	0	0	0	0	0
1,2,4-Trimethylbenzene	0	0.47	0.4	0.5	0.5	0.47	0.46
1-ethenyl-4-methylbenzene	0	0	0	0	0	0	0.04
1-ethenyl-3-methylbenzene	0	0	0	0	0	0	0.05
1-ethyl-3,5-dimethylbenzene	0	0.11	0.2	0.43	0.1	0	1
Indene	0	0	0	0	0	0	0
1-ethenyl-3,5-dimethylbenzene	0	0	0	0	0	0	0
1-methyleneindene	0	0	0	0	0	0	0
Naphthalene	0	0	0	0	0	0	0
3,5-dimethylbenzaldehyde	0	0.13	0.12	0.28	0	0	0.36
acenaphthylene	0	0	0	0	0	0	0
Benzene, 1,1'-methylenebis[3-methyl-	0	0	0	0	0	0	0
Fluorene	0	0	0	0	0	0	0
Benzene, 1,2-dimethyl-4-(phenylmethyl)-	0	0	0	0	0	0	0
2,4-dimethyldiphenylmethane	0	0	0.04	0.07	0	0	0
2,3,5-trimethyldiphenylmethane	0	0	0.04	0.07	0	0	0
3,3'-dimethyldiphenylmethane	0	0	0	0	0	0	0
2,4,2',3'-tetramethylbiphenyl	0	0	0	0	0	0	0
2,3,2',3'-tetramethylbiphenyl	0	0	0	0	0	0	0
benzene,1,1'-(1,2-ethanediyl)bi[3,5-dimethyl	0.05	0.56	0.73	1.47	0.46	0.07	2.9
Phenanthrene	0	0	0	0	0	0	0
2-phenylnapthalene	0	0	0	0	0	0	0
9-methylantracene	0	0	0	0	0	0	0
9-ethenylantracene	0	0	0	0	0	0	0
cyclopentaphenanthrene	0	0	0	0	0	0	0
Fluoranthene	0	0	0	0	0	0	0
Pyrene	0	0	0	0	0	0	0
2-methylfluoranthene	0	0	0	0	0	0	0
2,3-benzofluorene	0	0	0	0	0	0	0
ethylbenzaldehyde	0	0	0	0	0	0	0.46
3-methylbenzaldehyde	0	0	0	0	0	0	0
methylindene	0	0	0	0	0	0	0
PRE CARBON	739.08	739.08	739.08	739.08	739.08	739.08	739.08
POST CARBON	728.56	779.34	760.91	780.74	751.43	755.48	770.66

1,3,5-trimethylbenzene oxidation, average P5 =19.69 atm, $\phi = 1.79$, reaction time = 1.40 – 2.47 ms (page 2/3)

Temperature (K)	1379.4	1362.6	1413.6	1475.2	1446.7	1483.3	1532.8	1570.2
Pressure (atm)	22.38	22.31	22.61	21.51	21.39	20.01	22.03	20.82
Rxn Time (s)	0	0	0	0	0	0	0	0
O2	505.3	515.1	416	327.5	356.3	309.6	182.4	119.4
CO	49.6	35.22	115.02	236.41	177.2	259.82	394.61	459.98
CH4	17.29	13.44	23.95	24.19	24.46	23.13	17.22	13.86
CO2	4.23	2.65	8.24	23.22	14.85	26.47	48.29	55.46
C2H4	8.77	6.93	13.89	11.64	13.13	10.85	5.8	4.11
C2H6	5.46	5.96	3.55	2.11	2.34	1.82	1.06	0.84
C2H2	23.3	13.9	72.93	129.12	99.1	125.87	116.23	106.79
C3H6	0.29	0.23	0.14	0.11	0.12	0.09	0.09	0.07
C3H4-a	0.93	0.77	1.48	1.2	1.26	1.11	0.84	0.57
C3H4-p	2.33	2.04	3.5	3.13	3.26	3.18	1.57	0.9
1-BUTENE	0	0	0	0.27	0.36	0	0	0
1,3-BUTADIENE	0.47	0.36	0.44	0.28	0.37	0.23	0.13	0
BENZENE	7.36	5.03	10.68	6.05	9.62	6.01	2.58	1.49
TOLUENE	7.08	5.38	6.12	2.15	4.08	2	0.7	0.4
ETHYLBENZENE	0.25	0.2	0.2	0.05	0.15	0.06	0	0.03
m+p-xylene	5.96	6.01	2.71	0.56	1.27	0.76	0.2	0.17
135tmb-GC2	19.68	28.79	6.31	1.62	3.28	1.54	0.94	0.5
Vinylacetylene	1.28	0.79	1.76	1.26	1.6	1.15	0.54	0.32
Diacetylene	2.79	1.58	7.78	10.98	10.81	11.57	7.97	6.27
o-xylene	1.87	1.3	1.94	1.05	1.52	0.94	0.35	0.25
Styrene	4.36	3.42	3.36	1.23	1.89	1.06	0.36	0.22
Phenylacetylene	1.83	1.36	1.5	0.51	1.11	0.53	0.18	0
1,2,4-Trimethylbenzene	0.48	0.56	0.13	0	0	0	0	0
1-ethenyl-4-methylbenzene	1.61	1.41	0.59	0.09	0.24	0.06	0.02	0
1-ethenyl-3-methylbenzene	1.93	1.81	0.86	0.14	0.39	0.14	0.04	0
1-ethyl-3,5-dimethylbenzene	0	1.19	0.41	0.06	0.22	0	0	0
Indene	2.13	1.53	1.95	0.8	1.48	0.88	0.32	0.16
1-ethenyl-3,5-dimethylbenzene	0.2	0.3	0	0	0	0	0	0
1-methyleneindene	0.37	0.31	0.09	0	0.08	0	0	0
Naphthalene	0.93	0.27	1.3	0.72	1.17	0.69	0.24	0.09
3,5-dimethylbenzaldehyde	1.01	1.33	0.3	0	0.11	0	0	0
acenaphthylene	0.24	0.16	0.52	0.44	0.6	0.39	0.21	0.11
Benzene, 1,1'-methylenebis[3-methyl-	0.04	0.03	0	0	0	0	0	0
Fluorene	0.08	0.06	0.12	0.07	0.09	0.06	0	0
Benzene, 1,2-dimethyl-4-(phenylmethyl)	0.16	0.17	0.07	0	0	0	0	0
2,4-dimethyldiphenylmethane	0.2	0.22	0	0	0.02	0	0	0
2,3,5-trimethyldiphenylmethane	0.2	0.22	0	0	0.02	0	0	0
3,3'-dimethyldiphenylmethane	0.04	0.04	0	0	0	0	0	0
2,4,2',3'-tetramethylbiphenyl	0.02	0.01	0	0	0	0	0	0
2,3,2',3'-tetramethylbiphenyl	0	0	0	0	0	0	0	0
benzene,1,1'-(1,2-ethanediyl)bi[3,5-dimeth	0.79	0.99	0.2	0.07	0.1	0.04	0.04	0.03
Phenanthrene	0.11	0.11	0.23	0.1	0.12	0.06	0	0
2-phenylnaphthalene	0.08	0.08	0.03	0	0	0	0	0
9-methylantracene	0.07	0.06	0.03	0	0	0	0	0
9-ethenylantracene	0.03	0.02	0.03	0.03	0.04	0.02	0.03	0.02
cyclopentaphenanthrene	0.18	0.16	0.05	0.01	0.03	0	0	0
Fluoranthene	0.02	0.02	0.04	0.03	0.05	0.03	0.02	0.01
Pyrene	0.02	0.01	0.05	0.02	0.03	0.02	0	0
2-methylfluoranthene	0.01	0.01	0	0	0	0	0	0
2,3-benzofluorene	0.01	0.01	0.02	0.02	0.03	0.03	0.02	0.02
ethylbenzaldehyde	0.37	0.96	0	0	0	0	0	0
3-methylbenzaldehyde	0.24	0.29	0.06	0.04	0.07	0	0	0
methylindene	0.15	0.21	0.24	0	0	0	0	0
PRE CARBON	739.08	739.08	739.08	739.08	739.08	739.08	739.08	739.08
POST CARBON	682.25	682.09	699.31	755.22	726.09	767.29	796.19	810.21

1,3,5-trimethylbenzene oxidation, average P5 =19.69 atm, ϕ = 1.79, reaction time = 1.40 – 2.47 ms (page 3/3)

Shock number	37	38
Temperature (K)	1598.1	1620.5
Pressure (atm)	21.08	18.69
Rxn Time (s)	0	0
O2	94.9	52.2
CO	504.93	522.09
CH4	9.59	8.15
CO2	68.16	70.48
C2H4	1.73	1.48
C2H6	0.52	0.57
C2H2	76.27	64.42
C3H6	0	0
C3H4-a	0	0
C3H4-p	0	0
1-BUTENE	0	0
1,3-BUTADIENE	0	0
BENZENE	0.63	0.4
TOLUENE	0.14	0.14
ETHYLBENZENE	0	0
m-+p-xylene	0	0
135tmb-GC2	0.41	0.25
Vinylacetylene	0.17	0.1
Diacetylene	4.14	3.06
o-xylene	0.14	0
Styrene	0.11	0
Phenylacetylene	0	0
1,2,4-Trimethylbenzene	0	0
1-ethenyl-4-methylbenzene	0	0
1-ethenyl-3-methylbenzene	0	0
1-ethyl-3,5-dimethylbenzene	0	0
Indene	0	0
1-ethenyl-3,5-dimethylbenzene	0	0
1-methyleneindene	0	0
Naphthalene	0	0
3,5-dimethylbenzaldehyde	0	0
acenaphthylene	0.05	0
Benzene, 1,1'-methylenebis[3-methyl-	0	0
Fluorene	0	0
Benzene, 1,2-dimethyl-4-(phenylmethyl)	0	0
2,4-dimethyldiphenylmethane	0	0
2,3,5-trimethyldiphenylmethane	0	0
3,3'-dimethyldiphenylmethane	0	0
2,4,2',3'-tetramethylbiphenyl	0	0
2,3,2',3'-tetramethylbiphenyl	0	0
benzene,1,1'-(1,2-ethanediyl)bi[3,5-dimeth	0.05	0
Phenanthrene	0	0
2-phenylnapthalene	0	0
9-methylantracene	0	0
9-ethenylantracene	0	0
cyclopentaphenanthrene	0	0
Fluoranthene	0	0
Pyrene	0	0
2-methylfluoranthene	0	0
2,3-benzofluorene	0	0
ethylbenzaldehyde	0	0
3-methylbenzaldehyde	0	0
methylindene	0	0
PRE CARBON	739.08	739.08
POST CARBON	769	751.87

1,3,5-trimethylbenzene oxidation, average P5 =49.7 atm, $\phi = 0.51$, reaction time = 1.26 – 2.80 ms (page 1/2)

Shock number	2	4	6	12	14	18	20
Temperature (K)	1240	1018	1134	1264	1338	1283	1293
Pressure (atm)	49.94	41.12	47.67	53.13	54.18	52.17	52.86
Rxn Time (s)	0	0	0	0	0	0	0
O ₂	1964	2010	2027	1979	1774	1961	1962
CO	2.21	2.62	2.35	3.69	182.71	17.39	29.05
CH ₄	0	0	0	1.84	12.06	2.68	4.54
CO ₂	2.19	1.31	1.47	2.05	28.26	3.4	3.63
C ₂ H ₄	0	0	0	0	6.5	1.16	1.13
C ₂ H ₆	0	0	0	0.4	3.02	0.73	1.32
C ₂ H ₂	0	0	0	0	17.09	0	2.24
C ₃ H ₆	0	0	0	0	0.3	0.17	0.18
C ₃ H ₄ -a	0	0	0	0	0.63	0.16	0.29
C ₃ H ₄ -p	0	0	0	0	1.99	0.36	1.04
1-BUTENE	0	0	0	0	0.49	0.05	0
1,3-BUTADIENE	0	0	0	0.06	1.43	0.12	0.15
BENZENE	0.08	0	0	0.62	7.59	0.99	2.07
TOLUENE	0.22	0	0	1.19	5.52	1.67	3.12
ETHYLBENZENE	0	0	0	0.02	0.24	0.05	0.09
m+p-xylene	0.54	0	0	1.99	3.21	2.57	3.94
135tmb-GC2	78.47	86.94	85.81	61.11	17.97	49.9	44.79
Vinylacetylene	0	0	0	0.09	1.43	0.18	0.33
Diacetylene	0	0	0	0	0.57	0	0
o-Xylene	0	0	0	0	0.34	0	0.14
Styrene	0	0	0	0.15	1.13	0.35	0.52
Phenylacetylene	0	0	0	0	0.36	0.04	0.13
1,2,4-Trimethylbenzene	0.41	0.47	0.48	0.44	0.12	0.39	0.4
1-ethenyl-4-methylbenzene	0	0	0	0	0.29	0	0.22
1-ethenyl-3-methylbenzene	0	0	0	0	0.32	0.21	0.24
1-ethyl-3,5-dimethylbenzene	0	0	0	1.84	1.48	2.11	2.61
Indene	0	0	0	0	0.32	0	0.13
1-ethenyl-3,5-dimethylbenzene	0	0	0	0.15	0.39	0.24	0.47
3,5-dimethylbenzaldehyde	3.15	0	0	2.65	1.6	2.36	2.07
acenaphthylene	0	0	0	0	0.05	0.12	0.13
Benzene, 1,1'-methylenebis[3-methyl-	0	0	0	0	0.02	0.02	0
Benzene, 1,2-dimethyl-4-(phenylmethyl)	0	0	0	0.05	0.04	0.07	0.07
1,8-dimethylnaphthalene	0	0	0	0	0	0.25	0.06
2,4-dimethyldiphenylmethane	0.14	0	0	0.13	0.05	0.1	0.09
2,3,5-trimethyldiphenylmethane	0	0	0	0.02	0.01	0.01	0.02
3,3'-dimethyldiphenylmethane	0	0	0	0.02	0.01	0.01	0.01
2,4,2',3'-tetramethylbiphenyl	0.05	0	0	0.06	0.01	0.03	0.04
2,3,2',3'-tetramethylbiphenyl	0	0	0	0.01	0.01	0	0.01
benzene,1,1'-(1,2-ethanediy)bi[3,5-dimeth	3.56	0	1.39	2.75	0.79	1.14	1.2
Phenanthrene	0.08	0	0	0.14	0.06	0.4	0.12
2-methylantracene	0	0	0	0.01	0	0.16	0.06
2-phenylnaphthalene	0	0	0	0.06	0.02	0	0
9-methylantracene	0	0	0	0	0.02	0	0
9-ethenylnanthracene	0	0	0	0	0.02	0.01	0.05
cyclopentaphenanthrene	0	0	0	0	0.02	0.06	0.02
Pyrene	0.02	0	0	0	0	0.02	0.02
3-methylbenzaldehyde	0	0	0	0	0.66	0.15	0.28
methyleneindene	0	0	0	0.4	0.31	0.21	0.28
2,4,6-trimethylbenzaldehyde	0	0	0	0	0.18	0	0.08
1-ethyl-3-methylbenzene	0.87	0	0	3.2	1.2	3.61	2.52
1,3-diethyl-5-methylbenzene	0	0	0	0.06	0.14	0	0
1-methylindene	0.52	0	0	0.2	0.09	0.09	0.14
Ethylbenzaldehyde	2.27	0	0	2.64	2.18	2.77	3.02
3,6-dimethylphenanthrene	0	0	0	0	0.18	0.32	0.28
Fluoranthene	0	0	0	0	0.08	1.07	0.34
Pyrene	0.02	0	0	0	0	0.02	0.02
1,3,5-cycloheptatriene	0	0	0	0	0	0.53	0.77
Naphthalene	0	0	0	0	0.09	0	0
cpd	0	0	0	0	0	0.18	0.26
mecpd	0	0	0	0	0	0.25	0.41
4-methylphenanthrene	0	0	0	0	0	0.32	0.02
1,1'-biphenyl-3,3'-4,4'-tetramethyl	0	0	0	0	0	0.15	0.07
Precarb	699.56	699.56	699.56	699.56	699.56	699.56	699.56
Postcarb	773.12	704.62	714.58	697.69	658.08	702.1	687.35

1,3,5-trimethylbenzene oxidation, average P5 =49.7 atm, $\phi = 0.51$, reaction time = 1.26 – 2.80 ms (page 2/2)

Shock number	24	26	28	32	34	36	38	43
Temperature (K)	1383	1368	1478	1408	1439	1520	1561	1317
Pressure (atm)	49.03	51.59	52.67	46.52	48.29	49.78	50.06	52.35
Rxn Time (s)	0	0	0	0	0	0	0	0
O2	1533	1665	1114	1412	1180	1089	1026	1936
CO	362.39	346.21	72.23	331.8	168.69	61.36	36.08	87.38
CH4	8.03	10.02	0.42	4.22	1.25	0.3	0.28	8.86
CO2	170.92	125.48	676.34	295.62	535.53	685.3	715.27	7.18
C2H4	4.46	5.97	0	2.23	0.47	0	0	4.13
C2H6	1.41	1.47	0	0.74	0.28	0	0	3.42
C2H2	16.52	20.01	0	7.95	2.48	0	0	9.51
C3H6	0.33	0.4	0	0.11	0	0	0	0.22
C3H4-a	0.4	0.45	0	0.2	0	0	0	0.57
C3H4-p	0.98	1.4	0	0.26	0	0	0	1.55
1-BUTENE	0	0	0	0	0	0	0	0.06
1,3-BUTADIENE	0.29	0.32	0	0.15	0	0	0	0.32
BENZENE	5.13	6.27	0.17	2.36	0.85	0	0	5.07
TOLUENE	2.39	2.79	0.08	1.25	0.45	0	0	6
ETHYLBENZENE	0.12	0.14	0	0.03	0	0	0	0.22
m-p-xylene	1.22	1.53	0	0.67	0.18	0	0	4.98
135tmb-GC2	6.01	7.01	0.29	3.27	1.08	0	0	28.4
Vinylacetylene	0.85	1.01	0	0.43	0	0	0	0.91
Diacetylene	0.34	0.38	0	0.18	0	0	0	0.34
o-Xylene	0.1	0.13	0	0.07	0	0	0	0.4
Styrene	0.45	0.54	0	0	0	0	0	1.23
Phenylacetylene	0.18	0.24	0	0.09	0	0	0	0.28
1,2,4-Trimethylbenzene	0	0	0	0	0	0	0	0.3
1-ethenyl-4-methylbenzene	0.09	0.15	0	0	0	0	0	0.36
1-ethenyl-3-methylbenzene	0.18	0.24	0	0	0	0	0	0.31
1-ethyl-3,5-dimethylbenzene	0.15	0.2	0	0.06	0	0	0	2.46
Indene	0.19	0.22	0	0.1	0	0	0	0.27
1-ethenyl-3,5-dimethylbenzene	0.09	0.11	0	0	0	0	0	0.64
3,5-dimethylbenzaldehyde	0.26	0.27	0	0.15	0.18	0	0	1.78
acenaphthylene	0.03	0.04	0	0	0	0	0	0.05
Benzene, 1,1'-methylenbis[3-methyl-	0.01	0	0	0	0	0	0	0
Benzene, 1,2-dimethyl-4-(phenylmethyl)-	0	0.03	0	0	0	0	0	0.05
1,8-dimethylnaphthalene	0.04	0	0	0	0	0	0	0
2,4-dimethyldiphenylmethane	0.02	0.02	0	0	0	0	0	0
2,3,5-trimethyldiphenylmethane	0	0	0	0	0	0	0	0
3,3'-dimethyldiphenylmethane	0	0	0	0	0	0	0	0
2,4,2',3'-tetramethylbiphenyl	0	0	0	0	0	0	0	0
2,3,2',3'-tetramethylbiphenyl	0	0	0	0	0	0	0	0
benzene,1,1'-(1,2-ethanediyl)bi[3,5-dimethyl	0.14	0.14	0.06	0.1	0.07	0	0	0.62
Phenanthrene	0	0	0	0	0	0	0	0.08
2-methylantracene	0	0	0	0	0	0	0	0.01
2-phenylnaphthalene	0	0	0	0	0	0	0	0
9-methylantracene	0	0	0	0	0	0	0	0.21
9-ethenylnanthracene	0	0	0	0	0	0	0	0.05
cyclopentaphenanthrene	0	0	0	0	0	0	0	0
Pyrene	0	0	0	0	0	0	0	0
3-methylbenzaldehyde	0.1	0.16	0	0	0	0	0	0.52
methyleneindene	0	0.05	0	0	0	0	0	0.31
2,4,6-trimethylbenzaldehyde	0.05	0	0	0	0	0	0	0.15
1-ethyl-3-methylbenzene	0	0	0	0	0	0	0	2.1
1,3-diethyl-5-methylbenzene	0	0	0	0	0	0	0	0.16
1-methylindene	0	0.19	0	0	0	0	0	0
Ethylbenzaldehyde	0.74	1.32	0	0.52	0.19	0	0	3.23
3,6-dimethylphenanthrene	0	0	0	0	0	0	0	0.25
Fluoranthene	0	0	0	0	0	0	0	0.02
Pyrene	0	0	0	0	0	0	0	0
1,3,5-cycloheptatriene	0	0	0	0	0	0	0	0.61
Naphthalene	0.06	0.08	0.02	0	0	0	0	0.05
cpd	0	0	0	0	0	0	0	0.38
mecpd	0	0	0	0	0	0	0	0.59
4-methylphenanthrene	0	0	0	0	0	0	0	0
1,1'-biphenyl-3,3'-4,4'-tetramethyl	0	0	0	0	0	0	0	0.01
Precarb	699.56	699.56	699.56	699.56	699.56	699.56	699.56	699.56
Postcarb	729.55	710.85	755.81	725.57	736.33	746.96	751.64	663.58

1,3,5-trimethylbenzene oxidation average P5 =50.23 atm, $\phi = 0.95$, reaction time = 1.13 – 1.697 ms (page 1/3)

Shock number	24	26	28	32	34	36	38	43
Temperature (K)	1383	1368	1478	1408	1439	1520	1561	1317
Pressure (atm)	49.03	51.59	52.67	46.52	48.29	49.78	50.06	52.35
Rxn Time (s)	0	0	0	0	0	0	0	0
O2	1533	1665	1114	1412	1180	1089	1026	1936
CO	362.39	346.21	72.23	331.8	168.69	61.36	36.08	87.38
CH4	8.03	10.02	0.42	4.22	1.25	0.3	0.28	8.86
CO2	170.92	125.48	676.34	295.62	535.53	685.3	715.27	7.18
C2H4	4.46	5.97	0	2.23	0.47	0	0	4.13
C2H6	1.41	1.47	0	0.74	0.28	0	0	3.42
C2H2	16.52	20.01	0	7.95	2.48	0	0	9.51
C3H6	0.33	0.4	0	0.11	0	0	0	0.22
C3H4-a	0.4	0.45	0	0.2	0	0	0	0.57
C3H4-p	0.98	1.4	0	0.26	0	0	0	1.55
1-BUTENE	0	0	0	0	0	0	0	0.06
1,3-BUTADIENE	0.29	0.32	0	0.15	0	0	0	0.32
BENZENE	5.13	6.27	0.17	2.36	0.85	0	0	5.07
TOLUENE	2.39	2.79	0.08	1.25	0.45	0	0	6
ETHYLBENZENE	0.12	0.14	0	0.03	0	0	0	0.22
m-p-xylene	1.22	1.53	0	0.67	0.18	0	0	4.98
135tmb-GC2	6.01	7.01	0.29	3.27	1.08	0	0	28.4
Vinylacetylene	0.85	1.01	0	0.43	0	0	0	0.91
Diacetylene	0.34	0.38	0	0.18	0	0	0	0.34
o-Xylene	0.1	0.13	0	0.07	0	0	0	0.4
Styrene	0.45	0.54	0	0	0	0	0	1.23
Phenylacetylene	0.18	0.24	0	0.09	0	0	0	0.28
1,2,4-Trimethylbenzene	0	0	0	0	0	0	0	0.3
1-ethenyl-4-methylbenzene	0.09	0.15	0	0	0	0	0	0.36
1-ethenyl-3-methylbenzene	0.18	0.24	0	0	0	0	0	0.31
1-ethyl-3,5-dimethylbenzene	0.15	0.2	0	0.06	0	0	0	2.46
Indene	0.19	0.22	0	0.1	0	0	0	0.27
1-ethenyl-3,5-dimethylbenzene	0.09	0.11	0	0	0	0	0	0.64
3,5-dimethylbenzaldehyde	0.26	0.27	0	0.15	0.18	0	0	1.78
acenaphthylene	0.03	0.04	0	0	0	0	0	0.05
Benzene, 1,1'-methylenebis[3-methyl-	0.01	0	0	0	0	0	0	0
Benzene, 1,2-dimethyl-4-(phenylmethyl)-	0	0.03	0	0	0	0	0	0.05
1,8-dimethylnaphthalene	0.04	0	0	0	0	0	0	0
2,4-dimethyldiphenylmethane	0.02	0.02	0	0	0	0	0	0
2,3,5-trimethyldiphenylmethane	0	0	0	0	0	0	0	0
3,3'-dimethyldiphenylmethane	0	0	0	0	0	0	0	0
2,4,2',3'-tetramethylbiphenyl	0	0	0	0	0	0	0	0
2,3,2',3'-tetramethylbiphenyl	0	0	0	0	0	0	0	0
benzene,1,1'-(1,2-ethanediyl)bi[3,5-dimethyl	0.14	0.14	0.06	0.1	0.07	0	0	0.62
Phenanthrene	0	0	0	0	0	0	0	0.08
2-methylantracene	0	0	0	0	0	0	0	0.01
2-phenylnaphthalene	0	0	0	0	0	0	0	0
9-methylantracene	0	0	0	0	0	0	0	0.21
9-ethenylnanthracene	0	0	0	0	0	0	0	0.05
cyclopentaphenanthrene	0	0	0	0	0	0	0	0
Pyrene	0	0	0	0	0	0	0	0
3-methylbenzaldehyde	0.1	0.16	0	0	0	0	0	0.52
methyleneindene	0	0.05	0	0	0	0	0	0.31
2,4,6-trimethylbenzaldehyde	0.05	0	0	0	0	0	0	0.15
1-ethyl-3-methylbenzene	0	0	0	0	0	0	0	2.1
1,3-diethyl-5-methylbenzene	0	0	0	0	0	0	0	0.16
1-methylindene	0	0.19	0	0	0	0	0	0
Ethylbenzaldehyde	0.74	1.32	0	0.52	0.19	0	0	3.23
3,6-dimethylphenanthrene	0	0	0	0	0	0	0	0.25
Fluoranthene	0	0	0	0	0	0	0	0.02
Pyrene	0	0	0	0	0	0	0	0
1,3,5-cycloheptatriene	0	0	0	0	0	0	0	0.61
Naphthalene	0.06	0.08	0.02	0	0	0	0	0.05
cpd	0	0	0	0	0	0	0	0.38
mecpd	0	0	0	0	0	0	0	0.59
4-methylphenanthrene	0	0	0	0	0	0	0	0
1,1'-biphenyl-3,3'-4,4'-tetramethyl	0	0	0	0	0	0	0	0.01
Precarb	699.56	699.56	699.56	699.56	699.56	699.56	699.56	699.56
Postcarb	729.55	710.85	755.81	725.57	736.33	746.96	751.64	663.58

1,3,5-trimethylbenzene oxidation average P5 =50.23 atm, ϕ = 0.95, reaction time = 1.13 – 1.697 ms (page 2/3)

Shock number	18	24	26	30	32	34	36	38
Temperature (K)	1321	1349	1382	1481	1402	1411	1436	1500
Pressure (atm)	51.24	48.57	46.34	47.67	46.53	47.05	43.64	47.92
Rxn Time (s)	0	0	0	0	0	0	0	0
O2	885	902	881	420	885	851	804	347
CO	9.71	34.83	105.83	172.22	137.54	210.13	236.52	142.67
CH4	5.4	8.88	14.75	2.21	16.16	15.41	14.93	1.54
CO2	1.64	2.66	8.94	415.19	14.07	51.76	71.33	470.88
C2H4	1.04	2.28	6.66	0.75	8.3	8.14	7.69	0
C2H6	1.88	3	3.7	0.32	3.68	2.18	1.98	0.21
C2H2	1.95	5.5	20.81	4.56	28.29	42.27	40.91	3.23
C3H6	0	0.23	0.29	0	0.31	0.43	0.26	0
C3H4-a	0.23	0.6	0.75	0	0.91	0.77	0.68	0
C3H4-p	0.49	1.02	1.73	0	2.47	1.88	1.44	0
1-BUTENE	0	0	0	0	0	0	0.34	0
1,3-BUTADIENE	0.12	0.24	0.42	0.06	0.48	0.38	0.35	0
BENZENE	2.13	4.23	8.49	0.97	9.29	8.63	7.76	0.76
TOLUENE	3.15	5.18	6.59	0.41	5.12	3.9	3.41	0.32
ETHYLBENZENE	0.1	0.2	0.25	0	0.2	0.12	0	0
m-p-xylene	4.14	5.35	4.24	0.21	2.88	1.7	1.47	0.16
135tmb-GC2	38.37	28.55	12.24	0.72	7.32	5.35	4.08	0.74
Vinylacetylene	0.26	0.6	1.38	0.16	1.61	1.37	1.22	0
Diacetylene	0.04	0.13	0.4	0.06	0.47	0.56	0.48	0
o-xylene	0.11	0.29	0.87	0.12	0.92	0.72	0.59	0.11
Styrene	0.86	1.54	2.26	0.32	2.31	1.2	1.08	0.16
Phenylacetylene	0.35	0.71	0.8	0	0.64	0.42	0.38	0
1,2,4-Trimethylbenzene	0.5	0.51	0.31	0	0.12	0	0	0
1-ethenyl-4-methylbenzene	0.48	0.75	0.65	0	0.4	0.2	0.14	0
1-ethenyl-3-methylbenzene	0.62	0.91	0.96	0	0.68	0.33	0.26	0
1-ethyl-3,5-dimethylbenzene	2	1.78	1.21	0	0.8	0.42	0	0
Indene	0.38	0.67	1.13	0	0.89	0.72	0.67	0
1-ethenyl-3,5-dimethylbenzene	0.45	0.58	0.36	0	0.26	0.13	0	0
1-methyleneindene	0.75	0.75	0.5	0	0.17	0.04	0	0
Naphthalene	2.76	2.75	0.72	0	0.59	0.69	0.44	0
3,5-dimethylbenzaldehyde	3.88	2.35	2.07	0.21	0.84	0.67	0.57	0.23
acenaphthylene	0.02	0.04	0.1	0	0.11	0.1	0.1	0
Benzene, 1,1'-methylenebis[3-methyl-Fluorene	0.04	0.07	0.05	0	0.05	0	0	0
Benzene, 1,2-dimethyl-4-(phenylmethyl)-	0.15	0.15	0.12	0	0.13	0.04	0.05	0
2,4-dimethyldiphenylmethane	0.18	0.18	0.11	0	0.11	0.04	0.03	0
2,3,5-trimethyldiphenylmethane	0.03	0.04	0.02	0	0.02	0	0	0
3,3'-dimethyldiphenylmethane	0.02	0.02	0.02	0	0.01	0.01	0	0
2,4,2',3'-tetramethylbiphenyl	0.02	0.01	0	0	0	0.01	0	0
2,3,2',3'-tetramethylbiphenyl	0.01	0.01	0	0	0	0	0	0
benzene,1,1'-(1,2-ethanediyl)bi[3,5-dimethyl	1.68	1.19	0.53	0.13	0.28	0.25	0.18	0.08
Phenanthrene	0.25	1.26	0.59	0	0.04	0.27	0.11	0
2-methylantracene	0.02	0.05	0.01	0	0	0	0	0
2-phenylnapthalene	0.07	0.05	0.04	0	0.03	0	0.02	0
9-methylantracene	0.07	0.04	0.11	0	0.05	0.01	0.02	0
9-ethenylnapthalene	0.01	0.02	0.03	0	0.02	0.02	0.01	0
cyclopentaphenanthrene	0.06	0.04	0.03	0	0.01	0.01	0.02	0
Fluoranthene	0	0	0.02	0	0.02	0.02	0.02	0
Pyrene	0	0	0	0	0	0.01	0.02	0
2-methylfluoranthene	0	0	0	0	0	0	0	0
2,3-benzofluorene	0	0	0	0	0	0.01	0.02	0
Precarb	656.01	656.01	656.01	656.01	656.01	656.01	656.01	656.01
Postcarb	611.45	615.81	585.65	626.48	541.85	604.44	604.7	642.46

1,3,5-trimethylbenzene oxidation average P5 =50.23 atm, $\phi = 0.95$, reaction time = 1.13 – 1.697 ms (page 3/3)

Shock number	40	42	44	46	49
Temperature (K)	1456	1527	1550	1639	1588
Pressure (atm)	46	45.13	43.59	43.77	41.21
Rxn Time (s)	0	0	0	0	0
O2	491	255	151	111	137
CO	259.54	130.33	106.37	71.77	101.2
CH4	4.51	1.06	0	0	0.58
CO2	282.92	515.09	525.74	575.83	543.47
C2H4	1.6	0	0	0	0
C2H6	0.65	0.11	0	0	0.17
C2H2	10.21	1.65	0	0	0.62
C3H6	0.13	0	0	0	0
C3H4-a	0.21	0	0	0	0
C3H4-p	0.38	0	0	0	0
1-BUTENE	0	0	0	0	0
1,3-BUTADIENE	0.1	0	0	0	0
BENZENE	1.99	0.37	0.15	0.08	0.17
TOLUENE	1.1	0.18	0	0	0.08
ETHYLBENZENE	0	0	0	0	0
m-+p-xylene	0.59	0	0	0	0
135tmb-GC2	1.73	0.46	0.28	0.07	0.58
Vinylacetylene	0.3	0	0	0	0
Diacetylene	0.09	0	0	0	0
o-xylene	0.19	0	0	0	0
Styrene	0.39	0	0	0	0
Phenylacetylene	0.16	0	0	0	0
1,2,4-Trimethylbenzene	0	0	0	0	0
1-ethenyl-4-methylbenzene	0	0	0	0	0
1-ethenyl-3-methylbenzene	0	0	0	0	0
1-ethyl-3,5-dimethylbenzene	0	0	0	0	0
Indene	0.21	0	0	0	0
1-ethenyl-3,5-dimethylbenzene	0	0	0	0	0
1-methyleneindene	0	0	0	0	0
Naphthalene	0.22	0	0	0	0
3,5-dimethylbenzaldehyde	0.26	0.17	0.03	0	0.09
acenaphthylene	0.03	0	0	0	0
Benzene, 1,1'-methylenebis[3-methyl-	0	0	0	0	0
Fluorene	0.01	0	0	0	0
Benzene, 1,2-dimethyl-4-(phenylmethyl)-	0.01	0	0	0	0
2,4-dimethyldiphenylmethane	0.01	0	0	0	0
2,3,5-trimethyldiphenylmethane	0	0	0	0	0
3,3'-dimethyldiphenylmethane	0	0	0	0	0
2,4,2',3'-tetramethylbiphenyl	0	0	0	0	0
2,3,2',3'-tetramethylbiphenyl	0	0	0	0	0
benzene,1,1'-(1,2-ethanediy)bi[3,5-dimethyl	0.09	0.04	0.06	0	0
Phenanthrene	0	0	0	0	0
2-methylantracene	0	0	0	0	0
2-phenylnapthalene	0	0	0	0	0
9-methylantracene	0.01	0	0	0	0
9-ethenylantracene	0	0	0	0	0
cyclopentaphenanthrene	0.01	0	0	0	0
Fluoranthene	0	0	0	0	0
Pyrene	0	0	0	0	0
2-methylfluoranthene	0	0	0	0	0
2,3-benzofluorene	0	0	0	0	0
Precarb	656.01	656.01	656.01	656.01	656.01
Postcarb	631	659.8	636.84	648.69	654.5

1,3,5-trimethylbenzene oxidation average P5 =50.23 atm, $\phi = 0.95$, reaction time = 1.13 – 1.697 ms (page 1/3)

Shock number	10	14	16	18	20	23	25
Temperature (K)	1058.7	1214.7	1244.6	1347.7	1229.3	1286	1356.3
Pressure (atm)	48.57	51.72	49.17	51.8	43.06	45.8	50.35
Rxn Time (s)	0	0	0	0	0	0	0
O2	551.19	552.8	551.13	503.86	563.73	560.63	502.01
CO	0	0	0	20.86	0	1.23	33.23
CH4	0	0	0	12.16	0	2.31	15.42
CO2	0	0	0	1.77	0	1.27	2.06
C2H4	0	0	0	3.44	0	0	5.09
C2H6	0	0	0	3.77	0	0.43	4.2
C2H2	0	0	0	8.35	0	0	13.06
C3H6	0	0	0	0.13	0	0	0.16
C3H4-a	0	0	0	0.55	0	0	0.71
C3H4-p	0	0	0	1.2	0	0	1.63
1-BUTENE	0	0	0	0	0	0	0
1,3-BUTADIENE	0	0	0	0.23	0	0	0.3
BENZENE	0	0	0	4.73	0	0.36	6.04
TOLUENE	0	0.15	0.07	5.67	0	0.81	6.61
ETHYLBENZENE	0	0	0	0.19	0	0	0.38
m+p-xylene	0	0.28	0.22	6.62	0	2.21	6.81
135tmb-GC2	86.82	82.18	82.21	34.75	82.56	71.86	27.83
Vinylacetylene	0	0	0	0.6	0	0	0.84
Diacetylene	0	0	0	0.69	0	0	1.09
Styrene	0	0	0	2.45	0	0.09	2.98
1,2,4-Trimethylbenzene	0	0	0	0.64	0	0.68	0.52
1-ethenyl-4-methylbenzene	0	0	0	1.48	0	0	1.55
1-ethenyl-3-methylbenzene	0	0	0	1.59	0	0.33	1.69
1-ethyl-3,5-dimethylbenzene	0	0	0.15	1.71	0	1.72	1.4
Indene	0	0	0	1.42	0	0.1	1.64
1-ethenyl-3,5-dimethylbenzene	0	0	0	0.71	0	0.13	0.61
1-methyleneindene	0	0	0	0.43	0	0.31	0.65
Naphthalene	0	0	0	0.23	0	0	0.88
3,5-dimethylbenzaldehyde	0	0	0	2.73	0	2.26	2.45
acenaphthylene	0	0	0	0.07	0	0	0.11
Benzene, 1,1'-methylenebis[3-methyl-Fluorene	0	0	0	0.1	0	0	0.14
Benzene, 1,2-dimethyl-4-(phenylmethyl)-	0	0	0	0.3	0	0.09	0.28
2,4-dimethyldiphenylmethane	0	0.04	0.04	0.39	0	0.22	0.3
2,3,5-trimethyldiphenylmethane	0	0	0	0.08	0	0.03	0.06
3,3'-dimethyldiphenylmethane	0	0	0	0.04	0	0.04	0.03
2,4,2',3'-tetramethylbiphenyl	0	0	0	0.02	0	0.01	0.02
2,3,2',3'-tetramethylbiphenyl	0	0	0	0.02	0	0.01	0.02
benzene,1,1'-(1,2-ethanediyl)bi[3,5-dimeth	0	1.86	3.92	2.43	1.98	4.55	1.42
Phenanthrene	0	0	0	0.36	0	0.16	0.41
2-methylantracene	0	0	0	0.02	0	0.02	0.02
2-phenylanthracene	0	0	0	0.04	0	0.01	0.04
9-methylantracene	0	0	0	0.12	0	0	0.08
9-ethenylantracene	0	0	0	0.02	0	0	0.02
cyclopentaphenanthrene	0	0	0	0.16	0	0.01	0.14
Fluoranthene	0	0	0	0.02	0	0	0.02
Pyrene	0	0	0	0.01	0	0	0.01
2-methylfluoranthene	0	0	0	0.01	0	0	0.01
2,3-benzofluorene	0	0	0	0.02	0	0	0.01
Phenylacetylene	0	0	0	0.93	0	0	1.12
1-methylfluorene	0	0	0	0.15	0	0	0
o-xylene	0	0	0	0.72	0	0.04	0.93
PRE CARBON	770.57	770.57	770.57	770.57	770.57	770.57	770.57
POST CARBON	781.4	777.11	814.92	720.42	778.76	821.87	700.21

1,3,5-trimethylbenzene oxidation average P5 =50.23 atm, $\phi = 0.95$, reaction time = 1.13 – 1.697 ms (page 2/3)

Shock number	27	29	35	39	41	43	48	50
Temperature (K)	1250.7	1307.8	1425.7	1574.5	1471.4	1484.5	1548.6	1508.3
Pressure (atm)	41.98	45.86	45.22	51.8	43.98	41.1	42.21	40.88
Rxn Time (s)	0	0	0	0	0	0	0	0
O2	536.93	535.93	444.72	43.67	340.99	302.07	122.54	221.05
CO	0	3.46	117.5	505.67	248.91	286.55	464.45	350.72
CH4	0	4.29	25.12	10.59	26.55	27.64	17.12	23.32
CO2	0	1.07	7.31	80.14	24.09	32.22	63.89	44.34
C2H4	0	0	11.48	0	10.79	10.68	4.25	7.36
C2H6	0	1.24	3.33	0	1.78	1.8	0.71	1.22
C2H2	0	0	57.29	65.82	101.1	129.12	104.6	119.56
C3H6	0	0	0.22	0	0.19	0.13	0.07	0.1
C3H4-a	0	0	1.12	0.3	1.06	1.08	0.46	0.8
C3H4-p	0	0	2.8	0.5	2.71	2.57	0.86	2.03
1-BUTENE	0	0	0.4	0	0.27	0	0	0
1,3-BUTADIENE	0	0.07	0.41	0.04	0.28	0.27	0.07	0.16
BENZENE	0	0.98	12.09	0.6	8.53	7.54	1.41	3.81
TOLUENE	0.06	1.78	7.17	0.16	2.79	1.08	0.34	1.11
ETHYLBENZENE	0	0.14	0.07	0	0	0	0	0
m-+p-xylene	0.3	3.32	3.42	0	1.05	0.3	0	0.37
135tmb-GC2	81.5	60.19	9.9	0.29	2.17	0.85	0.44	0.97
Vinylacetylene	0	0.12	1.71	0.16	1.27	1.21	0.37	0.74
Diacetylene	0	0	5.22	3.5	8.26	8.88	5.59	7.59
Styrene	0	0.52	2.58	0.07	0.71	0	0	0
1,2,4-Trimethylbenzene	0.37	0.64	0.22	0	0	0	0	0
1-ethenyl-4-methylbenzene	0	0.44	0.7	0	0	0	0	0
1-ethenyl-3-methylbenzene	0	0.56	1.06	0	0.3	0	0	0
1-ethyl-3,5-dimethylbenzene	0.26	2.16	0.64	0	0.16	0	0	0
Indene	0	0.27	1.92	0	1.07	0.47	0.18	0.42
1-ethenyl-3,5-dimethylbenzene	0	0.32	0.12	0	0	0	0	0
1-methyleneindene	0	0.41	0.15	0	0.06	0	0	0
Naphthalene	0	0	1.52	0	1.03	0.65	0.12	0.5
3,5-dimethylbenzaldehyde	0	3.14	0.88	0	0.22	0.24	0	0
acenaphthylene	0	0	0.35	0.04	0.3	0.29	0.11	0.21
Benzene, 1,1'-methylenebis[3-methyl-Fluorene	0	0	0.06	0	0	0	0	0
Benzene, 1,2-dimethyl-4-(phenylmethyl)-	0	0.13	0.1	0	0	0.08	0	0.03
2,4-dimethyldiphenylmethane	0.05	0	0.08	0	0.02	0	0	0
2,3,5-trimethyldiphenylmethane	0	0.05	0	0	0	0	0	0
3,3'-dimethyldiphenylmethane	0	0.04	0	0	0	0	0	0
2,4,2',3'-tetramethylbiphenyl	0	0.01	0	0	0	0	0	0
2,3,2',3'-tetramethylbiphenyl	0	0.01	0	0	0	0	0	0
benzene,1,1'-(1,2-ethanediyl)bi[3,5-dimethyl	3.92	3.17	0	0	0.08	0.14	0	0.06
Phenanthrene	0	0.21	0.32	0	0.15	0.14	0	0
2-methylantracene	0	0.01	0	0	0	0	0	0
2-phenylnaphthalene	0	0	0.04	0	0	0	0	0
9-methylantracene	0	0.04	0.07	0	0	0	0	0
9-ethenylnaphthalene	0	0	0.09	0	0.06	0	0.02	0.04
cyclopentaphenanthrene	0	0.04	0.04	0	0.01	0.01	0	0
Fluoranthene	0	0.01	0.1	0	0.08	0.07	0.01	0.04
Pyrene	0	0	0.06	0	0.04	0.05	0	0.02
2-methylfluoranthene	0	0	0	0	0	0	0	0
2,3-benzofluorene	0	0	0.05	0	0.07	0.07	0.02	0.06
Phenylacetylene	0	0	1.65	0	0.61	0.31	0	0
1-methylfluorene	0	0	0.37	0	0	0	0	0
o-xylene	0	0.05	1.43	0.05	0.82	0.75	0.14	0.34
PRE CARBON	770.57	770.57	770.57	770.57	770.57	770.57	770.57	770.57
POST CARBON	813.58	743.68	716.27	753.97	734.11	778.93	813.78	777.93

1,3,5-trimethylbenzene oxidation average P5 =50.23 atm, $\phi = 0.95$, reaction time = 1.13 – 1.697 ms (page 3/3)

Shock number	52	54	56
Temperature (K)	1623.39	1645.02	1409.39
Pressure (atm)	41.13	39.43	48.25
Rxn Time (s)	0	0	0
O2	49.2	26.69	445.63
CO	521.79	545.18	110.78
CH4	11.25	8.65	23.4
CO2	73.95	88.49	7.77
C2H4	0	0.63	11.57
C2H6	0	0.24	3.3
C2H2	71.22	53.13	52.57
C3H6	0	0	0.2
C3H4-a	0	0	1.2
C3H4-p	0	0	2.88
1-BUTENE	0	0	0
1,3-BUTADIENE	0	0	0.45
BENZENE	0.47	0.27	9.07
TOLUENE	0.1	0.07	7.86
ETHYLBENZENE	0	0	0.15
m-+p-xylene	0	0	5.92
135tmb-GC2	0.15	0.09	11.67
Vinylacetylene	0.23	0.09	1.9
Diacetylene	3.69	2.28	5.06
Styrene	0	0	3.27
1,2,4-Trimethylbenzene	0	0	0.25
1-ethenyl-4-methylbenzene	0	0	0.77
1-ethenyl-3-methylbenzene	0	0	1.36
1-ethyl-3,5-dimethylbenzene	0	0	0.68
Indene	0	0	1.87
1-ethenyl-3,5-dimethylbenzene	0	0	0.15
1-methyleneindene	0	0	0.17
Naphthalene	0	0	1.42
3,5-dimethylbenzaldehyde	0	0	0.94
acenaphthylene	0	0	0.28
Benzene, 1,1'-methylenebis[3-methyl-	0	0	0.07
Fluorene	0	0	0.15
Benzene, 1,2-dimethyl-4-(phenylmethyl)-	0	0	0.12
2,4-dimethyldiphenylmethane	0	0	0.09
2,3,5-trimethyldiphenylmethane	0	0	0
3,3'-dimethyldiphenylmethane	0	0	0
2,4,2',3'-tetramethylbiphenyl	0	0	0
2,3,2',3'-tetramethylbiphenyl	0	0	0
benzene,1,1'-(1,2-ethanediyl)bi[3,5-dimethyl	0	0	0.51
Phenanthrene	0	0	0.37
2-methylantracene	0	0	0
2-phenylnaphthalene	0	0	0.06
9-methylantracene	0	0	0.09
9-ethenylantracene	0	0	0.11
cyclopentaphenanthrene	0	0	0.05
Fluoranthene	0	0	0.1
Pyrene	0	0	0.06
2-methylfluoranthene	0	0	0
2,3-benzofluorene	0	0	0.05
Phenylacetylene	0	0	1.85
1-methylfluorene	0	0	0
o-xylene	0	0	1.39
PRE CARBON	770.57	770.57	770.57
POST CARBON	769.98	762.76	737.57

1,3,5-Trimethylbenzene Pyrolysis

Experimental data for 1,3,5-trimethylbenzene pyrolysis, $\Phi = \infty$, average P5 = 49 atm (Page 1/3)

Shock	7	9	11	5	13	17	15
T5 Dec	1165.00	1202.96	1242.74	1261.60	1273.14	1285.96	1327.72
P5 /atm	48.96	51.59	53.60	67.67	54.32	51.46	53.54
Reac. Time	1.57E-03	1.64E-03	1.68E-03	1.76E-03	1.74E-03	1.67E-03	1.68E-03
CH4	0.00	0.00	0.00	0.00	1.04	1.14	3.63
C2H4	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C2H6	0.00	0.00	0.00	0.00	0.36	0.28	1.19
C2H2	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C3H6	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C3H4-a	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C3H4-p	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1-BUTENE	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1,3-BUTADIENE	0.00	0.00	0.00	0.00	0.00	0.00	0.03
BENZENE	0.00	0.00	0.00	0.05	0.04	0.06	0.42
TOLUENE	0.00	0.00	0.00	0.00	0.05	0.04	0.50
ETHYLBENZENE	0.00	0.00	0.00	0.06	0.00	0.00	0.00
m+p-xylene	0.00	0.00	0.00	0.51	0.57	0.83	2.72
135tmb-GC2	51.39	50.72	48.62	48.94	41.63	41.63	34.94
Vinylacetylene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Diacetylene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
o-Xylene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Styrene	0.00	0.00	0.00	0.00	0.00	0.00	0.77
Phenylacetylene	0.00	0.00	0.00	0.00	0.00	0.00	0.23
1,2,4-Trimethylbenzene	0.00	0.20	0.00	0.28	0.00	0.25	0.34
1-ethenyl-4-methylbenzene	0.00	0.00	0.00	0.00	0.00	0.00	0.29
1-ethenyl-3-methylbenzene	0.00	0.00	0.00	0.00	0.00	0.00	0.49
1-ethyl-3,5-dimethylbenzene	0.00	0.00	0.00	0.32	0.48	0.44	0.93
Indene	0.00	0.00	0.00	0.00	0.00	0.00	0.28
Benzene, 1,1'-methylenebis[3-methyl-	0.00	0.00	0.00	0.00	0.00	0.00	0.06
benzene, 1,2-dimethyl-4-(phenylmethyl	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,4-dimethyldiphenylmethane	0.00	0.04	0.10	0.33	0.32	0.25	0.65
3,3'-dimethyldiphenylmethane	0.00	0.00	0.04	0.11	0.10	0.11	0.25
2,4,2',3'-tetramethylbiphenyl	0.00	0.00	0.00	0.01	0.01	0.01	0.03
2,3,2',3'-tetramethylbiphenyl	0.00	0.00	0.00	0.00	0.01	0.00	0.02
benzene,1,1'-(1,2-ethanediyl)bi[3,5-dimet	0.57	0.89	3.13	6.48	4.76	4.64	5.35
Phenanthrene	0.00	0.00	0.00	0.10	0.07	0.08	0.55
2-methylantracene	0.00	0.00	0.00	0.00	0.00	0.00	0.09
2-phenylinaphthalene	0.00	0.00	0.00	0.00	0.00	0.00	0.10
9-methylantracene	0.00	0.00	0.00	0.00	0.00	0.00	0.06
9-ethenylantracene	0.00	0.00	0.00	0.00	0.00	0.00	0.07
cyclopentaphenanthrene	0.00	0.00	0.00	0.00	0.00	0.00	0.13
Pyrene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
methyleneindene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1-methylindene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Naphthalene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1,1'-biphenyl-3,3'-4,4'-tetramethyl	0.00	0.00	0.00	0.00	0.00	0.00	0.10
Fluorene (13)	0.00	0.00	0.00	0.00	0.00	0.00	0.01
Fluoranthene (16)	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2-methylfluoranthene (17)	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,3-benzofluorene (17)	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1-methylfluorene (14)	0.00	0.00	0.05	0.14	0.00	0.11	0.19
decahydrotriphenylene/o-terphenyl	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9-phenylantracene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1,2-benzanthracene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
chrysene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Triacetylene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1-methylnaphthalene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2-methylnaphthalene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Azulene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2-ethenylnaphthalene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Acenaphthene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Indane	0.00	0.00	0.00	0.00	0.00	0.00	0.11
1-ethynyl-3-methylbenzene	0.00	0.00	0.00	0.00	0.00	0.00	0.03
1,2-dihydronaphthalene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
diphenylethyne	0.00	0.00	0.00	0.00	0.00	0.00	0.21
1,1'-Biphenyl, 4-ethenyl-	0.00	0.00	0.00	0.00	0.00	0.00	0.03
4-methylphenanthrene	0.00	0.00	0.00	0.00	0.00	0.00	0.09
1-methylphenanthrene	0.00	0.00	0.00	0.00	0.00	0.00	0.14
Precarb	462.51	462.51	462.51	462.51	462.51	462.51	462.51
Postcarb	472.75	474.77	496.76	577.79	479.84	482.06	516.70

Experimental data for 1,3,5-trimethylbenzene pyrolysis, $\Phi = \infty$, average P5 = 49 atm (Page 2/3)

Shock	21	26	19	24	28	30	32
T5 Dec	1344.63	1371.36	1405.89	1407.33	1442.77	1482.20	1503.25
P5 /atm	49.65	49.97	55.45	51.47	47.08	44.74	43.08
Reac. Time	1.58E-03	1.58E-03	1.57E-03	1.56E-03	1.30E-03	1.53E-03	1.55E-03
CH4	4.77	9.20	17.30	15.79	21.43	22.71	23.61
C2H4	0.00	3.07	4.52	5.22	9.89	9.89	8.20
C2H6	1.76	3.15	2.33	2.78	2.18	1.50	0.67
C2H2	0.00	2.41	12.65	11.12	28.45	49.93	59.72
C3H6	0.00	0.12	0.16	0.14	0.20	0.18	0.11
C3H4-a	0.00	0.44	0.52	0.68	0.81	0.85	0.84
C3H4-p	0.00	0.69	1.22	1.10	1.44	1.75	1.72
1-BUTENE	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1,3-BUTADIENE	0.06	0.14	0.20	0.20	0.20	0.16	0.13
BENZENE	0.62	1.68	5.30	4.75	7.21	7.22	8.00
TOLUENE	0.83	2.13	4.59	4.86	3.98	2.27	1.57
ETHYLBENZENE	0.00	0.08	0.00	0.11	0.07	0.00	0.00
m-p-xylene	2.80	4.76	2.83	3.71	1.40	0.54	0.33
135tmb-GC2	25.51	22.47	6.50	8.57	3.77	1.43	0.84
Vinylacetylene	0.00	0.11	0.25	0.19	0.31	0.35	0.32
Diacetylene	0.00	0.27	1.91	1.44	4.42	8.46	13.04
o-Xylene	0.20	0.28	0.86	0.96	1.04	0.97	0.95
Styrene	1.11	2.07	3.02	3.17	2.73	1.75	1.18
Phenylacetylene	0.32	0.95	1.58	1.71	1.45	0.99	0.84
1,2,4-Trimethylbenzene	0.36	0.53	0.00	0.23	0.00	0.00	0.00
1-ethenyl-4-methylbenzene	0.52	1.15	0.73	0.88	0.32	0.00	0.00
1-ethenyl-3-methylbenzene	0.47	1.34	0.84	1.41	0.56	0.40	0.26
1-ethyl-3,5-dimethylbenzene	0.67	0.79	0.21	0.25	0.07	0.00	0.00
Indene	0.46	1.12	1.77	1.96	1.64	1.23	0.98
Benzene, 1,1'-methylenebis[3-methyl-	0.08	0.13	0.21	0.02	0.05	0.25	0.00
Benzene, 1,2-dimethyl-4-(phenylmethyl)-	0.00	0.10	0.18	0.16	0.18	0.16	0.14
2,4-dimethyldiphenylmethane	0.34	0.47	0.09	0.18	0.00	0.00	0.00
3,3'-dimethyldiphenylmethane	0.13	0.14	0.04	0.05	0.00	0.00	0.00
2,4,2',3'-tetramethylbiphenyl	0.01	0.01	0.00	0.00	0.00	0.00	0.00
2,3,2',3'-tetramethylbiphenyl	0.02	0.03	0.02	0.02	0.00	0.02	0.01
benzene,1,1'-(1,2-ethanediy)bi[3,5-dimethyl	2.85	1.93	0.61	0.55	0.13	0.12	0.08
Phenanthrene	0.44	0.56	0.89	0.88	0.65	0.62	0.48
2-methylanthracene	0.13	0.17	0.19	0.12	0.10	0.04	0.03
2-phenylnaphthalene	0.13	0.16	0.19	0.16	0.08	0.03	0.00
9-methylanthracene	0.13	0.08	0.00	0.06	0.05	0.00	0.00
9-ethenylanthracene	0.02	0.07	0.08	0.08	0.07	0.05	0.03
cyclopentaphenanthrene	0.23	0.24	0.19	0.19	0.11	0.03	0.03
Pyrene	0.03	0.04	0.10	0.02	0.12	0.11	0.18
methyleneindene	0.00	0.06	0.13	0.13	0.14	0.09	0.08
1-methylindene	0.00	0.07	0.19	0.11	0.08	0.03	0.00
Naphthalene	0.00	0.25	1.31	1.06	1.86	2.11	2.24
1,1'-biphenyl-3,3'-4,4'-tetramethyl	0.05	0.11	0.08	0.10	0.05	0.04	0.04
Fluorene (13)	0.03	0.05	0.16	0.16	0.13	0.12	0.12
Fluoranthene (16)	0.00	0.04	0.11	0.12	0.19	0.19	0.19
2-methylfluoranthene (17)	0.05	0.04	0.00	0.00	0.12	0.00	0.13
2,3-benzofluorene (17)	0.03	0.04	0.06	0.02	0.13	0.17	0.19
1-methylfluorene (14)	0.49	0.06	0.58	0.51	0.18	0.18	0.14
decahydrotriphenylene/o-terphenyl	0.03	0.05	0.05	0.01	0.16	0.02	0.11
9-phenylanthracene	0.00	0.00	0.00	0.00	0.05	0.02	0.08
1,2-benzanthracene	0.00	0.00	0.00	0.00	0.00	0.04	0.05
chrysene	0.00	0.00	0.00	0.00	0.00	0.14	0.13
Triacetylene	0.00	0.00	0.00	0.00	0.00	0.61	1.51
1-methylnaphthalene	0.00	0.03	0.05	0.06	0.06	0.05	0.04
2-methylnaphthalene	0.00	0.06	0.11	0.08	0.08	0.06	0.06
Azulene	0.00	0.00	0.02	0.01	0.02	0.04	0.02
2-ethenylnaphthalene	0.00	0.01	0.04	0.03	0.04	0.07	0.05
Acenaphthene	0.00	0.02	0.06	0.03	0.04	0.05	0.05
Indane	0.12	0.13	0.06	0.16	0.00	0.00	0.00
1-ethynyl-3-methylbenzene	0.10	0.29	0.04	0.25	0.08	0.06	0.00
1,2-dihydronaphthalene	0.00	0.10	0.15	0.11	0.14	0.07	0.00
diphenylethyne	0.13	0.09	0.03	0.02	0.01	0.00	0.00
1,1'-Biphenyl, 4-ethenyl-	0.04	0.06	0.02	0.05	0.02	0.01	0.01
4-methylphenanthrene	0.10	0.15	0.14	0.10	0.06	0.02	0.02
1-methylphenanthrene	0.26	0.00	0.29	0.09	0.11	0.03	0.05
Precarb	462.51	462.51	462.51	462.51	462.51	462.51	462.51
Postcarb	401.87	458.60	383.12	404.77	384.28	384.25	405.81

Experimental data for 1,3,5-trimethylbenzene pyrolysis, $\Phi = \infty$, average P5 = 49 atm (Page 3/3)

Shock	36	42	40	38	49	34
T5 Dec	1528.62	1568.02	1589.39	1598.86	1654.22	1662.69
P5 /atm	39.92	45.40	44.30	44.08	41.18	46.59
Reac. Time	1.55E-03	1.34E-03	1.38E-03	1.55E-03	1.29E-03	1.30E-03
CH4	22.48	18.53	14.62	14.45	6.66	5.28
C2H4	7.13	4.06	1.98	1.69	0.59	0.00
C2H6	0.55	0.27	0.18	0.15	0.14	0.00
C2H2	73.09	106.75	121.04	127.36	152.71	157.50
C3H6	0.00	0.00	0.00	0.21	0.00	0.00
C3H4-a	0.79	0.36	0.34	0.23	0.00	0.00
C3H4-p	1.50	1.25	0.48	0.54	0.00	0.00
1-BUTENE	0.00	0.00	0.00	0.00	0.00	0.00
1,3-BUTADIENE	0.09	0.05	0.03	0.03	0.00	0.00
BENZENE	7.14	3.80	2.29	2.03	0.58	0.38
TOLUENE	0.00	0.25	0.12	0.00	0.02	0.00
ETHYLBENZENE	0.00	0.00	0.00	0.00	0.00	0.00
m-+p-xylene	0.16	0.16	0.00	0.00	0.00	0.00
135tmb-GC2	0.67	0.37	0.24	0.21	0.09	0.00
Vinylacetylene	0.24	0.16	0.08	0.08	0.00	0.00
Diacetylene	16.87	25.67	28.59	27.29	30.39	31.80
o-Xylene	0.72	0.32	0.00	0.00	0.00	0.00
Styrene	0.76	0.26	0.24	0.16	0.00	0.00
Phenylacetylene	0.54	0.21	0.03	0.00	0.00	0.00
1,2,4-Trimethylbenzene	0.00	0.00	0.00	0.00	0.00	0.00
1-ethenyl-4-methylbenzene	0.00	0.00	0.00	0.00	0.00	0.00
1-ethenyl-3-methylbenzene	0.00	0.00	0.00	0.00	0.00	0.00
1-ethyl-3,5-dimethylbenzene	0.00	0.00	0.00	0.00	0.00	0.00
Indene	0.78	0.27	0.14	0.23	0.00	0.00
Benzene, 1,1'-methylenebis[3-methyl-	0.15	0.00	0.00	0.00	0.00	0.00
Benzene, 1,2-dimethyl-4-(phenylmethyl)-	0.10	0.05	0.00	0.00	0.00	0.00
2,4-dimethyldiphenylmethane	0.00	0.00	0.00	0.00	0.00	0.00
3,3'-dimethyldiphenylmethane	0.00	0.00	0.00	0.00	0.00	0.00
2,4,2',3'-tetramethylbiphenyl	0.00	0.00	0.00	0.00	0.00	0.00
2,3,2',3'-tetramethylbiphenyl	0.00	0.00	0.00	0.00	0.00	0.00
benzene,1,1'-(1,2-ethanediy)bi[3,5-dimethyl	0.09	0.07	0.05	0.05	0.00	0.04
Phenanthrene	0.38	0.14	0.08	0.07	0.00	0.00
2-methylantracene	0.01	0.00	0.00	0.00	0.00	0.00
2-phenylnaphthalene	0.00	0.00	0.00	0.00	0.00	0.00
9-methylantracene	0.00	0.00	0.00	0.00	0.00	0.00
9-ethenylantracene	0.02	0.01	0.00	0.00	0.00	0.00
cyclopentaphenanthrene	0.02	0.02	0.00	0.00	0.00	0.00
Pyrene	0.09	0.08	0.05	0.03	0.02	0.02
methyleneindene	0.05	0.00	0.00	0.00	0.00	0.00
1-methylindene	0.00	0.00	0.00	0.00	0.00	0.00
Naphthalene	1.95	0.67	0.50	0.31	0.00	0.00
1,1'-biphenyl-3,3'-4,4'-tetramethyl	0.02	0.00	0.00	0.00	0.00	0.00
Fluorene (13)	0.08	0.00	0.00	0.00	0.00	0.00
Fluoranthene (16)	0.18	0.12	0.04	0.03	0.00	0.00
2-methylfluoranthene (17)	0.01	0.00	0.00	0.00	0.00	0.00
2,3-benzofluorene (17)	0.19	0.20	0.07	0.03	0.00	0.01
1-methylfluorene (14)	0.06	0.06	0.00	0.00	0.00	0.00
decahydrotriphenylene/o-terphenyl	0.01	0.00	0.00	0.00	0.00	0.00
9-phenylantracene	0.05	0.06	0.03	0.03	0.00	0.03
1,2-benzanthracene	0.10	0.24	0.00	0.02	0.00	0.07
chrysene	0.00	0.03	0.00	0.17	0.00	0.03
Triacetylene	3.33	7.20	9.44	10.39	12.80	11.11
1-methylnaphthalene	0.01	0.00	0.00	0.00	0.00	0.00
2-methylnaphthalene	0.03	0.00	0.00	0.00	0.00	0.00
Azulene	0.01	0.00	0.00	0.00	0.00	0.00
2-ethenylnaphthalene	0.04	0.00	0.00	0.00	0.00	0.00
Acenaphthene	0.02	0.00	0.00	0.00	0.00	0.00
Indane	0.00	0.00	0.00	0.00	0.00	0.00
1-ethynyl-3-methylbenzene	0.00	0.00	0.00	0.00	0.00	0.00
1,2-dihydronaphthalene	0.00	0.00	0.00	0.00	0.00	0.00
diphenylethyne	0.00	0.00	0.00	0.00	0.00	0.00
1,1'-Biphenyl, 4-ethenyl-	0.01	0.00	0.00	0.00	0.00	0.00
4-methylphenanthrene	0.01	0.00	0.00	0.00	0.00	0.00
1-methylphenanthrene	0.07	0.02	0.01	0.01	0.00	0.00
Precarb	462.51	462.51	462.51	462.51	462.51	462.51
Postcarb	409.44	460.03	469.02	478.99	517.57	520.78

n-Propylbenzene Oxidation Model

!UIC npb Oxidation Model

!S. Gudiyella and K. Brezinsky, "High Pressure Study of n-Propylbenzene Oxidation"(2011)

!Contact: Prof. Kenneth Brezinsky, kenbrez@uic.edu

!Developed against High Temperature High Pressure Single Pulse Shock Tube species profiles

!Tested against flow reactor data of Litzinger et al., "Reactions of n-Propylbenzene During Gas Phase Oxidation", Combust. Sci. and Tech., 1986, Vol. 50, pp. 117-133

!Tested against jet stirred reactor data of Dagaut et al., "Experimental and Kinetic Modeling Study of the Oxidation of n-Propylbenzene", 2002, vol. 81 (2), pp 173-184

ELEMENTS H O C AR N HE END

SPECIES

PHC3H7 O2 CO CO2

CH4 C2H4 C2H6 C2H2

C3H8 AC3H4 PC3H4

C4H4 C4H2 C6H6 C6H5CH3 C6H5C2H

C6H5C2H3 C5H6 C6H5C2H5 C6H5CHO

C6H5OH C6H5C3H5 C6H5CH2OH

C6H5C3H5-2 PXYLENE

A2C2H INDENE C5H4O

A2 C4H6-13 FLUORENE

C14H14 C14H12

C8H6O C3H6 A2C2H

A3 C6H5CH2C6H5 C14H10

DIBZFUR

P2

C4H8-1

C4H10 C4H8-2 C4H6-12

H2CCCH AC3H5 HO2 C14H13

C2H5 C2H3 C2H CH3 CH2 CH CH2CHCHO

CH3HCO CH3CO CH2CO

CH3O CH2O HCCO HCO

H O H2O2 H2 H2O OH

N2 AR HE CH2HCO

CH2OH NC3H7 IC3H7 C4H5-N

C5H5 C5H5O C5H4OH C6H5

C6H5CH2 C6H5CO

OC6H4CH3 HOC6H4CH3 PC4H9 SC4H9 SC3H5 CH3OH

C4H5-I PC3H5

C C2 C2O C3H2

C6H2 CH2-S CH2CHCO CH3CHCO

H2C4O HCCOH HCOH

C2H5OH C2H5O PC2H4OH SC2H4OH C4H3-I C4H3-N

H2CC C4H71-1 C4H71-2 C4H71-3 C4H71-4 CH3CHCHCHO
 CH3CHCHCO CH2CHCHCHO C4H6-2 C4H5-2
 C6H5CHCH3 C6H5CH2CH2 C6H5CHCH
 C6H5CCH2 C6H4C2H
 APHC3H6 BPHC3H6 CPHC3H6 BPHPROPY
 C6H3 C6H5CH2OO C6H5CH2O
 R1C9H9 R2C9H9 R3C9H9 R13C9H9
 pc-C9H9 i-C9H9 n-C9H9
 R22C9H9 s-C9H8
 BZCOOH C6H5O C6H4CH3
 HOC6H4CH2 O-C6H4O2
 C14H11 C14H13OO C14H13OOH
 C14H12O2H-1O2 C14H12O2H-1O2
 C14H11O-1O2H C14H13O C14H12OOH
 HOC6H4CH2OO HOC6H4CH2O HOC6H4CH2OOH
 HOC6H4CHO HOC6H4CO C6H5CHOH
 C6H5OO C6H5OOH OC6H4OH C6H4OH
 P-C6H4O2 P-C6H3O2 C5H5OH
 C4H4O C#CC*CCJ C5H6-L
 C5H5OH CJ*CC*CC*O C*CC*CCJ*O
 CJ*CC*O C2H3CO C5H5OH C5H7
 C5H3O C*CCJC*C OC5H7O
 C*CCJC*COH HOC*CC*O HOC*CCJ*O
 C2H2OH OC4H6O OC4H5O HOCO
 C2H3CHO O-OC6H5OJ P-OC6H5OJ
 C*CC*CCJ C*CC*CC C*CC*CCOH
 C*CCJC*O O2CCHOOJ
 A2- INDENYL
 P2- A2C2H* A3- A3C2H
 C6H2 A1C2H3* C6H4C2H n-C8H7
 !SPECIES FROM UIC NPB PYR MODEL
 A2R5 A2R5- BGHIF A2CH3 A2CH2
 A3CH3 A3CH2 A4 C14H9 C5H4CH3 C5H4CH2
 HT1245 HD125Y m-TERPH p-TERPH HDY15
 p-TERPH A2C6H5-2
 END

REACTIONS

!S. Dooley et al., Combust. Flame, 157 (2010) 2333 - 2339

H+O2<=>O+OH	3.547E+15	-0.4060	16599.0
O+H2<=>H+OH	5.080E+04	2.6700	6290.0
H2+OH<=>H2O+H	2.160E+08	1.5100	3430.0
O+H2O<=>OH+OH	2.970E+06	2.0200	13400.0
H2+M<=>H+H+M	4.577E+19	-1.4000	104380.0
H2/2.5/ H2O/12/CO/1.9/ CO2/3.8/			
O+O+M<=>O2+M	6.165E+15	-0.5000	0.0
H2/2.5/ H2O/12/CO/1.9/ CO2/3.8/			

O+H+M<=>OH+M	4.714E+18	-1.0000	0.0
H2/2.5/ H2O/12/CO/1.9/ CO2/3.8/			
H+OH+M<=>H2O+M	3.800E+22	-2.0000	0.0
H2/2.5/ H2O/12/CO/1.9/ CO2/3.8/			
H+O2(+M) = HO2(+M)	1.475E+12	0.60	0.000E+00
LOW/9.042E+19 -1.50 4.922E+02/			
TROE/0.5 1E-30 1E+30/			
H2/3.0/ H2O/16/ O2/1.1/ CO/2.7/ CO2/5.4/			
HO2+H<=>H2+O2	1.660E+13	0.0000	823.0
HO2+H<=>OH+OH	7.079E+13	0.0000	295.0
HO2+O<=>O2+OH	3.250E+13	0.0000	0.0
HO2+OH<=>H2O+O2	2.890E+13	0.0000	-497.0
HO2+HO2<=>H2O2+O2	4.200E+14	0.0000	11982.0
DUPLICATE			
HO2+HO2<=>H2O2+O2	1.300E+11	0.0000	-1629.3
DUPLICATE			
H2O2(+M)<=>OH+OH(+M)	2.951E+14	0.0000	48430.0
LOW /1.202E+17 0.0000 45500.0/			
TROE/0.5 1E-30 1E+30/			
H2/2.5/ H2O/12/CO/1.9/ CO2/3.8/			
H2O2+H<=>H2O+OH	2.410E+13	0.0000	3970.0
H2O2+H<=>HO2+H2	4.820E+13	0.0000	7950.0
H2O2+O<=>OH+HO2	9.550E+06	2.0000	3970.0
H2O2+OH<=>HO2+H2O	1.000E+12	0.0000	0.0
DUPLICATE			
H2O2+OH<=>HO2+H2O	5.800E+14	0.0000	9557.0
DUPLICATE			
CO+O(+M)<=>CO2(+M)	1.800E+10	0.0000	2384.0
LOW /1.550E+24 -2.7900 4191.0/			
H2/2.5/ H2O/12/ CO/1.9/ CO2/3.8/			
CO+O2<=>CO2+O	2.530E+12	0.0000	47700.0
CO+HO2<=>CO2+OH	3.010E+13	0.0000	23000.0
CO+OH<=>CO2+H	2.229E+05	1.8900	-1158.7
CH4+H<=>CH3+H2	5.47E+07	1.97	11210
CH4+O<=>CH3+OH	3.15E+12	0.5	10290
CH4+OH<=>CH3+H2O	5.72E+06	1.96	2639
CH4+HO2<=>CH3+H2O2	1.81E+11	0	18580
CH2OH+H=CH3OH	9.635e+13	0.00	0.000e+00
CH3+H(+M)<=>CH4(+M)	1.270E+16	-0.6300	383.0
LOW /2.477E+33 -4.7600 2440.0/			
TROE/ 0.7830 74.00 2941.00 6964.00 /			
H2/2.0/ H2O/6.0/CO/1.5/ CO2/2.0/			
CH3+O<=>CH2O+H	8.43E+13	0	0
CH3+O2<=>CH3O+O	1.99E+18	-1.57	29230
CH3+O2<=>CH2O+OH	3.51E-01	3.524	7380
CH3+CH3(+M)<=>C2H6(+M)	2.277E+15	-0.6900	174.9
LOW /8.054E+31 -3.7500 981.6/			
TROE/0.0 570.0 0.00000001 1.E+30/			

H2O/5/ CO/2/ CO2/3/			
CH3+HO2<=>CH4+O2	3.16E+12	0	0
CH3+OH<=>CH2+H2O	5.60E+07	1.6	5420
OH+CH3(+M)<=>CH3OH(+M)	2.790E+18	-1.4300	1330.0
LOW /4.000E+36 -5.9200 3140.0/			
TROE/ .4120 195.0 5900.00 6394.00/			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/			
CH2+H2<=>CH3+H	5.00E+05	2	7230
CH3O+H<=>CH3+OH	3.20E+13	0	0
CH3+CH3<=>H+C2H5	4.99E+12	0.1	10600
CH4+CH2<=>CH3+CH3	2.46E+06	2	8270
CH4+CH2-S<=>CH3+CH3	1.60E+13	0	-570
CH3+OH<=>CH2-S+H2O	2.50E+13	0	0
CH2+H(+M)<=>CH3(+M)	2.50E+16	-0.8	0
LOW /3.200E+27 -3.1400 1230.0/			
TROE/ 0.6800 78.00 1995.00 5590.00 /			
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/			
CH2-S+H2<=>CH3+H	7.00E+13	0	0
CH2O+H<=>HCO+H2	5.740E+07	1.9000	2748.6
CH2O+O<=>HCO+OH	1.810E+13	0.0000	3080.0
CH2O+OH<=>HCO+H2O	3.430E+09	1.1800	-447.0
CH2O+M<=>HCO+H+M	3.300E+39	-6.3000	99900.0
H2/2.5/ H2O/12.0/ CO/1.9/ CO2/3.8/			
CH2O+M<=>CO+H2+M	3.100E+45	-8.0000	97510.0
H2/2.5/ H2O/12.0/ CO/1.9/ CO2/3.8/			
CH2O+HO2<=>HCO+H2O2	4.110E+04	2.5000	10210.0
CH2O+CH3<=>HCO+CH4	3.636E-06	5.4200	998.0
HCO+M =H+CO+M	4.7485e+11	0.659	1.4874e+04
H2/2.5/ H2O/6/ CO/1.9/ CO2/3.8/			
HCO+O2<=>CO+HO2	7.580E+12	0.0000	410.0
HCO+OH<=>CO+H2O	3.020E+13	0.0000	0.0
HCO+O<=>CO2+H	3.000E+13	0.0000	0.0
HCO+H<=>CO+H2	7.230E+13	0.0000	0.0
HCO+O<=>CO+OH	3.020E+13	0.0000	0.0
HCO+HO2<=>CO2+OH+H	3.000E+13	0.0000	0.0
HCO+CH3<=>CO+CH4	2.650E+13	0.0000	0.0
HCO+HCO<=>H2+CO+CO	3.000E+12	0.0000	0.0
HCO+HCO<=>CH2O+CO	3.000E+13	0.0000	0.0
CH3OH+OH<=>CH2OH+H2O	7.100E+06	1.8000	-596.0
CH3OH+OH<=>CH3O+H2O	1.000E+06	2.1000	496.7
CH3OH+O<=>CH2OH+OH	3.880E+05	2.5000	3080.0
CH3OH+H<=>CH2OH+H2	3.200E+13	0.0000	6095.0
CH3OH+H<=>CH3O+H2	8.000E+12	0.0000	6095.0
CH3OH+HO2=CH2OH+H2O2	3.980e+13	0.00	1.940e+04
H+CH2OH(+M)<=>CH3OH(+M)	1.055E+12	0.5000	86.0
LOW /4.360E+31 -4.6500 5080.0/			
TROE/ .600 100.00 90000.0 10000.0 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/			

H+CH3O(+M)<=>CH3OH(+M)	2.430E+12	0.5150	50.0
LOW /4.660E+41 -7.4400 14080.0/			
TROE/ .700 100.00 90000.0 10000.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/			
CH3OH+O2<=>CH2OH+HO2	2.050E+13	0.0000	44900.0
CH3OH+HCO<=>CH2OH+CH2O	9.635E+03	2.9000	13110.0
CH3OH+CH3<=>CH2OH+CH4	3.190E+01	3.1700	7172.0
CH3O+CH3OH<=>CH3OH+CH2OH	3.000E+11	0.0000	4060.0
CH2-S+H2O(+M) = CH3OH(+M)	4.820e+17	-1.16	1.145e+03
LOW / 1.880e+38 -6.360 5040.00/			
TROE/ .6027 208.00 3922.00 10180.0 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/			
CH3O+M<=>CH2O+H+M	8.300E+17	-1.2000	15500.0
CH3O+H<=>CH2O+H2	2.000E+13	0.0000	0.0
CH3O+OH<=>CH2O+H2O	1.800E+13	0.0000	0.0
CH3O+O<=>CH2O+OH	6.000E+12	0.0000	0.0
CH3O+O2<=>CH2O+HO2	9.033E+13	0.0000	11980.0
DUPLICATE			
CH3O+O2<=>CH2O+HO2	2.200E+10	0.0000	1748.0
DUPLICATE			
CH3O+H<=>CH2-S+H2O	1.600E+13	0.0000	0.0
CH3O+CH3<=>CH2O+CH4	1.200E+13	0.0000	0.0
CH3O+HO2<=>CH2O+H2O2	3.000E+11	0.0000	0.0
CH3O+CO<=>CH3+CO2	1.600E+13	0.0000	11800.0
CH3O+HCO<=>CH3OH+CO	9.000E+13	0.0000	0.0
CH3O+CH3O<=>CH3OH+CH2O	6.000E+13	0.0000	0.0
CH2OH+M<=>CH2O+H+M	1.000E+14	0.0000	25100.0
CH2OH+H<=>CH2O+H2	6.000E+12	0.0000	0.0
CH2OH+H<=>CH3+OH	9.635E+13	0.0000	0.0
CH2OH+OH<=>CH2O+H2O	2.400E+13	0.0000	0.0
CH2OH+O<=>CH2O+OH	4.200E+13	0.0000	0.0
CH2OH+O2<=>CH2O+HO2	2.410E+14	0.0000	5017.0
DUPLICATE			
CH2OH+O2<=>CH2O+HO2	1.510E+15	-1.0000	0.0
DUPLICATE			
CH2OH+HO2<=>CH2O+H2O2	1.200E+13	0.0000	0.0
CH2OH+HCO<=>CH3OH+CO	1.000E+13	0.0000	0.0
CH2OH+HCO<=>CH2O+CH2O	1.500E+13	0.0000	0.0
CH2OH+CH2OH<=>CH3OH+CH2O	3.000E+12	0.0000	0.0
CH2OH+CH3O<=>CH3OH+CH2O	2.400E+13	0.0000	0.0
CH2+H<=>CH+H2	1.000e+18	-1.56	0.000e+00
DUP			
CH2+H<=>CH+H2	2.700e+11	0.67	2.570e+04
DUP			
CH2+OH<=>CH2O+H	2.000E+13	0.0000	0.0
CH2+OH<=>CH+H2O	1.130e+07	2.00	3.000e+03
CH2+O<=>HCO+H	8.000E+13	0.0000	0.0
CH2+O2=HCO+OH	1.320e+13	0.00	1.500e+03

CH3+CH2=C2H4+H	4.000e+13	0.00	0.000e+00
!CH2+CH2<=>C2H2+H2	3.200E+13	0.0000	0.0
CH2+HO2<=>CH2O+OH	2.000E+13	0.0000	0.0
CH2+CH2<=>C2H2+H2	3.200E+13	0.0000	0.0
CH2-S+M<=>CH2+M	9.000E+12	0.0000	600.0
H2O/0.0/ CO/0.0/ CO2/0.0/			
CH2-S+C2H6 = CH3+C2H5	1.200e+14	0.00	0.000e+00
CH2-S+O2<=>H+OH+CO	2.800E+13	0.0000	0.0
CH2-S+O2<=>CO+H2O	1.200E+13	0.0000	0.0
CH2-S+O<=>CO+H2	1.500E+13	0.0000	0.0
CH2-S+O<=>HCO+H	1.500E+13	0.0000	0.0
CH2-S+OH<=>CH2O+H	3.000E+13	0.0000	0.0
CH2-S+H<=>CH+H2	3.000E+13	0.0000	0.0
CH3+CH2-S<=>C2H4+H	1.200E+13	0.0000	-570.0
CH2-S+CO2<=>CH2O+CO	1.400E+13	0.0000	0.0
CH2-S+H2O<=>CH2+H2O	3.000E+13	0.0000	0.0
CH2-S+CO<=>CH2+CO	9.000E+12	0.0000	0.0
CH2-S+CO2<=>CH2+CO2	7.000E+12	0.0000	0.0
CH+O2<=>HCO+O	3.300E+13	0.0000	0.0
CH+H<=>C+H2	5.000E+13	0.0000	0.0
CH+O<=>CO+H	5.700E+13	0.0000	0.0
CH+OH<=>HCO+H	3.000E+13	0.0000	0.0
CH2+H<=>CH+H2	2.700E+11	0.6700	25700.0
DUP			
CH+H2O<=>H+CH2O	1.713E+13	0.0000	-755.0
CH+CO2<=>HCO+CO	1.700E+12	0.0000	685.0
CH+CH2O<=>H+CH2CO	9.460E+13	0.0000	-515.0
C2H6+CH3<=>C2H5+CH4	1.510E-07	6.0000	6047.0
C2H6+H<=>C2H5+H2	1.150E+08	1.9000	7530.0
C2H6+O<=>C2H5+OH	3.550E+06	2.4000	5830.0
C2H6+OH<=>C2H5+H2O	1.480E+07	1.9000	950.0
C2H6+O2<=>C2H5+HO2	6.030E+13	0.0000	51870.0
C2H6+HO2<=>C2H5+H2O2	3.460E+01	3.6100	16920.0
C2H6+CH3O<=>C2H5+CH3OH	2.410E+11	0.0000	7090.0
C2H5+H(+M)<=>C2H6(+M)	5.210E+17	-0.9900	1580.0
LOW /1.990E+41 -7.0800 6685.0/			
TROE / 8.4200E-01 1.2500E+02 2.2190E+03 6.8820E+03 /			
H2/2/ H2O/6/ CO/1.5/ CO2/2/ CH4/2/ C2H6/3/			
C2H6+CH<=>C2H5+CH2	1.100E+14	0.0000	-260.0
C2H5+H<=>C2H4+H2	2.000E+12	0.0000	0.0
C2H5OH(+M) = C2H5+OH(+M)	2.400e+23	-1.62	9.954e+04
LOW / 5.1100e+85 -1.8800e+01 1.1877e+05 /			
TROE / 5.0000e-01 6.5000e+02 8.0000e+02 1.0000e+15 / !TROE fall-off reaction			
H2/2/ H2O/5/ CO/2/ CO2/3/			
C2H5OH(+M) = C2H4+H2O(+M)	2.790e+13	0.09	6.614e+04
LOW / 2.5700e+83 -1.8850e+01 8.6453e+04 /			
TROE / 7.0000e-01 3.5000e+02 8.0000e+02 3.8000e+03 / !TROE fall-off reaction			

H2O/5/			
C2H5+O<=>CH3HCO+H	1.100E+14	0.0000	0.0
C2H5+HO2<=>C2H5O+OH	1.100E+13	0.0000	0.0
C2H5+O2<=>C2H4+HO2	7.561E+14	-1.0100	4749.0
DUP			
C2H5+O2<=>C2H4+HO2	4.000E-01	3.8800	13620.0
DUP			
C2H5+O2<=>CH3HCO+OH	8.265E+02	2.4100	5285.0
C3H8(+M)<=>CH3+C2H5(+M)	1.290E+37	-5.8400	97380.0
LOW /5.640E+74 -15.7400 98714.0/			
TROE / 3.1000E-01 5.0000E+01 3.0000E+03 9.0000E+03 /			
H2/2/ H2O/6/ CO/1.5/ CO2/2/ CH4/2/ C2H6/3/			
C2H5+C2H<=>H2CCCH+CH3	1.810E+13	0.0000	0.0
C4H10(+M)<=>C2H5+C2H5(+M)	2.720E+15	0.0000	75610.0
LOW /4.720E+18 0.0000 49576.0/			
TROE / 7.2000E-01 1.5000E+03 1.0000E-10 1.0000E+10 /			
CH+CH4<=>C2H4+H	6.000E+13	0.0000	0.0
H+C2H4(+M)<=>C2H5(+M)	8.100E+11	0.4540	1820.0
LOW /9.000E+41 -7.6200 6970.0/			
TROE/ .9753 210.00 984.00 4374.00 /			
H2/2/ H2O/6/ CO/1.5/ CO2/2/ CH4/2/ C2H6/3/			
!C2H4+H<=>C2H3+H2	5.070E+07	1.9300	12950.0
C2H4+OH<=>C2H3+H2O	1.800E+06	2.0000	2500.0
C2H4+O<=>CH3+HCO	8.564E+06	1.8800	183.0
C2H4+O<=>CH2HCO+H	4.986E+06	1.8800	183.0
C2H4+CH3<=>C2H3+CH4	6.620E+00	3.7000	9500.0
C2H4(+M)<=>C2H2+H2(+M)	8.000E+12	0.4400	88770.0
LOW /1.580E+51 -9.3000 97800.0/			
TROE / 7.3500E-01 1.8000E+02 1.0350E+03 5.4170E+03 /			
H2/2/ H2O/6/ CO/1.5/ CO2/2/ CH4/2/ C2H6/3/			
C2H3+H(+M)<=>C2H4(+M)	1.360E+14	0.1700	660.0
LOW /1.400E+30 -3.8600 3320.0/			
TROE / 7.8200E-01 2.0750E+02 2.6630E+03 6.0950E+03 /			
H2/2/ H2O/6/ CO/1.5/ CO2/2/ CH4/2/ C2H6/3/			
C2H4+O2<=>C2H3+HO2	4.000E+13	0.0000	58200.0
C2H4+CH3O<=>C2H3+CH3OH	1.200E+11	0.0000	6750.0
C4H6-13+H<=>C2H4+C2H3	5.450E+30	-4.5100	21877.0
C2H3+H<=>C2H2+H2	3.000E+13	0.0000	0.0
C2H3+O2<=>HCO+CH2O	4.580E+16	-1.3900	1015.0
C2H3+O2<=>HO2+C2H2	1.337E+06	1.6100	-384.0
C2H3+O2<=>O+CH2HCO	1.000E+11	0.2900	11.0
C2H3+OH<=>C2H2+H2O	5.000E+12	0.0000	0.0
CH3+C2H3<=>CH4+C2H2	3.920E+11	0.0000	0.0
C2H3+CH3(+M) = C3H6(+M)	2.500E+13	0.0	0.0
LOW / 4.270E+58 -11.940 9769.80/			
TROE / 0.175 1340.6 60000.0 10139.8 /			
H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/C2H2/3.00/ C2H4/3.00/			
C2H2+H(+M)<=>C2H3(+M)	5.600E+12	0.0000	2400.0

LOW /3.800E+40 -7.2700 7220.0/
 TROE / 7.5100E-01 9.8500E+01 1.3020E+03 4.1670E+03 /
 H2/2/ H2O/6/ CO/1.5/ CO2/2/ CH4/2/ C2H6/3/
 C2H2+OH<=>C2H+H2O 3.370E+07 2.0000 14000.0
 C2H2+OH<=>CH2CO+H 3.236E+13 0.0000 12000.0
 C2H2+OH<=>CH3+CO 4.830E-04 4.0000 -2000.0
 O+C2H2<=>C2H+OH 4.600E+19 -1.4000 28950.0
 C2H2+O<=>CH2+CO 6.940E+06 2.0000 1900.0
 C2H2+O<=>HCCO+H 1.350E+07 2.0000 1900.0
 C2H+H(+M)<=>C2H2(+M) 1.000E+17 0.0000 0.0
 LOW /3.750E+33 -4.8000 1900.0/
 TROE / 6.4600E-01 1.3200E+02 1.3150E+03 5.5660E+03 /
 H2/2/ H2O/6/ CO/1.5/ CO2/2/ CH4/2/ C2H6/3/
 C2H2+O2<=>HCCO+OH 2.000E+08 1.5000 30100.0
 CH3HCO+OH<=>CH3CO+H2O 2.000E+06 1.8000 1300.0
 CH3HCO+H<=>CH3CO+H2 1.110E+13 0.0000 3110.0
 CH3HCO+O<=>CH3CO+OH 5.940E+12 0.0000 1868.0
 CH3HCO+HO2<=>CH3CO+H2O2 3.010E+12 0.0000 11920.0
 CH3HCO+O2<=>CH3CO+HO2 3.010E+13 0.0000 39150.0
 CH3HCO+CH3<=>CH3CO+CH4 1.760E+03 2.7900 4950.0
 CH3HCO+H<=>C2H5O 8.000E+12 0.0000 6400.0
 CH3HCO+OH<=>CH2HCO+H2O 1.720E+05 2.4000 815.0
 CH3+HCO<=>CH3HCO 1.750E+13 0.0000 0.0
 CH2CO + H = CH2HCO 5.000E+13 0.00 1.230e+04
 CH2HCO+O2 = CH2O+CO+OH 2.000e+13 0.00 4.200e+03
 CH3CO(+M)<=>CH3+CO(+M) 3.000E+12 0.0000 16720.0
 LOW /1.200E+15 0.0000 12518.0/
 CH3CO+H<=>CH2CO+H2 2.000E+13 0.0000 0.0
 CH3CO+O<=>CH2CO+OH 2.000E+13 0.0000 0.0
 CH3CO+CH3<=>CH2CO+CH4 5.000E+13 0.0000 0.0
 CH2CO+H<=>CH3+CO 1.100E+13 0.0000 3400.0
 CH2CO+H<=>HCCO+H2 2.000E+14 0.0000 8000.0
 CH2CO+O<=>CH2+CO2 1.750E+12 0.0000 1350.0
 CH2CO+O<=>HCCO+OH 1.000E+13 0.0000 8000.0
 CH2CO+OH<=>HCCO+H2O 1.000E+13 0.0000 2000.0
 CH2CO+OH<=>CH2OH+CO 2.000E+12 0.0000 -1010.0
 H+HCCOH<=>H+CH2CO 1.000E+13 0.0000 0.0
 !HCCO+OH<=>H2+CO+CO 1.000E+14 0.0000 0.0
 !H+HCCO<=>CH2-S+CO 1.100E+13 0.0000 0.0
 !HCCO+O<=>H+CO+CO 8.000E+13 0.0000 0.0
 !HCCO+O2<=>OH+CO+CO 4.200E+10 0.0000 850.0
 !HCCO+M<=>CH+CO+M 6.500E+15 0.0000 58820.0
 C2H5O+O2<=>CH3HCO+HO2 4.280E+10 0.0000 1097.0
 CH3+CH2O<=>C2H5O 3.000E+11 0.0000 6336.0
 C2H5OH(+M)<=>CH3HCO+H2(+M) 7.240E+11 0.1000 91010.0
 LOW /4.460E+87 -19.4200 115580.0/
 TROE / 9.0000E-01 9.0000E+02 1.1000E+03 3.5000E+03 /
 H2O/5/

C2H5OH+O2<=>PC2H4OH+HO2	2.000E+13	0.0000	52800.0
C2H5OH+O2<=>SC2H4OH+HO2	1.500E+13	0.0000	50150.0
C2H5OH+OH<=>PC2H4OH+H2O	1.740E+11	0.2700	600.0
C2H5OH+OH<=>SC2H4OH+H2O	4.640E+11	0.1500	0.0
C2H5OH+OH<=>C2H5O+H2O	7.460E+11	0.3000	1634.0
C2H5OH+H<=>PC2H4OH+H2	1.230E+07	1.8000	5098.0
C2H5OH+H<=>SC2H4OH+H2	2.580E+07	1.6500	2827.0
C2H5OH+H<=>C2H5O+H2	1.500E+07	1.6000	3038.0
C2H5OH+HO2<=>PC2H4OH+H2O2	1.230E+04	2.5500	15750.0
C2H5OH+HO2<=>SC2H4OH+H2O2	8.200E+03	2.5500	10750.0
C2H5OH+HO2<=>C2H5O+H2O2	2.500E+12	0.0000	24000.0
C2H5OH+O<=>PC2H4OH+OH	9.410E+07	1.7000	5459.0
C2H5OH+O<=>SC2H4OH+OH	1.880E+07	1.8500	1824.0
C2H5OH+O<=>C2H5O+OH	1.580E+07	2.0000	4448.0
C2H5OH+CH3<=>PC2H4OH+CH4	1.330E+02	3.1800	9362.0
C2H5OH+CH3<=>SC2H4OH+CH4	4.440E+02	2.9000	7690.0
C2H5OH+CH3<=>C2H5O+CH4	1.340E+02	2.9200	7452.0
C2H5OH+C2H5<=>PC2H4OH+C2H6	5.000E+10	0.0000	13400.0
C2H5OH+C2H5<=>SC2H4OH+C2H6	5.000E+10	0.0000	10400.0
C2H4+OH<=>PC2H4OH	4.170E+20	-2.8400	1240.0
SC2H4OH+M<=>CH3HCO+H+M	1.000E+14	0.0000	25000.0
SC2H4OH+O2<=>CH3HCO+HO2	3.810E+06	2.0000	1641.0
NC3H7+H<=>C3H8	1.000E+14	0.0000	0.0
IC3H7+H<=>C3H8	1.000E+14	0.0000	0.0
C3H8+O2<=>IC3H7+HO2	2.000E+13	0.0000	49640.0
C3H8+O2<=>NC3H7+HO2	6.000E+13	0.0000	52290.0
H+C3H8<=>H2+IC3H7	1.300E+06	2.4000	4471.0
H+C3H8<=>H2+NC3H7	1.330E+06	2.5400	6756.0
C3H8+O<=>IC3H7+OH	5.490E+05	2.5000	3140.0
C3H8+O<=>NC3H7+OH	3.710E+06	2.4000	5505.0
C3H8+OH<=>NC3H7+H2O	1.054E+10	0.9700	1586.0
C3H8+OH<=>IC3H7+H2O	4.670E+07	1.6100	-35.0
C3H8+HO2<=>IC3H7+H2O2	5.880E+04	2.5000	14860.0
C3H8+HO2<=>NC3H7+H2O2	8.100E+04	2.5000	16690.0
CH3+C3H8<=>CH4+IC3H7	6.400E+04	2.1700	7520.0
CH3+C3H8<=>CH4+NC3H7	9.040E-01	3.6500	7154.0
IC3H7+C3H8<=>NC3H7+C3H8	3.000E+10	0.0000	12900.0
C2H3+C3H8<=>C2H4+IC3H7	1.000E+11	0.0000	10400.0
C2H3+C3H8<=>C2H4+NC3H7	1.000E+11	0.0000	10400.0
C2H5+C3H8<=>C2H6+IC3H7	1.000E+11	0.0000	10400.0
C2H5+C3H8<=>C2H6+NC3H7	1.000E+11	0.0000	10400.0
C3H8+AC3H5<=>NC3H7+C3H6	7.940E+11	0.0000	20500.0
C3H8+AC3H5<=>IC3H7+C3H6	7.940E+11	0.0000	16200.0
C3H8+CH3O<=>NC3H7+CH3OH	3.000E+11	0.0000	7000.0
C3H8+CH3O<=>IC3H7+CH3OH	3.000E+11	0.0000	7000.0
NC3H7<=>CH3+C2H4	9.970E+40	-8.6000	41430.0
NC3H7<=>H+C3H6	8.780E+39	-8.1000	46580.0
NC3H7+O2<=>C3H6+HO2	3.000E-19	0.0000	3000.0

H+C3H6<=>IC3H7	2.640E+13	0.0000	2160.0
IC3H7+H<=>C2H5+CH3	2.000E+13	0.0000	0.0
IC3H7+O2<=>C3H6+HO2	4.500E-19	0.0000	5020.0
IC3H7+OH<=>C3H6+H2O	2.410E+13	0.0000	0.0
IC3H7+O<=>CH3HCO+CH3	4.818E+13	0.0000	0.0
!TC3H5 in the mech replaced with PC3H5			
C3H6<=>SC3H5+H	7.710E+69	-16.0900	140000.0
C3H6<=>PC3H5+H	5.620E+71	-16.5800	139300.0
C3H6+O<=>C2H5+HCO	1.580E+07	1.7600	-1216.0
C3H6+O<=>CH2CO+CH3+H	2.500E+07	1.7600	76.0
C3H6+O<=>CH3CHCO+H+H	2.500E+07	1.7600	76.0
C3H6+O<=>AC3H5+OH	5.240E+11	0.7000	5884.0
C3H6+O<=>SC3H5+OH	1.200E+11	0.7000	8959.0
C3H6+O<=>PC3H5+OH	6.030E+10	0.7000	7632.0
C3H6+OH<=>AC3H5+H2O	3.120E+06	2.0000	-298.0
C3H6+OH<=>SC3H5+H2O	2.110E+06	2.0000	2778.0
C3H6+OH<=>PC3H5+H2O	1.110E+06	2.0000	1451.0
C3H6+HO2<=>AC3H5+H2O2	2.700E+04	2.5000	12340.0
C3H6+HO2<=>SC3H5+H2O2	1.800E+04	2.5000	27620.0
C3H6+HO2<=>PC3H5+H2O2	9.000E+03	2.5000	23590.0
C3H6+H<=>C2H4+CH3	3.300E+24	-3.0400	15610.0
C3H6+H<=>AC3H5+H2	1.730E+05	2.5000	2490.0
C3H6+H<=>PC3H5+H2	4.000E+05	2.5000	9790.0
C3H6+H<=>SC3H5+H2	8.040E+05	2.5000	12283.0
C3H6+O2<=>AC3H5+HO2	4.000E+12	0.0000	39900.0
C3H6+O2<=>SC3H5+HO2	2.000E+12	0.0000	62900.0
C3H6+O2<=>PC3H5+HO2	1.400E+12	0.0000	60700.0
C3H6+CH3<=>AC3H5+CH4	2.210E+00	3.5000	5675.0
C3H6+CH3<=>SC3H5+CH4	1.348E+00	3.5000	12850.0
C3H6+CH3<=>PC3H5+CH4	8.400E-01	3.5000	11660.0
C3H6+C2H5<=>AC3H5+C2H6	1.000E+11	0.0000	9800.0
AC3H5+H(+M)<=>C3H6(+M)	2.000E+14	0.0000	0.0
LOW /1.330E+60 -12.0000 5967.8/			
TROE / 0.020 1096.6 1096.6 6859.5 /			
H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/			
AC3H5+H<=>AC3H4+H2	1.800E+13	0.0000	0.0
AC3H5+O<=>CH2CHCHO+H	6.000E+13	0.0000	0.0
AC3H5+OH<=>CH2CHCHO+H+H	1.600E+20	-1.5600	26330.0
AC3H5+OH<=>AC3H4+H2O	6.000E+12	0.0000	0.0
AC3H5+O2<=>AC3H4+HO2	2.180E+21	-2.8500	30755.0
AC3H5+O2<=>CH3CO+CH2O	7.140E+15	-1.2100	21046.0
AC3H5+O2<=>CH2CHCHO+OH	2.470E+13	-0.4500	23017.0
AC3H5+HCO<=>C3H6+CO	6.000E+13	0.0000	0.0
AC3H5+CH3(+M)<=>C4H8-1(+M)	1.000E+14	-0.3200	-262.3
LOW /3.910E+60 -12.8100 6250.0/			
TROE / 0.104 1606.0 60000.0 6118.4 /			
H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/			
AC3H5+CH3<=>AC3H4+CH4	3.000E+12	-0.3200	-131.0

AC3H5<=>PC3H5	4.860E+53	-12.8100	75883.0
AC3H5<=>SC3H5	9.700E+48	-11.7300	73700.0
C2H2+CH3<=>AC3H5	1.040E+51	-11.8900	36476.0
AC3H5+C2H5<=>C2H6+AC3H4	4.000E+11	0.0000	0.0
AC3H5+C2H5<=>C2H4+C3H6	4.000E+11	0.0000	0.0
AC3H5+C2H3<=>C2H4+AC3H4	1.000E+12	0.0000	0.0
AC3H5+AC3H5<=>AC3H4+C3H6	8.430E+10	0.0000	-262.0
C2H2+CH3<=>SC3H5	2.400E+38	-8.2100	17100.0
SC3H5+H<=>PC3H4+H2	3.340E+12	0.0000	0.0
SC3H5+O<=>C2H4+HCO	6.000E+13	0.0000	0.0
SC3H5+OH<=>C2H4+HCO+H	5.000E+12	0.0000	0.0
SC3H5+O2<=>CH3HCO+HCO	1.000E+11	0.0000	0.0
SC3H5+HO2<=>C2H4+HCO+OH	2.000E+13	0.0000	0.0
SC3H5+HCO<=>C3H6+CO	9.000E+13	0.0000	0.0
SC3H5+CH3<=>PC3H4+CH4	1.000E+11	0.0000	0.0
C2H2+CH3<=>PC3H5	7.310E+25	-5.0600	21150.0
PC3H5<=>SC3H5	5.100E+52	-13.3700	57200.0
PC3H5+H<=>PC3H4+H2	3.340E+12	0.0000	0.0
PC3H5+O<=>CH3+CH2CO	6.000E+13	0.0000	0.0
PC3H5+OH<=>CH3+CH2CO+H	5.000E+12	0.0000	0.0
PC3H5+O2<=>CH3CO+CH2O	1.000E+11	0.0000	0.0
PC3H5+HO2<=>CH3+CH2CO+OH	2.000E+13	0.0000	0.0
PC3H5+HCO<=>C3H6+CO	9.000E+13	0.0000	0.0
PC3H5+CH3<=>PC3H4+CH4	1.000E+11	0.0000	0.0
C2H2+CH3<=>AC3H4+H	9.200E+10	0.5400	23950.0
AC3H4+H<=>H2CCCH+H2	1.300E+06	2.0000	5500.0
AC3H4+H<=>SC3H5	2.600E+31	-6.2300	18700.0
AC3H4+H<=>PC3H5	6.980E+44	-9.7000	14032.0
AC3H4+H<=>AC3H5	7.340E+54	-12.0900	26187.0
AC3H4+O<=>C2H4+CO	2.000E+07	1.8000	1000.0
AC3H4+OH<=>H2CCCH+H2O	5.300E+06	2.0000	2000.0
AC3H4+CH3<=>H2CCCH+CH4	1.300E+12	0.0000	7700.0
AC3H4+C2H<=>C2H2+H2CCCH	1.000E+13	0.0000	0.0
AC3H4+AC3H4<=>AC3H5+H2CCCH	5.000E+14	0.0000	64746.7
AC3H4+AC3H5<=>H2CCCH+C3H6	2.000E+11	0.0000	7700.0
PC3H4<=>AC3H4	3.120E+58	-13.0700	92680.0
PC3H4+H<=>AC3H4+H	1.930E+18	-1.0100	11523.0
PC3H4+H<=>PC3H5	9.620E+47	-10.5500	15910.0
PC3H4+H<=>SC3H5	1.000E+34	-6.8800	8900.0
PC3H4+H<=>AC3H5	9.020E+59	-13.8900	33953.0
PC3H4+H<=>H2CCCH+H2	1.300E+06	2.0000	5500.0
PC3H4+H2CCCH<=>AC3H4+H2CCCH	6.140E+06	1.7400	10450.0
PC3H4+O<=>HCCO+CH3	7.300E+12	0.0000	2250.0
PC3H4+O<=>C2H4+CO	1.000E+13	0.0000	2250.0
PC3H4+OH<=>H2CCCH+H2O	1.000E+06	2.0000	100.0
PC3H4+C2H<=>C2H2+H2CCCH	1.000E+13	0.0000	0.0
PC3H4+CH3<=>H2CCCH+CH4	1.800E+12	0.0000	7700.0
C2H2+CH3<=>PC3H4+H	2.510E+11	0.5600	15453.0

PC3H4+C2H3<=>H2CCCH+C2H4	1.000E+12	0.0000	7700.0
PC3H4+AC3H5<=>H2CCCH+C3H6	1.000E+12	0.0000	7700.0
H2CCCH+H<=>PC3H4	1.500E+13	0.0000	0.0
H2CCCH+H<=>AC3H4	2.500E+12	0.0000	0.0
H2CCCH+H<=>C3H2+H2	5.000E+13	0.0000	1000.0
H2CCCH+O<=>CH2O+C2H	2.000E+13	0.0000	0.0
H2CCCH+OH<=>C3H2+H2O	2.000E+13	0.0000	0.0
H2CCCH+O2<=>CH2CO+HCO	3.000E+10	0.0000	2868.0
H2CCCH+HO2<=>OH+CO+C2H3	8.000E+11	0.0000	0.0
H2CCCH+HO2<=>AC3H4+O2	3.000E+11	0.0000	0.0
H2CCCH+HO2<=>PC3H4+O2	2.500E+12	0.0000	0.0
H2CCCH+HCO<=>AC3H4+CO	2.500E+13	0.0000	0.0
H2CCCH+HCO<=>PC3H4+CO	2.500E+13	0.0000	0.0
H2CCCH+HCCO<=>C4H4+CO	2.500E+13	0.0000	0.0
H2CCCH+CH<=>C4H3-I+H	5.000E+13	0.0000	0.0
H2CCCH+CH2<=>C4H4+H	5.000E+13	0.0000	0.0
H2CCCH+CH3(+M)<=>C4H6-12(+M)	1.500E+12	0.0000	0.0
LOW /2.600E+57 -11.9400 9770.0/			
TROE /0.175 1340.6 60000.0 9769.8/			
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/			
C3H2+H<=>H2CCCH	1.000E+13	0.0000	0.0
C3H2+O<=>C2H2+CO	6.800E+13	0.0000	0.0
C3H2+OH<=>HCO+C2H2	6.800E+13	0.0000	0.0
C3H2+O2<=>HCCO+H+CO	2.000E+12	0.0000	1000.0
C3H2+CH<=>C4H2+H	5.000E+13	0.0000	0.0
C3H2+CH2<=>C4H3-N+H	5.000E+13	0.0000	0.0
C3H2+CH3<=>C4H4+H	5.000E+12	0.0000	0.0
C3H2+HCCO<=>C4H3-N+CO	1.000E+13	0.0000	0.0
C3H2+O2<=>HCO+HCCO	5.000E+13	0.0000	0.0
CH3CHCO+OH<=>C2H5+CO2	1.730E+12	0.0000	-1010.0
CH3CHCO+OH<=>SC2H4OH+CO	2.000E+12	0.0000	-1010.0
CH3CHCO+H<=>C2H5+CO	4.400E+12	0.0000	1459.0
CH3CHCO+O<=>CH3HCO+CO	3.200E+12	0.0000	-437.0
CH2CHCHO+H<=>CH2CHCO+H2	1.340E+13	0.0000	3300.0
CH2CHCHO+O<=>CH2CHCO+OH	5.940E+12	0.0000	1868.0
CH2CHCHO+H<=>C2H4+HCO	2.000E+13	0.0000	3500.0
CH2CHCHO+O<=>CH2CO+HCO+H	5.000E+07	1.7600	76.0
CH2CHCHO+OH<=>CH2CHCO+H2O	9.240E+06	1.5000	-962.0
CH2CHCHO+O2<=>CH2CHCO+HO2	1.005E+13	0.0000	40700.0
CH2CHCHO+HO2<=>CH2CHCO+H2O2	3.010E+12	0.0000	11920.0
CH2CHCHO+CH3<=>CH2CHCO+CH4	2.608E+06	1.7800	5911.0
CH2CHCHO+C2H3<=>CH2CHCO+C2H4	1.740E+12	0.0000	8440.0
CH2CHCHO+CH3O<=>CH2CHCO+CH3OH	1.000E+12	0.0000	3300.0
C2H3+CO<=>CH2CHCO	1.510E+11	0.0000	4810.0
CH2CHCO+O2<=>CH2HCO+CO2	5.400E+20	-2.7200	7000.0
CH2CHCO+O<=>C2H3+CO2	1.000E+14	0.0000	0.0
C4H4+H<=>C4H5-I	4.900E+51	-11.9200	17700.0
C4H4+H<=>C4H3-N+H2	6.650E+05	2.5300	12240.0

C4H4+H<=>C4H3-I+H2	3.330E+05	2.5300	9240.0
C4H4+OH<=>C4H3-N+H2O	3.100E+07	2.0000	3430.0
C4H4+OH<=>C4H3-I+H2O	1.550E+07	2.0000	430.0
C4H4+O<=>H2CCCH+HCO	6.000E+08	1.4500	-860.0
C4H4+H<=>C4H5-N	1.300E+51	-11.9200	16500.0
C4H3-I+H<=>C4H4	3.400E+43	-9.0100	12120.0
H2CC+C2H2(+M)<=>C4H4(+M)	3.500E+05	2.0550	-2400.0
LOW /1.400E+60 -12.5990 7417.0/			
TROE /0.980 56.0 580.0 4164.0 /			
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/			
C2H2/3.00/ C2H4/3.00/			
H2CC+H<=>C2H2+H	1.000E+14	0.0000	0.0
H2CC+OH<=>CH2CO+H	2.000E+13	0.0000	0.0
H2CC+O2<=>HCO+HCO	1.000E+13	0.0000	0.0
C4H3-N<=>C4H3-I	4.100E+43	-9.4900	53000.0
C4H3-N+H<=>C4H3-I+H	2.500E+20	-1.6700	10800.0
C4H3-N+H<=>C2H2+H2CC	6.300E+25	-3.3400	10014.0
C4H3-N+H<=>C4H4	2.000E+47	-10.2600	13070.0
C4H3-N+H<=>C4H2+H2	3.000E+13	0.0000	0.0
C4H3-N+OH<=>C4H2+H2O	2.000E+12	0.0000	0.0
C4H3-I+H<=>C2H2+H2CC	2.800E+23	-2.5500	10780.0
C4H3-I+H<=>C4H2+H2	6.000E+13	0.0000	0.0
C4H3-I+OH<=>C4H2+H2O	4.000E+12	0.0000	0.0
C4H3-I+O2<=>HCCO+CH2CO	7.860E+16	-1.8000	0.0
C4H3-I+CH2<=>AC3H4+C2H	2.000E+13	0.0000	0.0
C4H2+H<=>C4H3-N	1.100E+42	-8.7200	15300.0
C4H2+H<=>C4H3-I	1.100E+30	-4.9200	10800.0
C4H10(+M)<=>NC3H7+CH3(+M)	4.280E+14	0.0000	69900.0
LOW /5.340E+17 0.0000 42959.0/			
TROE / 7.2000E-01 1.5000E+03 1.0000E-10 1.0000E+10 /			
PC4H9+H<=>C4H10	3.610E+13	0.0000	0.0
SC4H9+H<=>C4H10	3.610E+13	0.0000	0.0
C4H10+O2<=>PC4H9+HO2	6.000E+13	0.0000	52340.0
C4H10+O2<=>SC4H9+HO2	4.000E+13	0.0000	49800.0
C4H10+AC3H5<=>PC4H9+C3H6	7.940E+11	0.0000	20500.0
C4H10+AC3H5<=>SC4H9+C3H6	3.160E+11	0.0000	16400.0
C4H10+C2H5<=>PC4H9+C2H6	1.580E+11	0.0000	12300.0
C4H10+C2H5<=>SC4H9+C2H6	1.000E+11	0.0000	10400.0
C4H10+C2H3<=>PC4H9+C2H4	1.000E+12	0.0000	18000.0
C4H10+C2H3<=>SC4H9+C2H4	8.000E+11	0.0000	16800.0
C4H10+CH3<=>PC4H9+CH4	9.040E-01	3.6500	7154.0
C4H10+CH3<=>SC4H9+CH4	3.020E+00	3.4600	5481.0
C4H10+H<=>PC4H9+H2	1.880E+05	2.7500	6280.0
C4H10+H<=>SC4H9+H2	2.600E+06	2.4000	4471.0
C4H10+OH<=>PC4H9+H2O	1.054E+10	0.9700	1586.0
C4H10+OH<=>SC4H9+H2O	9.340E+07	1.6100	-35.0
C4H10+O<=>PC4H9+OH	1.130E+14	0.0000	7850.0
C4H10+O<=>SC4H9+OH	5.620E+13	0.0000	5200.0

C4H10+HO2<=>PC4H9+H2O2	8.100E+04	2.5000	16690.0
C4H10+HO2<=>SC4H9+H2O2	1.176E+05	2.5000	14860.0
C4H10+CH3O<=>PC4H9+CH3OH	3.000E+11	0.0000	7000.0
C4H10+CH3O<=>SC4H9+CH3OH	6.000E+11	0.0000	7000.0
C4H10+C2H5O<=>PC4H9+C2H5OH	3.000E+11	0.0000	7000.0
C4H10+C2H5O<=>SC4H9+C2H5OH	6.000E+11	0.0000	7000.0
C4H10+PC4H9<=>SC4H9+C4H10	1.000E+11	0.0000	10400.0
C2H5+C2H4<=>PC4H9	1.320E+04	2.4800	6130.0
C3H6+CH3<=>SC4H9	1.760E+04	2.4800	6130.0
C4H8-1+H<=>PC4H9	2.500E+11	0.5100	2620.0
C4H8-2+H<=>SC4H9	2.500E+11	0.5100	2620.0
C4H8-1+H<=>SC4H9	4.240E+11	0.5100	1230.0
PC4H9+O2<=>C4H8-1+HO2	2.000E-18	0.0000	5000.0
SC4H9+O2<=>C4H8-1+HO2	2.000E-18	0.0000	5000.0
SC4H9+O2<=>C4H8-2+HO2	2.000E-18	0.0000	5000.0
C2H3+C2H5<=>C4H8-1	9.000E+12	0.0000	0.0
C4H8-1+O2<=>C4H71-3+HO2	2.000E+13	0.0000	37190.0
C4H8-1+H<=>C4H71-1+H2	7.810E+05	2.5000	12290.0
C4H8-1+H<=>C4H71-2+H2	3.900E+05	2.5000	5821.0
C4H8-1+H<=>C4H71-3+H2	3.376E+05	2.3600	207.0
C4H8-1+H<=>C4H71-4+H2	6.651E+05	2.5400	6756.0
C4H8-1+OH<=>C4H71-1+H2O	2.140E+06	2.0000	2778.0
C4H8-1+OH<=>C4H71-2+H2O	2.220E+06	2.0000	1451.0
C4H8-1+OH<=>C4H71-3+H2O	2.764E+04	2.6400	-1919.0
C4H8-1+OH<=>C4H71-4+H2O	5.270E+09	0.9700	1586.0
C4H8-1+CH3<=>C4H71-3+CH4	3.690E+00	3.3100	4002.0
C4H8-1+CH3<=>C4H71-4+CH4	4.520E-01	3.6500	7154.0
C4H8-1+HO2<=>C4H71-3+H2O2	4.820E+03	2.5500	10530.0
C4H8-1+HO2<=>C4H71-4+H2O2	2.380E+03	2.5500	16490.0
C4H8-1+CH3O<=>C4H71-3+CH3OH	4.000E+01	2.9000	8609.0
C4H8-1+CH3O<=>C4H71-4+CH3OH	2.170E+11	0.0000	6458.0
C4H8-1+AC3H5<=>C4H71-3+C3H6	7.900E+10	0.0000	12400.0
H+C4H71-3<=>C4H8-2	5.000E+13	0.0000	0.0
C4H8-2+O2<=>C4H71-3+HO2	4.000E+13	0.0000	39390.0
C4H8-2+H<=>C4H71-3+H2	3.460E+05	2.5000	2492.0
C4H8-2+OH<=>C4H71-3+H2O	6.240E+06	2.0000	-298.0
C4H8-2+CH3<=>C4H71-3+CH4	4.420E+00	3.5000	5675.0
C4H8-2+HO2<=>C4H71-3+H2O2	1.928E+04	2.6000	13910.0
C4H8-2+CH3O<=>C4H71-3+CH3OH	1.800E+01	2.9500	11990.0
C2H2+C2H5<=>C4H71-1	2.000E+11	0.0000	7800.0
AC3H4+CH3<=>C4H71-2	2.000E+11	0.0000	7800.0
C2H4+C2H3<=>C4H71-4	2.000E+11	0.0000	7800.0
C4H6-13+H<=>C4H71-3	4.000E+13	0.0000	1300.0
C4H71-3+C2H5<=>C4H8-1+C2H4	2.590E+12	0.0000	-131.0
C4H71-3+CH3O<=>C4H8-1+CH2O	2.410E+13	0.0000	0.0
C4H71-3+O<=>CH2CHCHO+CH3	6.030E+13	0.0000	0.0
AC3H5+C4H71-3<=>C3H6+C4H6-13	6.310E+12	0.0000	0.0
C4H71-3+O2<=>C4H6-13+HO2	1.000E+09	0.0000	0.0

H+C4H71-3<=>C4H6-13+H2	3.160E+13	0.0000	0.0
C2H5+C4H71-3<=>C4H6-13+C2H6	3.980E+12	0.0000	0.0
C2H3+C4H71-3<=>C2H4+C4H6-13	3.980E+12	0.0000	0.0
C4H71-3+C4H71-3<=>C4H8-1+C4H6-13	1.600E+12	0.0000	0.0
C4H71-4<=>C4H6-13+H	1.850E+48	-10.5000	51770.0
C4H6-13<=>C4H5-I+H	5.700E+36	-6.2700	112353.0
C4H6-13<=>C4H5-N+H	5.300E+44	-8.6200	123608.0
C4H6-13<=>C4H4+H2	2.500E+15	0.0000	94700.0
C4H6-13+H<=>C4H5-N+H2	1.330E+06	2.5300	12240.0
C4H6-13+H<=>C4H5-I+H2	6.650E+05	2.5300	9240.0
C4H6-13+H<=>PC3H4+CH3	2.000E+12	0.0000	7000.0
C4H6-13+H<=>AC3H4+CH3	2.000E+12	0.0000	7000.0
C4H6-13+O<=>C4H5-N+OH	7.500E+06	1.9000	3740.0
C4H6-13+O<=>C4H5-I+OH	7.500E+06	1.9000	3740.0
C4H6-13+O<=>CH3CHCHCO+H	1.500E+08	1.4500	-860.0
C4H6-13+O<=>CH2CHCHCHO+H	4.500E+08	1.4500	-860.0
C4H6-13+OH<=>C4H5-N+H2O	6.200E+06	2.0000	3430.0
C4H6-13+OH<=>C4H5-I+H2O	3.100E+06	2.0000	430.0
C4H6-13+CH3<=>C4H5-N+CH4	2.000E+14	0.0000	22800.0
C4H6-13+CH3<=>C4H5-I+CH4	1.000E+14	0.0000	19800.0
C4H6-13+C2H3<=>C4H5-N+C2H4	5.000E+13	0.0000	22800.0
C4H6-13+C2H3<=>C4H5-I+C2H4	2.500E+13	0.0000	19800.0
C4H6-13+H2CCCH<=>C4H5-N+AC3H4	1.000E+13	0.0000	22500.0
C4H6-13+H2CCCH<=>C4H5-I+AC3H4	5.000E+12	0.0000	19500.0
C4H6-13+AC3H5<=>C4H5-N+C3H6	1.000E+13	0.0000	22500.0
C4H6-13+AC3H5<=>C4H5-I+C3H6	5.000E+12	0.0000	19500.0
C4H6-12<=>C4H5-I+H	4.200E+15	0.0000	92600.0
C4H6-12+H<=>C4H5-I+H2	1.700E+05	2.5000	2490.0
C4H6-12+CH3<=>C4H5-I+CH4	7.000E+13	0.0000	18500.0
C4H6-12+O<=>C4H5-I+OH	1.800E+11	0.7000	5880.0
C4H6-12+OH<=>C4H5-I+H2O	3.100E+06	2.0000	-298.0
C4H6-12<=>C4H6-13	3.000E+13	0.0000	65000.0
C4H6-2<=>C4H6-13	3.000E+13	0.0000	65000.0
C4H6-2<=>C4H6-12	3.000E+13	0.0000	67000.0
C4H6-2+H<=>C4H6-12+H	2.000E+13	0.0000	4000.0
C4H6-2+H<=>C4H5-2+H2	3.400E+05	2.5000	2490.0
C4H6-2+H<=>CH3+PC3H4	2.600E+05	2.5000	1000.0
C4H6-2<=>H+C4H5-2	5.000E+15	0.0000	87300.0
C4H6-2+CH3<=>C4H5-2+CH4	1.400E+14	0.0000	18500.0
C4H5-N+HCO<=>C4H6-13+CO	5.000E+12	0.0000	0.0
C4H5-N+H2O2<=>C4H6-13+HO2	1.210E+10	0.0000	-596.0
C4H5-N+HO2<=>C4H6-13+O2	6.000E+11	0.0000	0.0
C4H5-I+HCO<=>C4H6-13+CO	5.000E+12	0.0000	0.0
C4H5-I+HO2<=>C4H6-13+O2	6.000E+11	0.0000	0.0
C4H5-I+H2O2<=>C4H6-13+HO2	1.210E+10	0.0000	-596.0
C4H5-I+HO2<=>C2H3+CH2CO+OH	6.600E+12	0.0000	0.0
C4H5-I+O2<=>CH2CO+CH2HCO	2.160E+10	0.0000	2500.0
C4H5-2<=>C4H5-I	1.500E+67	-16.8900	59100.0

C4H5-2+H<=>C4H5-I+H	3.100E+26	-3.3500	17423.0
C4H5-2+HO2<=>OH+C2H2+CH3CO	8.000E+11	0.0000	0.0
C4H5-2+O2<=>CH3CO+CH2CO	2.160E+10	0.0000	2500.0
C4H5-N<=>C4H5-I	1.500E+67	-16.8900	59100.0
C4H5-N+H<=>C4H5-I+H	3.100E+26	-3.3500	17423.0
C4H5-I+H<=>C4H4+H2	3.000E+13	0.0000	0.0
C4H5-I+H<=>H2CCCH+CH3	2.000E+13	0.0000	2000.0
C4H5-I+OH<=>C4H4+H2O	4.000E+12	0.0000	0.0
C4H5-N+H<=>C4H4+H2	1.500E+13	0.0000	0.0
C4H5-N+OH<=>C4H4+H2O	2.000E+12	0.0000	0.0
C4H5-N+HO2<=>C2H3+CH2CO+OH	6.600E+12	0.0000	0.0
C4H5-N+O2<=>CH2CHCHCHO+O	3.000E+11	0.2900	11.0
C4H5-N+O2<=>HCO+CH2CHCHO	9.200E+16	-1.3900	1010.0
CH3CHCHCHO<=>C3H6+CO	3.900E+14	0.0000	69000.0
CH3CHCHCHO+H<=>CH2CHCHCHO+H2	1.700E+05	2.5000	2490.0
CH3CHCHCHO+H<=>CH3CHCHCO+H2	1.000E+05	2.5000	2490.0
CH3CHCHCHO+H<=>CH3+CH2CHCHO	4.000E+21	-2.3900	11180.0
CH3CHCHCHO+H<=>C3H6+HCO	4.000E+21	-2.3900	11180.0
CH3CHCHCHO+CH3<=>CH2CHCHCHO+CH4	2.100E+00	3.5000	5675.0
CH3CHCHCHO+CH3<=>CH3CHCHCO+CH4	1.100E+00	3.5000	5675.0
CH3CHCHCHO+C2H3<=>CH2CHCHCHO+C2H4	2.210E+00	3.5000	4682.0
CH3CHCHCHO+C2H3<=>CH3CHCHCO+C2H4	1.110E+00	3.5000	4682.0
CH3CHCHCO+H<=>CH3CHCHCHO	1.000E+14	0.0000	0.0
CH2CHCHCHO+H<=>CH3CHCHCHO	1.000E+14	0.0000	0.0
CH2CHCHCHO=AC3H5+CO	1.00e14	0.0	25000.00
CH3CHCHCO=SC3H5 +CO	1.00e14	0.0	30000.00
C4H2+O<=>C3H2+CO	2.700E+13	0.0000	1720.0
C4H2+OH<=>H2C4O+H	6.600E+12	0.0000	-410.0
C4H2+C2H<=>C6H2+H	9.600E+13	0.0000	0.0
H2C4O+H<=>C2H2+HCCO	5.000E+13	0.0000	3000.0
H2C4O+OH<=>CH2CO+HCCO	1.000E+07	2.0000	2000.0
!TOLUENE SUBMECHANISM!!			
!BASED ON HP LIM OF ADDITION REACTION FROM KLIPPENSTEIN			
!PROC. COMBUST. INST 31 (2007) 221-229			
C6H5CH3(+M) = C6H5CH2+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/			
!BASED ON HP LIM OF ADDITION REACTION FROM KLIPPENSTEIN			
!PROC. COMBUST. INST 31 (2007) 221-229			
C6H5CH3(+M) = C6H5+CH3(+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/			
!OEHSCHLAGER C&F (2006)195-208			
C6H5CH3+O2 = C6H5CH2+HO2	2.18E+7	2.5	46045.0
!BAULCH,D.L.; COBOS,C.J.			
!EVALUATED KINETIC DATA FOR COMBUSTION MODELLING. SUPPLEMENT I			
!J. PHYS. CHEM. REF. DATA 23, 847-1033 (1994)			
C6H5CH3+HO2 = C6H5CH2+H2O2	3.97E+11	0.00	14069.38

!OEHLSCHLAEGER, J. PHYS. CHEM. A, VOL. 110, NO. 32, 2006			
C6H5CH3+H = C6H5CH2+H2	6.47E+0	3.98	3384.0
!TAKAMASA SETA, MASAKAZU NAKAJIMA, AND AKIRA MIYOSHI			
!J. PHYS. CHEM. A, 2006, 110 (15), 5081-5090			
C6H5CH3+OH = C6H5CH2+H2O	1.770E+05	2.39	-602.0
!HOFFMANN,A.; KLATT,M.; WAGNER,H.GG.			
!Z. PHYS. CHEM. (NEUE FOLGE) 168, 1-12 (1990)			
C6H5CH3+O = C6H5CH2+OH	6.3E+11	0.0	0.0
!2 PARAMETER FIT TO AVAILABLE RATE DATA ON NIST KINETIC DATA BASE (ONLINE)			
C6H5CH3+CH3 = C6H5CH2+CH4	2.939E+11	0.0	9245.0
!SAKAI ET AL			
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418			
C6H5CH3+HCO = C6H5CH2+CH2O	3.77E+13	0.0	23787.4
!3 PARAMETER FIT FROM NIST ONLINE DATA BASE. VERY LIMITED DATA SET.			
!C6H5CH3+C6H5 = C6H6+C6H5CH2	2.68E-01	3.95	877.06
!BOUNACEUR ET AL			
!INT J CHEM KINET 37: 25-49, 2005			
C6H5CH3+C2H3 = C6H5CH2+C2H4	4.0E+12	0.0	8000.0
!BOUNACEUR ET AL			
!INT J CHEM KINET 37: 25-49, 2005			
C6H5CH3+AC3H5 = C6H5CH2+C3H6	1.6E+12	0.0	15100.0
!BOUNACEUR ET AL			
!INT J CHEM KINET 37: 25-49, 2005			
C6H5CH3+H2CCCH = C6H5CH2+PC3H4	1.6E+12	0.0	15100.0
!BOUNACEUR ET AL			
!INT J CHEM KINET 37: 25-49, 2005			
C6H5CH3+C4H5-I = C6H5CH2+C4H6-13	1.6E+12	0.0	15100.0
!BOUNACEUR ET AL			
!INT J CHEM KINET 37: 25-49, 2005			
C6H5CH3+C4H5-N = C6H5CH2+C4H6-13	1.6E+12	0.0	15100.0
!BOUNACEUR ET AL			
!INT J CHEM KINET 37: 25-49, 2005			
C6H5CH3+C5H5 = C6H5CH2+C5H6	1.6E+12	0.0	11100.0
!BOUNACEUR ET AL			

!INT J CHEM KINET 37: 25-49, 2005
 $\text{C}_6\text{H}_5\text{CH}_3 + \text{C}_6\text{H}_5 = \text{C}_6\text{H}_5\text{CH}_2 + \text{C}_6\text{H}_6$ 7.9E+13 0.0 12000.0

!SAKAI ET AL
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418
 $\text{C}_6\text{H}_5\text{CH}_3 + \text{C}_6\text{H}_5\text{O} = \text{C}_6\text{H}_5\text{CH}_2 + \text{C}_6\text{H}_5\text{OH}$ 5.43E+12 0.00 20923.0
!TST,SAKAI

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
 $\text{C}_6\text{H}_5\text{CH}_3 + \text{C}_6\text{H}_4\text{CH}_3 = \text{C}_6\text{H}_5\text{CH}_2 + \text{C}_6\text{H}_5\text{CH}_3$ 7.9E+13 0.0 12000.0

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
 $\text{C}_6\text{H}_5\text{CH}_3 + \text{OC}_6\text{H}_4\text{CH}_3 = \text{C}_6\text{H}_5\text{CH}_2 + \text{HOC}_6\text{H}_4\text{CH}_3$ 1.6E+11 0.0 15100.0

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
 $\text{C}_6\text{H}_5\text{CH}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{OO} = \text{C}_6\text{H}_5\text{CH}_2 + \text{BZCOOH}$ 4.0E+11 0.0 14000.0

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
 $\text{C}_6\text{H}_5\text{CH}_3 + \text{C}_6\text{H}_5\text{CH}_2\text{O} = \text{C}_6\text{H}_5\text{CH}_2 + \text{C}_6\text{H}_5\text{CH}_2\text{OH}$ 1.6E+11 0.0 11100.0

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
 $\text{C}_6\text{H}_5\text{CH}_3 + \text{HOC}_6\text{H}_4\text{CH}_2 = \text{C}_6\text{H}_5\text{CH}_2 + \text{HOC}_6\text{H}_4\text{CH}_3$ 1.6E+11 0.0 15100.0

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
!BOUNACEUR LIKENED THIS RATES TO BENZENE. I HAVE CORRECTED THE
!A-FACTOR BY *5/6 TO ACCOUNT FOR ONE POSITION MISSING
 $\text{C}_6\text{H}_5\text{CH}_3 + \text{H} = \text{C}_6\text{H}_4\text{CH}_3 + \text{H}_2$ 5.0E+8 1.0 16800.0

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
!BOUNACEUR LIKENED THIS RATES TO BENZENE. I HAVE CORRECTED THE
!A-FACTOR BY *5/6 TO ACCOUNT FOR ONE POSITION MISSING
 $\text{C}_6\text{H}_5\text{CH}_3 + \text{O} = \text{C}_6\text{H}_4\text{CH}_3 + \text{OH}$ 1.66E+13 0.0 14700.0

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
!BOUNACEUR LIKENED THIS RATES TO BENZENE. I HAVE CORRECTED THE
!A-FACTOR BY *5/6 TO ACCOUNT FOR ONE POSITION MISSING
 $\text{C}_6\text{H}_5\text{CH}_3 + \text{OH} = \text{C}_6\text{H}_4\text{CH}_3 + \text{H}_2\text{O}$ 1.33E+8 1.42 1450.0

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005

!BOUNACEUR LIKENED THIS RATES TO BENZENE. I HAVE CORRECTED THE
 !A-FACTOR BY *5/6 TO ACCOUNT FOR ONE POSITION MISSING
 $\text{C}_6\text{H}_5\text{CH}_3 + \text{HO}_2 = \text{C}_6\text{H}_4\text{CH}_3 + \text{H}_2\text{O}_2$ 3.33E+11 0.0 28900.0

!BOUNACEUR ET AL
 !INT J CHEM KINET 37: 25-49, 2005
 !BOUNACEUR LIKENED THIS RATES TO BENZENE. I HAVE CORRECTED THE
 !A-FACTOR BY *5/6 TO ACCOUNT FOR ONE POSITION MISSING
 $\text{C}_6\text{H}_5\text{CH}_3 + \text{CH}_3 = \text{C}_6\text{H}_4\text{CH}_3 + \text{CH}_4$ 1.6E+12 0.0 15000.0

!BOUNACEUR ET AL
 !INT J CHEM KINET 37: 25-49, 2005
 $\text{C}_6\text{H}_5\text{CH}_3 + \text{O} = \text{OC}_6\text{H}_4\text{CH}_3 + \text{H}$ 1.7E+13 0.0 3600.0

!TAKAMASA SETA, MASAKAZU NAKAJIMA, AND AKIRA MIYOSHI
 !J. PHYS. CHEM. A, 2006, 110 (15), 5081-5090
 !BENZENE A-FACTOR *5/6 TO ACCOUNT FOR ONE POSITION MISSING
 $\text{C}_6\text{H}_5\text{CH}_3 + \text{OH} = \text{HOC}_6\text{H}_4\text{CH}_3 + \text{H}$ 110.0 3.25 5590.0

!ELLIS, C.; SCOTT, M.S.; WALKER, R.W.,
 !COMBUST. FLAME 132, 291-304 (2003)
 $\text{C}_6\text{H}_5\text{CH}_3 + \text{H} = \text{C}_6\text{H}_6 + \text{CH}_3$ 9.494E+05 2.00 944.0

!BOUNACEUR ET AL
 !INT J CHEM KINET 37: 25-49, 2005
 $\text{C}_6\text{H}_5\text{CH}_2 = \text{C}_5\text{H}_5 + \text{C}_2\text{H}_2$ 6.0E+13 0.0 70000.0

!BOUNACEUR ET AL
 !INT J CHEM KINET 37: 25-49, 2005
 $\text{C}_6\text{H}_5\text{CH}_2 = \text{H}_2\text{CCCH} + \text{C}_4\text{H}_4$ 2.0E+14 0.0 83600.0

!SAKAI ET AL
 !PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418
 $\text{C}_6\text{H}_5\text{CH}_2 + \text{O} = \text{C}_6\text{H}_5\text{CHO} + \text{H}$ 2.11E+14 0.0 0.0 !SAKAI

!SAKAI ET AL
 !PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418
 $\text{C}_6\text{H}_5\text{CH}_2 + \text{O} = \text{C}_6\text{H}_5 + \text{CH}_2\text{O}$ 1.19E+14 0.0 0.0 !SAKAI

!HIPPLER, H.; REIHS, C.; TROE, J.,
 !SYMP. INT. COMBUST. PROC., 23 37-43, 1991
 $\text{C}_6\text{H}_5\text{CH}_2 + \text{OH} = \text{C}_6\text{H}_5\text{CH}_2\text{OH}$ 2.0E13 0.0 0.0

!DA SILVA ET AL.
 !PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 287-294
 $\text{C}_6\text{H}_5\text{CH}_2 + \text{HO}_2 = \text{BZCOOH}$ 3.37E+11 0.02 -3460.0
 !300 < T < 700 K

!C6H5CH2+HO2 = BZCOOH !700 < T < 2000 K	3.70E+37	-16.33	-67470.0
!C6H5CH2+HO2 = C6H5CH2O+OH !300 < T < 800 K	7.48E-2	4.92	2500.0
!C6H5CH2+HO2 = C6H5CH2O+OH !800 < T < 2000 K	1.19E+9	1.03	-2250.0

!WKM

!3 PARAM FIT TO THE TWO EXPRESSIONS ABOVE,
!CREATES ERRORS BUT NOT IMPORTANT.

C6H5CH2+HO2 = BZCOOH	6.75E+44	-17.47518	-45232.0
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!WKM

!CHOSEN TO IMPROVE AGREEMENT WITH HIGH PRESSURE SHOCK TUBE
EXPERIMENTS

!SHEN ET AL. PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 165-172

!APPROXIMATELY A FACTOR OF 2 INCREASE ON DA SILVA'S NUMBER ABOVE (800 -
2000)

C6H5CH2+HO2 = C6H5CH2O+OH	1.0E+13	0.0	0.0
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!ERGUT ET AL

!COMBUSTION AND FLAME 144 (2006) 757-772

C6H5CH2+CH3 = C6H5C2H5	1.19E+13	0.0	221.0
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!BOUNACEUR ET AL

!INT J CHEM KINET 37: 25-49, 2005

C6H4CH3+O2 = OC6H4CH3+O	2.6E13	0.0	6100.0
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!BOUNACEUR ET AL

!INT J CHEM KINET 37: 25-49, 2005

C6H4CH3+O2 = O-C6H4O2+CH3	3.0E+13	0.0	9000.0
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!BOUNACEUR ET AL

!INT J CHEM KINET 37: 25-49, 2005

C6H4CH3+H = C6H5CH3	1.0E+14	0.0	0.0
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!BOUNACEUR ET AL

!INT J CHEM KINET 37: 25-49, 2005

C6H4CH3+H = C6H5CH2+H	1.0E+13	0.0	0.0
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!BOUNACEUR ET AL

!INT J CHEM KINET 37: 25-49, 2005

C6H4CH3+O = OC6H4CH3	1.0E+14	0.0	0.0
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!BOUNACEUR ET AL

!INT J CHEM KINET 37: 25-49, 2005

C6H4CH3+OH = HOC6H4CH3	1.0E+13	0.0	0.0
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!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
 $C_6H_4CH_3+HO_2 = OC_6H_4CH_3+OH$ 5.0E+12 0.0 0.0

!MURAKAMI ET AL.
!J. PHYS. CHEM. A 2007, 111, 13200-13208
!THE OTHER PATHWAYS WERE NOT INCLUDED AS THE DISSOCIATION IS
DOMINANT
!THROUGHOUT THE REGIME (~95%)
 $C_6H_5CH_2OO(+M) = C_6H_5CH_2+O_2(+M)$ 4.17000E+36 -7.06798 3.22350E+04
LOW / 1.79700E-06 5.40000E+00 -7.63000E+03/
TROE /6.114198E-01 9.999806E+09 1.037924E+00 1.786062E+09/

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
 $C_6H_5CH_2OO+H = BZCOOH$ 1.0E+14 0.0 0.0

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
 $C_6H_5CH_2OO+HO_2 = BZCOOH+O_2$ 2.0E+11 0.00 0.0

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
 $C_6H_5CH_2OO+C_6H_5CH_2OO = C_6H_5CH_2OH+C_6H_5CHO+O_2$ 1.4E+10 0.0 -720.0

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
 $C_6H_5CH_2OO+C_6H_5CH_2OO = C_6H_5CH_2O+C_6H_5CH_2O+O_2$ 6.3E+10 0.0 -720.0

!WKM
!ESTIMATED
 $C_6H_5CH_2O+OH = BZCOOH$ 2.0E13 0.0 0.0

!SAKAI ET AL
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418
!!!!!!!!!!!!!!!!!!PRESSURE DEPENDANCE!!!!!!!!!!!!!!!!!!!!!!
 $C_6H_5CH_2O = C_6H_5CHO+H$ 2.73E+09 0.0 7289.0
!SAKAI,1ATM
 $C_6H_5CH_2O = C_6H_5+CH_2O$ 3.29E+08 0.0 10268.0
!SAKAI,1ATM
 $C_6H_5CH_2O = C_6H_5CHO+H$ 1.99E+13 0.0 18728.0
!SAKAI,HPLIMIT
 $C_6H_5CH_2O = C_6H_5+CH_2O$ 8.55E+13 0.0 26017.0
!SAKAI,HPLIMIT

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
 $C_6H_5CH_2O+O_2 = C_6H_5CHO+HO_2$ 6.0E+10 0.0 1600.0

!BOUNACEUR ET AL			
!INT J CHEM KINET 37: 25-49, 2005			
OC6H4CH3 = C6H6+CO+H	7.6E+11	0.0	43800.0
!BOUNACEUR ET AL			
!INT J CHEM KINET 37: 25-49, 2005			
OC6H4CH3+H = HOC6H4CH3	1.0E+14	0.0	0.0
!SAKAI ET AL			
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418			
C6H5CH2+C6H5CH2 = C14H14	5.00E+12	0.0	454.0
!OEHLSCHLAEGER2005			
!SAKAI ET AL			
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418			
C14H14 = C14H13+H	1.00E+16	0.0	83660.0
!OEHLSCHLAEGER2005			
!SAKAI ET AL			
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418			
C14H14+H = C14H13+H2	3.16E+12	0.0	0.0
!OEHLSCHLAEGER2005			
!SAKAI ET AL			
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418			
C14H14+O2 = C14H13+HO2	2.80E+12	0.0	35000.0
!OEHLSCHLAEGER2005			
!SAKAI ET AL			
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418			
C14H14+O = C14H13+OH	8.40E+11	0.0	-2000.0
!OEHLSCHLAEGER2005			
!SAKAI ET AL			
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418			
C14H14+OH = C14H13+H2O	7.00E+09	1.0	-1100.0
!OEHLSCHLAEGER2005			
!SAKAI ET AL			
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418			
C14H14+HO2 = C14H13+H2O2	5.40E+11	0.0	12000.0
!OEHLSCHLAEGER2005			
!SAKAI ET AL			
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418			
C14H14+CH3 = C14H13+CH4	2.20E+12	0.0	9100.0
!OEHLSCHLAEGER2005			

!BOUNACEUR ET AL			
!INT J CHEM KINET 37: 25-49, 2005			
C14H14+AC3H5 = C14H13+C3H6	2.2E+12	0.0	9100.0
!SAKAI ET AL			
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418			
C14H14+C6H5CH2 = C14H13+C6H5CH3	2.20E+11	0.0	9100.0
!OEHLSCHLAEGER2005			
!SAKAI ET AL			
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418			
C14H14+C6H5 = C14H13+C6H6	1.06E+14	0.0	9949.0
!BOUNACEUR2005,TABLEV ESTIMATED AA			
!SAKAI ET AL			
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418			
C14H14+C6H5O = C14H13+C6H5OH	5.43E+12	0.0	20923.0
!EQUAL TO C6H5CH3+C6H5O			
!SAKAI ET AL			
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418			
C14H13 = C14H12+H	7.90E+15	0.0	51864.0
!OEHLSCHLAEGER2005			
!SAKAI ET AL			
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418			
C14H13+O2 = C6H5CHO+C6H5CH2O	3.94E+50	-11.5	4.225E+04
!C2H5+O2,A-FACTOR*(4/5)			
!SAKAI ET AL			
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418			
C14H13+HO2 = C6H5CH2+C6H5CHO+OH	1.920E+13	0.0	0.0 !EQUAL TO
C2H5+HO2			
!SAKAI ET AL			
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418			
C14H12+O2 = HO2+C14H11	4.00E+13	0.0	58200.0
!EQUAL TO C2H4+O2=C2H3+HO2			
!SAKAI ET AL			
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418			
C14H12+H = C14H11+H2	8.42E-03	4.62	2583.0 !EQUAL
TO C2H4+H=C2H3+H2			
!SAKAI ET AL			
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418			

C14H12+OH = C14H11+H2O TO C2H4+OH=C2H3+H2O	2.02E+13	0.0	5955.0 !EQUAL
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!SAKAI ET AL
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418
C14H12+O = C6H5CO+C6H5CH2

7.95E+03	1.66	657.4 !
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!SAKAI ET AL
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418
C14H11 => C6H5+C2H+C6H5

1.074E+25	-2.217	88474.6 !
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!SAKAI ET AL
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418
C14H11+O2 = C6H5CO+C6H5CHO
TO C2H3+O2=CH2O+HCO

1.70E+29	-5.31	6500.0 !EQUAL
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!WKM
!ESTIMATED
C14H12+O = C14H11+OH

4.2E+11	0.0	-1940.0
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!WKM
!ESTIMATED
C14H12+HO2 = C14H11+H2O2

2.7E+11	0.0	11640.0
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!WKM
!ESTIMATED
C14H12+CH3 = C14H11+CH4

1.1E+12	0.0	8827.0
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!WKM
!ESTIMATED
C14H12+AC3H5 = C14H11+C3H6

1.1E+12	0.0	8827.0
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!WKM
!ESTIMATED
C14H12+C6H5O = C14H11+C6H5OH

5.43E+12	0.0	20923.0
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!WKM
!ESTIMATED
C14H12+C6H5CH2 = C14H11+C6H5CH3

1.1E+11	0.0	8827.0
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!WKM
!LOW T CHEM OF BIBENZYL

!WKM
!ESTIMATED
C14H13+O2 = C14H13OO

8.0E+12	0.0	0.0
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!WKM

!ESTIMATED				
C14H13+HO2 = C14H13O+OH	7.0E+12	0.0	-1000.0	
!WKM				
!ESTIMATE FROM LLNL N-HEPTANE				
C6H5CH2+C6H5CHO = C14H13O	1.0E+11	0.0	12900.0	
!C7H15O-4=NC3H7CHO+NC3H7				
!WKM				
!ESTIMATED				
C14H13OOH+C6H5CH2 = C14H13OO+C6H5CH3	1.44E+10	0.0	17700.0	
!WKM				
!ESTIMATE FROM LLNL N-HEPTANE				
C14H13OO+HO2 = C14H13OOH+O2	1.750E+10	0.0	-3.275E+03	
!C7H15O2-1+HO2=C7H15O2H-1+O2				
!WKM				
!ESTIMATE FROM LLNL N-HEPTANE				
C14H13OO+H2O2 = C14H13OOH+HO2	2.400E+12	0.0	1.000E+04	
!H2O2+C7H15O2-1=HO2+C7H15O2H-1				
!WKM				
!ESTIMATED				
C14H13O+OH = C14H13OOH	2.0E+13	0.0	0.0	
!WKM				
!ESTIMATED FROM METHODS DESCRIBED IN CURRAN'S N-HEPTANE				
!C&F 114: 149-177 (1998)				
C14H13OO = C14H12OOH	2.59E+12	0.0	21374.0	
!WKM				
!ESTIMATE FROM LLNL N-HEPTANE				
C14H12+HO2 = C14H12OOH	1.0E+11	0.0	10530.0	
!WKM				
!ESTIMATE FROM LLNL N-HEPTANE				
C14H12OOH+O2 = C14H12O2H-1O2	8.0E+12	0.0	0.0	
!WKM				
!ESTIMATE FROM LLNL N-HEPTANE				
C14H12O2H-1O2 = C14H11O-1O2H+OH	1.295E+12	0.0	18374.0	
!WKM				
!ESTIMATE FROM LLNL N-HEPTANE				
C14H11O-1O2H = C6H5CHO+C6H5CO+OH	1.0E+16	0.0	43000.0	
!BOUNACEUR ET AL				

!INT J CHEM KINET 37: 25-49, 2005 C6H5CHO = C6H5CO+H	4.0E+15	0.0	83700.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CHO+O2 = C6H5CO+HO2	7.0E+11	0.0	39500.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CHO+H = C6H6+HCO	5.8E+13	0.0	8100.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CHO+H = C6H5CO+H2	4.0E+13	0.0	3200.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CHO+O = C6H5CO+OH	6.0E+12	0.0	1800.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CHO+OH = C6H5CO+H2O	7.8E+12	0.0	0.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CHO+HO2 = C6H5CO+H2O2	3.0E+12	0.0	11000.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CHO+CH3 = C6H5CO+CH4	2.0E-6	5.6	1500.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CHO+C2H5 = C6H5CO+C2H6	1.3E+12	0.0	7500.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CHO+AC3H5 = C6H5CO+C3H6	1.3E+12	0.0	11500.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CHO+C4H5-I = C6H5CO+C4H6-13	1.3E+12	0.0	11500.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CHO+C4H5-N = C6H5CO+C4H6-13	1.3E+12	0.0	7500.0
!BOUNACEUR ET AL			

!INT J CHEM KINET 37: 25-49, 2005 C6H5CHO+C5H5 = C6H5CO+C5H6	1.3E+11	0.0	11500.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CHO+C6H5 = C6H5CO+C6H6	1.3E+11	0.0	11500.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CHO+C6H5CH2 = C6H5CO+C6H5CH3	1.3E+11	0.0	11500.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CHO+C6H5O = C6H5CO+C6H5OH	1.3E+11	0.0	11500.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CHO+OC6H4CH3 = C6H5CO+HOC6H4CH3	1.3E+11	0.0	11500.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CHO+HOC6H4CH2 = C6H5CO+HOC6H4CH3	1.3E+11	0.0	11500.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CO = C6H5+CO	4.0E+14	0.0	29500.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 HOC6H4CH3+O2 = OC6H4CH3+HO2	1.0E+13	0.0	38900.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 HOC6H4CH3+O2 = HOC6H4CH2+HO2	2.1E+12	0.0	39700.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 HOC6H4CH3+H = C6H5OH+CH3	5.8E+13	0.0	8100.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 HOC6H4CH3+H = OC6H4CH3+H2	1.2E+14	0.0	12400.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 HOC6H4CH3+O = OC6H4CH3+OH	1.3E+13	0.0	2900.0
!BOUNACEUR ET AL			

!INT J CHEM KINET 37: 25-49, 2005 HOC6H4CH3+OH = OC6H4CH3+H2O	1.4E+8	1.4	-960.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 HOC6H4CH3+HO2 = OC6H4CH3+H2O2	1.0E+12	0.0	10000.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 HOC6H4CH3+CH3 = OC6H4CH3+CH4	1.8E+11	0.0	7700.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 HOC6H4CH3+C6H5 = OC6H4CH3+C6H6	4.9E+12	0.0	4400.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 HOC6H4CH3+C5H5 = OC6H4CH3+C5H6	4.9E+11	0.0	9400.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 HOC6H4CH3+AC3H5 = OC6H4CH3+C3H6	4.9E+11	0.0	9400.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 HOC6H4CH3+C4H5-I = OC6H4CH3+C4H6-13	4.9E+11	0.0	9400.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 HOC6H4CH3+C4H5-N = OC6H4CH3+C4H6-13	4.9E+11	0.0	9400.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 HOC6H4CH3+C6H5O = OC6H4CH3+C6H5OH	4.9E+11	0.0	9400.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 HOC6H4CH3+H = HOC6H4CH2+H2	1.2E+14	0.0	8400.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 HOC6H4CH3+O = HOC6H4CH2+OH	6.3E+11	0.0	0.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 HOC6H4CH3+OH = HOC6H4CH2+H2O	5.2E+9	1.0	870.0
!BOUNACEUR ET AL			

!INT J CHEM KINET 37: 25-49, 2005				
HOC6H4CH3+HO2 = HOC6H4CH2+H2O2	4.0E+11	0.0		14000.0
!BOUNACEUR ET AL				
!INT J CHEM KINET 37: 25-49, 2005				
HOC6H4CH3+CH3 = HOC6H4CH2+CH4	1.6E+12	0.0		11100.0
!BOUNACEUR ET AL				
!INT J CHEM KINET 37: 25-49, 2005				
HOC6H4CH3+AC3H5 = HOC6H4CH2+C3H6	1.6E+12	0.0		15100.0
!BOUNACEUR ET AL				
!INT J CHEM KINET 37: 25-49, 2005				
HOC6H4CH3+H2CCCH = HOC6H4CH2+PC3H4	1.6E+12	0.0		15100.0
!BOUNACEUR ET AL				
!INT J CHEM KINET 37: 25-49, 2005				
HOC6H4CH3+C4H5-I = HOC6H4CH2+C4H6-13	1.6E+12	0.0		15100.0
!BOUNACEUR ET AL				
!INT J CHEM KINET 37: 25-49, 2005				
HOC6H4CH3+C4H5-N = HOC6H4CH2+C4H6-13	1.6E+12	0.0		11100.0
!BOUNACEUR ET AL				
!INT J CHEM KINET 37: 25-49, 2005				
HOC6H4CH3+C5H5 = HOC6H4CH2+C5H6	1.6E+11	0.0		15100.0
!BOUNACEUR ET AL				
!INT J CHEM KINET 37: 25-49, 2005				
HOC6H4CH3+C6H5 = HOC6H4CH2+C6H6	7.9E+13	0.0		12000.0
!BOUNACEUR ET AL				
!INT J CHEM KINET 37: 25-49, 2005				
HOC6H4CH3+C6H5O = HOC6H4CH2+C6H5OH	1.6E+11	0.0		15100.0
!BOUNACEUR ET AL				
!INT J CHEM KINET 37: 25-49, 2005				
HOC6H4CH3+C6H4CH3 = OC6H4CH3+C6H5CH3	7.9E+13	0.0		12000.0
!BOUNACEUR ET AL				
!INT J CHEM KINET 37: 25-49, 2005				
HOC6H4CH3+OC6H4CH3 = HOC6H4CH2+HOC6H4CH3	1.6E+11	0.0		15100.0
!BOUNACEUR ET AL				
!INT J CHEM KINET 37: 25-49, 2005				
HOC6H4CH3+C6H5CH2OO = HOC6H4CH2+BZCOOH	4.0E+11	0.0		14000.0
!BOUNACEUR ET AL				

!INT J CHEM KINET 37: 25-49, 2005			
HOC6H4CH3+C6H5CH2O = HOC6H4CH2+C6H5CH2OH	1.6E+11	0.0	11100.0
!BOUNACEUR ET AL			
!INT J CHEM KINET 37: 25-49, 2005			
HOC6H4CH2+O2 = HOC6H4CH2OO	4.6E+11	0.0	-380.0
!BOUNACEUR ET AL			
!INT J CHEM KINET 37: 25-49, 2005			
HOC6H4CH2+O2 = HOC6H4CH2O+O	6.3E+12	0.0	40000.0
!BOUNACEUR ET AL			
!INT J CHEM KINET 37: 25-49, 2005			
HOC6H4CH2+H = HOC6H4CH3	1.0E+14	0.0	0.0
!BOUNACEUR ET AL			
!INT J CHEM KINET 37: 25-49, 2005			
HOC6H4CH2+HO2 = HOC6H4CH2OOH	5.0E+12	0.0	0.0
!BOUNACEUR ET AL			
!INT J CHEM KINET 37: 25-49, 2005			
HOC6H4CH2+CH3 = C6H5OH+C2H4	5.0E+12	0.0	0.0
!BOUNACEUR ET AL			
!INT J CHEM KINET 37: 25-49, 2005			
HOC6H4CH2OO = HOC6H4CHO+OH	3.4E+9	1.0	37500.0
!BOUNACEUR ET AL			
!INT J CHEM KINET 37: 25-49, 2005			
HOC6H4CH2O = HOC6H4CHO+H	2.0E+13	0.0	27500.0
!BOUNACEUR ET AL			
!INT J CHEM KINET 37: 25-49, 2005			
HOC6H4CH2O+O2 = HOC6H4CHO+HO2	6.0E+10	0.0	1600.0
!BOUNACEUR ET AL			
!INT J CHEM KINET 37: 25-49, 2005			
HOC6H4CHO+H = HOC6H4CO+H2	4.0E+13	0.0	3200.0
!BOUNACEUR ET AL			
!INT J CHEM KINET 37: 25-49, 2005			
HOC6H4CHO+O = HOC6H4CO+OH	6.0E+12	0.0	1800.0
!BOUNACEUR ET AL			
!INT J CHEM KINET 37: 25-49, 2005			
HOC6H4CHO+OH = HOC6H4CO+H2O	7.8E+12	0.0	0.0
!BOUNACEUR ET AL			

!INT J CHEM KINET 37: 25-49, 2005 HOC6H4CHO+HO2 = HOC6H4CO+H2O2	3.0E+12	0.0	11000.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 HOC6H4CHO+CH3 = HOC6H4CO+CH4	2.0E-6	5.6	1500.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 HOC6H4CO = C6H5O+CO	4.0E+14	0.0	29500.0
!WKM !ESTIMATED HOC6H4CH2O+OH = HOC6H4CH2OOH	2.0E+13	0.0	0.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CH2OH+O2 = C6H5CHOH+HO2	1.4E+12	0.0	34000.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CH2OH+O2 = C6H5CH2O+HO2	2.0E+14	0.0	41400.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CH2OH+H = C6H6+CH2OH	5.8E+13	0.0	8100.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CH2OH+H = C6H5CHOH+H2	8.0E+13	0.0	6400.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CH2OH+O = C6H5CHOH+OH	4.2E+11	0.0	-2000.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CH2OH+OH = C6H5CHOH+H2O	3.9E+9	1.0	-1100.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CH2OH+HO2 = C6H5CHOH+H2O2	2.7E+11	0.0	12000.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CH2OH+CH3 = C6H5CHOH+CH4	1.1E+12	0.0	9100.0
!BOUNACEUR ET AL			

!INT J CHEM KINET 37: 25-49, 2005
 $\text{C6H5CH2OH} + \text{H2CCCH} = \text{C6H5CHOH} + \text{PC3H4}$ 1.1E+12 0.0 13100.0

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
 $\text{C6H5CH2OH} + \text{AC3H5} = \text{C6H5CHOH} + \text{C3H6}$ 1.1E+12 0.0 13100.0

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
 $\text{C6H5CH2OH} + \text{C4H5-I} = \text{C6H5CHOH} + \text{C4H6-13}$ 1.1E+12 0.0 13100.0

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
 $\text{C6H5CH2OH} + \text{C4H5-N} = \text{C6H5CHOH} + \text{C4H6-13}$ 1.1E+12 0.0 13100.0

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
 $\text{C6H5CH2OH} + \text{C5H5} = \text{C6H5CHOH} + \text{C5H6}$ 1.1E+12 0.0 9100.0

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
 $\text{C6H5CH2OH} + \text{C6H5} = \text{C6H5CHOH} + \text{C6H6}$ 5.2E+13 0.0 10000.0

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
 $\text{C6H5CH2OH} + \text{C6H5O} = \text{C6H5CHOH} + \text{C6H5OH}$ 1.1E+11 0.0 13100.0

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
 $\text{C6H5CH2OH} + \text{C6H5CH2} = \text{C6H5CHOH} + \text{C6H5CH3}$ 1.1E+11 0.0 13100.0

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
 $\text{C6H5CH2OH} + \text{C6H4CH3} = \text{C6H5CHOH} + \text{C6H5CH3}$ 5.2E+13 0.0 10000.0

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
 $\text{C6H5CH2OH} + \text{OC6H4CH3} = \text{C6H5CHOH} + \text{HOC6H4CH3}$ 1.1E+11 0.0 13100.0

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
 $\text{C6H5CH2OH} + \text{HOC6H4CH2} = \text{C6H5CHOH} + \text{HOC6H4CH3}$ 1.1E+11 0.0 13100.0

!BOUNACEUR ET AL
!INT J CHEM KINET 37: 25-49, 2005
 $\text{C6H5CH2OH} + \text{C6H5CH2O} = \text{C6H5CHOH} + \text{C6H5CH2OH}$ 1.1E+11 0.0 9100.0

!BOUNACEUR ET AL

!INT J CHEM KINET 37: 25-49, 2005 C6H5CHOH = C6H5CHO+H	2.0E+14	0.0	23300.0
!ERGUT ET AL !COMBUSTION AND FLAME 144 (2006) 757-772 C6H5C2H5+H = C6H6+C2H5	1.20E+13	0.0	5100.0
!ERGUT ET AL !COMBUSTION AND FLAME 144 (2006) 757-772 C6H5C2H5+H = C6H5CHCH3+H2	3.97E+2	3.44	3120.0
!ERGUT ET AL !COMBUSTION AND FLAME 144 (2006) 757-772 C6H5C2H5+OH = C6H5CHCH3+H2O	5.17E+9	1.0	870.0
!ERGUT ET AL !COMBUSTION AND FLAME 144 (2006) 757-772 C6H5C2H5+O2 = C6H5CHCH3+HO2	1.81E+12	0.0	39740.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5C2H5+O2 = C6H5CH2CH2+HO2	1.2E+13	0.0	49000.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5C2H5+O = C6H5CHCH3+OH	3.9E+9	1.0	-1100.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5C2H5+HO2 = C6H5CHCH3+H2O2	2.7E+11	0.0	12000.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5C2H5+CH3 = C6H5CHCH3+CH4	1.1E+12	0.0	9100.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5C2H5+AC3H5 = C6H5CHCH3+C3H6	1.1E+12	0.0	13100.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5C2H5+C4H5-I = C6H5CHCH3+C4H6-13	1.1E+12	0.0	13100.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5C2H5+C4H5-N = C6H5CHCH3+C4H6-13	1.1E+12	0.0	13100.0
!BOUNACEUR ET AL			

!INT J CHEM KINET 37: 25-49, 2005				
$\text{C}_6\text{H}_5\text{C}_2\text{H}_5 + \text{C}_5\text{H}_5 = \text{C}_6\text{H}_5\text{CHCH}_3 + \text{C}_5\text{H}_6$	1.1E+12	0.0		9100.0
!BOUNACEUR ET AL				
!INT J CHEM KINET 37: 25-49, 2005				
$\text{C}_6\text{H}_5\text{C}_2\text{H}_5 + \text{C}_6\text{H}_5\text{O} = \text{C}_6\text{H}_5\text{CHCH}_3 + \text{C}_6\text{H}_5\text{OH}$	1.1E+12	0.0		13100.0
!BOUNACEUR ET AL				
!INT J CHEM KINET 37: 25-49, 2005				
$\text{C}_6\text{H}_5\text{C}_2\text{H}_5 + \text{C}_6\text{H}_5\text{CH}_2 = \text{C}_6\text{H}_5\text{CHCH}_3 + \text{C}_6\text{H}_5\text{CH}_3$	1.1E+12	0.0		13100.0
!BOUNACEUR ET AL				
!INT J CHEM KINET 37: 25-49, 2005				
$\text{C}_6\text{H}_5\text{C}_2\text{H}_5 + \text{OC}_6\text{H}_4\text{CH}_3 = \text{C}_6\text{H}_5\text{CHCH}_3 + \text{HOC}_6\text{H}_4\text{CH}_3$	1.1E+11	0.0		13100.0
!BOUNACEUR ET AL				
!INT J CHEM KINET 37: 25-49, 2005				
$\text{C}_6\text{H}_5\text{C}_2\text{H}_5 + \text{HOC}_6\text{H}_4\text{CH}_2 = \text{C}_6\text{H}_5\text{CHCH}_3 + \text{HOC}_6\text{H}_4\text{CH}_3$	1.1E+11	0.0		13100.0
!BOUNACEUR ET AL				
!INT J CHEM KINET 37: 25-49, 2005				
$\text{C}_6\text{H}_5\text{C}_2\text{H}_5 + \text{H} = \text{C}_6\text{H}_5\text{CH}_2\text{CH}_2 + \text{H}_2$	2.8E+7	2.0		7700.0
!BOUNACEUR ET AL				
!INT J CHEM KINET 37: 25-49, 2005				
$\text{C}_6\text{H}_5\text{C}_2\text{H}_5 + \text{O} = \text{C}_6\text{H}_5\text{CH}_2\text{CH}_2 + \text{OH}$	5.1E+13	0.0		7800.0
!BOUNACEUR ET AL				
!INT J CHEM KINET 37: 25-49, 2005				
$\text{C}_6\text{H}_5\text{C}_2\text{H}_5 + \text{OH} = \text{C}_6\text{H}_5\text{CH}_2\text{CH}_2 + \text{H}_2\text{O}$	2.7E+6	2.0		400.0
!BOUNACEUR ET AL				
!INT J CHEM KINET 37: 25-49, 2005				
$\text{C}_6\text{H}_5\text{C}_2\text{H}_5 + \text{HO}_2 = \text{C}_6\text{H}_5\text{CH}_2\text{CH}_2 + \text{H}_2\text{O}_2$	6.0E+11	0.0		17000.0
!BOUNACEUR ET AL				
!INT J CHEM KINET 37: 25-49, 2005				
$\text{C}_6\text{H}_5\text{C}_2\text{H}_5 + \text{CH}_3 = \text{C}_6\text{H}_5\text{CH}_2\text{CH}_2 + \text{CH}_4$	0.3	4.0		8200.0
!BOUNACEUR ET AL				
!INT J CHEM KINET 37: 25-49, 2005				
$\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2 = \text{C}_6\text{H}_5\text{C}_2\text{H}_3 + \text{H}$	1.6E+13	0.0		43500.0
!BOUNACEUR ET AL				
!INT J CHEM KINET 37: 25-49, 2005				
$\text{C}_6\text{H}_5\text{CH}_2\text{CH}_2 = \text{C}_2\text{H}_4 + \text{C}_6\text{H}_5$	7.1E+14	0.0		43500.0
!BOUNACEUR ET AL				

!INT J CHEM KINET 37: 25-49, 2005 C6H5CHCH3+O2 = C6H5C2H3+HO2	7.0E+11	0.0	15000.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CH2CH2+O2 = C6H5C2H3+HO2	1.5E+12	0.0	5000.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CHCH3+HO2 = C6H5CHO+CH3+OH	5.0E+12	0.0	0.0
!BOUNACEUR ET AL !INT J CHEM KINET 37: 25-49, 2005 C6H5CH2CH2+HO2 = C6H5CH2+CH2O+OH	5.0E+12	0.0	0.0
!ERGUT ET AL !COMBUSTION AND FLAME 144 (2006) 757-772 C6H5C2H5 = C6H5CHCH3+H	2.51E+15	0.0	81262.0
!ERGUT ET AL !COMBUSTION AND FLAME 144 (2006) 757-772 C6H5CHCH3 = C6H5C2H3+H	3.16E+13	0.0	50669.0
!ERGUT ET AL !COMBUSTION AND FLAME 144 (2006) 757-772 C6H5C2H3 = C6H6+C2H2	1.58E+11	0.0	58440.0
!ERGUT ET AL !COMBUSTION AND FLAME 144 (2006) 757-772 C6H5+C2H4 = C6H5C2H3+H	2.51E+12	0.0	6200.0
!ERGUT ET AL !COMBUSTION AND FLAME 144 (2006) 757-772 C6H5C2H3+O = C6H5+CH2HCO	3.5E+13	0.0	2832.0
!ERGUT ET AL !COMBUSTION AND FLAME 144 (2006) 757-772 C6H5C2H3+H = C6H5CCH2+H2	3.23E+7	2.095	15842.0
!ERGUT ET AL !COMBUSTION AND FLAME 144 (2006) 757-772 C6H5C2H3+OH = C6H5CCH2+H2O	2.11E+13	0.0	4571.0
!ERGUT ET AL !COMBUSTION AND FLAME 144 (2006) 757-772 C6H5CCH2+O2 = C6H5O+CH2CO	1.88E+12	0.0	7469.0
!ERGUT ET AL			

!COMBUSTION AND FLAME 144 (2006) 757-772			
C6H5CCH2+H = C6H5C2H3	1.11E+16	-0.817	690.0
!ERGUT ET AL			
!COMBUSTION AND FLAME 144 (2006) 757-772			
C6H5+C2H2 = C6H5CCH2	1.10E+41	-8.61	18152.0
!ERGUT ET AL			
!COMBUSTION AND FLAME 144 (2006) 757-772			
C6H5C2H3+H = C6H5CHCH+H2	5.07E+7	1.93	12951.0
!ERGUT ET AL			
!COMBUSTION AND FLAME 144 (2006) 757-772			
C6H5C2H3+OH = C6H5CHCH+H2O	2.02E+13	0.0	5955.0
!ERGUT ET AL			
!COMBUSTION AND FLAME 144 (2006) 757-772			
C6H5C2H3+O = C6H5CHCH+OH	7.55E+06	1.91	3736.0
!ERGUT ET AL			
!COMBUSTION AND FLAME 144 (2006) 757-772			
C6H5+C2H2 = C6H5CHCH	6.7E+34	-7.04	10987.0
!BOUNACEUR ET AL			
!INT J CHEM KINET 37: 25-49, 2005			
C6H5C2H3+O2 = C6H5CCH2+HO2	2.0E+13	0.0	57900.0
!WANG ET AL.			
!C&F, 110: 173. 1994			
C6H5+H(+M) = C6H6(+M)	1.0E+14	0.0	0.0
LOW / 6.6E+75 -16.3 7000.0 /			
TROE / 1.0 0.1 584.9 6113.0 /			
H2 /2.0/ H2O /6.0/ CH4 /2.0/ CO /1.5/ CO2 /2.0/			
!EMDEE ET AL.			
!J. PHYS. CHEM. 1992, 96, 2151-2161			
C6H6+O2 = C6H5+HO2	6.30E+13	0.0	60000.0
!ALZUETA ET AL.			
!IJCK 32: 498-522 (2000)			
C6H6+O = C6H5O+H	2.2E+13	0.0	4530.0
!ALZUETA ET AL.			
!IJCK 32: 498-522 (2000)			
C6H6+O = C6H5+OH	2.0E13	0.0	14700.0
!EMDEE ET AL.			
!J. PHYS. CHEM. 1992, 96, 2151-2161			

C6H6+H = C6H5+H2	2.50E+14	0.0	16000.0
!ESTIMATED			
C6H6+CH3 = C6H5+CH4	7.32E+12	0.0	18920.0
!ESTIMATED			
C6H6+HO2 = C6H5+H2O2	5.5E+12	0.0	28900.0
!CHEN&BOZ			
!J. PHYS. CHEM. A 108: 4632 - 4652 2004			
C6H6+OH = C6H5+H2O	1.20	4.1	-301.0
!TAKAMASA SETA, MASAKAZU NAKAJIMA, AND AKIRA MIYOSHI			
!J. PHYS. CHEM. A, 2006, 110 (15), 5081-5090			
C6H6+OH = C6H5OH+H	132.0	3.25	5590.0
!CHAOS ET AL.			
!PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007			
C6H5 => H+C4H2+C2H2	4.3E+12	0.62	77294.
!CHAOS ET AL.			
!PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007			
C6H5+CH2O = C6H6+HCO	8.55E+4	2.19	38.0
!CHAOS ET AL.			
!PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007			
C6H5+CH2O = C6H5CHO+H	2.91E+4	2.09	-411.0
!CHAOS ET AL.			
!PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007			
C6H5+HCO = C6H6+CO	8.55E+4	2.19	38.0
!DA COSTA ET AL.			
!INT J CHEM KINET 35: 503-524, 2003			
C6H5+HO2 = C6H5O+OH	5.0E+12	0.0	0.0
!FRANK ET AL.			
!SYMP (INT) COMBUST, [PROC] 1994, 25, 833.			
C6H5+O2 = C6H5O+O	2.6E+13	0.0	6120.0
!FRANK ET AL.			
!SYMP (INT) COMBUST, [PROC] 1994, 25, 833.			
C6H5+O2 = O-C6H4O2+H	3.0E+13	0.0	8980.0
!DA SILVA AND BOZZELLI			
!J PHYS CHEM 112: 3566-3575			
C6H5+O2 = C6H5OO	1.86E+13	-0.22	-711.0

!DA SILVA AND BOZZELLI			
!J PHYS CHEM 112: 3566-3575			
$C_6H_5OO = C_6H_5O + O$	1.27E+15	-0.246	38536.0
!CHAOS ET AL.			
!PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007			
$C_6H_5OO + C_6H_5CH_3 = C_6H_5OOH + C_6H_5CH_2$	4.0E+11	0.0	14000.0
!WKM			
!ESTIMATED			
$C_6H_5O + OH = C_6H_5OOH$	2.0E+13	0.0	0.0
!CHAOS ET AL.			
!PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007			
$C_6H_5OO + C_6H_5OH = C_6H_5OOH + C_6H_5O$	1.33E+11	0.0	14000.0
!WKM			
!ESTIMATED			
$C_6H_5 + C_2H_5 = C_6H_5C_2H_5$	5.0E+12	0.0	0.0
!WKM			
!ESTIMATED			
$C_6H_5 + C_2H_3 = C_6H_5C_2H_3$	5.0E+12	0.0	0.0
!DA COSTA ET AL.			
!INT J CHEM KINET 35: 503-524, 2003			
$C_6H_5OH + O_2 = C_6H_5O + HO_2$	1.0E+13	0.0	38800.0
!DA COSTA ET AL.			
!INT J CHEM KINET 35: 503-524, 2003			
$C_6H_5OH + O = OC_6H_4OH + H$	1.6E+13	0.0	3400.0
!DA COSTA ET AL.			
!INT J CHEM KINET 35: 503-524, 2003			
$C_6H_5OH + H = C_6H_5O + H_2$	1.2E+14	0.0	12400.0
!DA COSTA ET AL.			
!INT J CHEM KINET 35: 503-524, 2003			
$C_6H_5OH + O = C_6H_5O + OH$	1.3E+13	0.0	2900.0
!DA COSTA ET AL.			
!INT J CHEM KINET 35: 503-524, 2003			
$C_6H_5OH + OH = C_6H_5O + H_2O$	1.4E+8	1.4	-960.0
!DA COSTA ET AL.			
!INT J CHEM KINET 35: 503-524, 2003			
$C_6H_5OH + HO_2 = C_6H_5O + H_2O_2$	1.0E+12	0.0	10000.0

!DA COSTA ET AL. !INT J CHEM KINET 35: 503-524, 2003 $\text{C}_6\text{H}_5\text{OH} + \text{CH}_3 = \text{C}_6\text{H}_5\text{O} + \text{CH}_4$	1.8E+11	0.0	7700.0
!DA COSTA ET AL. !INT J CHEM KINET 35: 503-524, 2003 $\text{C}_6\text{H}_5\text{OH} + \text{C}_6\text{H}_5 = \text{C}_6\text{H}_5\text{O} + \text{C}_6\text{H}_6$	4.9E+12	0.0	4400.0
!DA COSTA ET AL. !INT J CHEM KINET 35: 503-524, 2003 $\text{C}_6\text{H}_5\text{OH} + \text{AC}_3\text{H}_5 = \text{C}_6\text{H}_5\text{O} + \text{C}_3\text{H}_6$	4.9E+11	0.0	9400.0
!DA COSTA ET AL. !INT J CHEM KINET 35: 503-524, 2003 $\text{C}_6\text{H}_5\text{OH} + \text{C}_4\text{H}_5\text{-I} = \text{C}_6\text{H}_5\text{O} + \text{C}_4\text{H}_6\text{-13}$	4.9E+11	0.0	9400.0
!DA COSTA ET AL. !INT J CHEM KINET 35: 503-524, 2003 $\text{C}_6\text{H}_5\text{OH} + \text{H} = \text{C}_6\text{H}_4\text{OH} + \text{H}_2$	1.7E+14	0.0	16000.0
!DA COSTA ET AL. !INT J CHEM KINET 35: 503-524, 2003 $\text{C}_6\text{H}_5\text{OH} + \text{O} = \text{C}_6\text{H}_4\text{OH} + \text{OH}$	2.0E+13	0.0	14700.0
!DA COSTA ET AL. !INT J CHEM KINET 35: 503-524, 2003 $\text{C}_6\text{H}_5\text{OH} + \text{OH} = \text{C}_6\text{H}_4\text{OH} + \text{H}_2\text{O}$	1.4E+13	0.0	4600.0
!DA COSTA ET AL. !INT J CHEM KINET 35: 503-524, 2003 $\text{C}_6\text{H}_5\text{OH} + \text{HO}_2 = \text{C}_6\text{H}_4\text{OH} + \text{H}_2\text{O}_2$	4.0E+11	0.0	28900.0
!DA COSTA ET AL. !INT J CHEM KINET 35: 503-524, 2003 $\text{C}_6\text{H}_5\text{OH} + \text{CH}_3 = \text{C}_6\text{H}_4\text{OH} + \text{CH}_4$	2.0E+12	0.0	15000.0
!DA COSTA ET AL. !INT J CHEM KINET 35: 503-524, 2003 $\text{C}_6\text{H}_4\text{OH} + \text{O}_2 = \text{OC}_6\text{H}_4\text{OH} + \text{O}$	2.1E+13	0.0	6100.0
!DA COSTA ET AL. !INT J CHEM KINET 35: 503-524, 2003 $\text{C}_6\text{H}_4\text{OH} + \text{H} = \text{C}_6\text{H}_5\text{OH}$	1.0E+14	0.0	0.0
!DA COSTA ET AL. !INT J CHEM KINET 35: 503-524, 2003 $\text{OC}_6\text{H}_4\text{OH} = \text{C}_5\text{H}_4\text{OH} + \text{CO}$	7.4E+11	0.0	43800.0

!WKM
 !REDUCED FROM 2.5E+14
 !EMDEE ET AL.
 !J. PHYS. CHEM. 1992, 96, 2151-2161
 $\text{C}_6\text{H}_5\text{O} + \text{H}(+\text{M}) = \text{C}_6\text{H}_5\text{OH}(+\text{M})$ 2.0E+14 0.0 0.0
 LOW /1.0E+94 -21.84 13880. /
 TROE /0.043 304.2 60000. 5896.4 /

!XU AND LIN
 !J PHYS CHEM 110 1672-1677 2006
 !WKM
 !A FACTOR *0.5 TO FIT PYROLYSIS DATA
 $\text{C}_6\text{H}_5\text{OH} = \text{C}_5\text{H}_6 + \text{CO}$ 4.31E15 -0.61 74115.

!BAULCH AND COBOS
 !EVALUATED KINETIC DATA FOR COMBUSTION MODELLING
 !J. PHYS. CHEM. REF. DATA 21, 411-429 (1992)
 !WKM
 !A FACTOR REDUCED FROM 2.5E+11 TO 2.0E+11
 !TO FIT DATA BENZENE FLOW REACTOR DATA (LOVELL)
 $\text{C}_6\text{H}_5\text{O} = \text{CO} + \text{C}_5\text{H}_5$ 2.0E+11 0.0 43900.0

!CHAOS ET AL.
 !PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007
 $\text{C}_6\text{H}_5\text{O} + \text{H} = \text{CO} + \text{C}_5\text{H}_6$ 1.E+13 0.0 0.0

!CHAOS ET AL.
 !PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007
 $\text{C}_6\text{H}_5\text{O} + \text{O} = \text{C}_5\text{H}_5 + \text{CO}_2$ 1.0E+13 0.0 0.0

!CHAOS ET AL.
 !PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007
 $\text{C}_6\text{H}_5\text{O} + \text{O} = \text{OC}_6\text{H}_4\text{OH}$ 2.6E+10 0.47 800.0

!WKM
 !ESTIMATED TO IMPROVE AGREEMENT WITH
 !TOLUENE FLOW REACTOR DATA. PATHWAY TO FORM
 !PARABENZOQUINONE REMOVED AS IT CAUSED IT TO BUILD
 !UP AND IT IS NOT SEEN IN THE EXPERIMENT
 $\text{C}_6\text{H}_5\text{O} + \text{HO}_2 = \text{O-OC}_6\text{H}_5\text{OJ} + \text{OH}$ 2.00E+12 0.0 0.0

!ESTIMATED FROM METHODS DESCRIBED IN CURRAN
 !INT J CHEM KINET 38: 250-275, 2006
 $\text{P-C}_6\text{H}_4\text{O}_2 + \text{H} = \text{P-OC}_6\text{H}_5\text{OJ}$ 4.0E+12 0.0 9740.0

!ESTIMATED FROM METHODS DESCRIBED IN CURRAN
 !INT J CHEM KINET 38: 250-275, 2006
 $\text{O-C}_6\text{H}_4\text{O}_2 + \text{H} = \text{O-OC}_6\text{H}_5\text{OJ}$ 4.0E+12 0.0 6960.0

!ALZUETA ET AL.			
!INT J CHEM KINET: 30: 683-697, 1998			
$\text{C6H5O} + \text{O} = \text{P-C6H4O2} + \text{H}$	4.25E+13	0.0	0.0
!ALZUETA ET AL.			
!INT J CHEM KINET: 30: 683-697, 1998			
$\text{C6H5O} + \text{O} = \text{O-C6H4O2} + \text{H}$	8.5E+13	0.0	0.0
!ALZUETA ET AL.			
!INT J CHEM KINET: 30: 683-697, 1998			
$\text{O-C6H4O2} = \text{C5H4O} + \text{CO}$	1.0E+12	0.0	40000.0
!ALZUETA ET AL.			
!INT J CHEM KINET: 30: 683-697, 1998			
$\text{P-C6H4O2} = \text{C5H4O} + \text{CO}$	3.7E+11	0.0	59000.0
!ALZUETA ET AL.			
!INT J CHEM KINET: 30: 683-697, 1998			
$\text{P-C6H4O2} + \text{H} = \text{C5H5O} + \text{CO}$	2.5E+13	0.0	4700.0
!ALZUETA ET AL.			
!INT J CHEM KINET: 30: 683-697, 1998			
$\text{P-C6H4O2} + \text{H} = \text{P-C6H3O2} + \text{H2}$	2.0E+12	0.0	8100.0
!ALZUETA ET AL.			
!INT J CHEM KINET: 30: 683-697, 1998			
$\text{P-C6H4O2} + \text{O} = \text{P-C6H3O2} + \text{OH}$	1.4E+13	0.0	14700.0
!ALZUETA ET AL.			
!INT J CHEM KINET: 30: 683-697, 1998			
$\text{P-C6H4O2} + \text{OH} = \text{P-C6H3O2} + \text{H2O}$	1.0E+6	2.0	4000.0
!ALZUETA ET AL.			
!INT J CHEM KINET: 30: 683-697, 1998			
$\text{P-C6H3O2} + \text{H} = \text{P-C6H4O2}$	1.0E+14	0.0	0.0
!ALZUETA ET AL.			
!INT J CHEM KINET: 30: 683-697, 1998			
$\text{P-C6H3O2} + \text{H} = 2\text{C2H2} + 2\text{CO}$	1.0E+14	0.0	0.0
!ALZUETA ET AL.			
!INT J CHEM KINET: 30: 683-697, 1998			
$\text{P-C6H3O2} + \text{O} = \text{C2H2} + \text{HCCO} + 2\text{CO}$	1.0E+14	0.0	0.0
!CHAOS ET AL.			
!PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007			
$\text{P-C6H4O2} + \text{O} = 2\text{CO} + \text{C2H2} + \text{CH2CO}$	3.000E+13	0.0	5000.0

!CHAOS ET AL.

!PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007

C5H5+H(+M) = C5H6(+M) 2.600E+14 0.0 0.0

LOW /4.400E+80 -18.28 12994/

TROE /0.0680 400.700 4135.8 5501.9/

CO /1.5/ CO2 /2.0/ H2O /6.0/ H2 /2.0/ CH4 /2.0/

!MACKIE ET AL.

!PHYS CHEM CHEM PHYS 3 2467 2001

!TROE FIT ADDED BY WKM (CHEMDIS)

C5H6(+M) = AC3H4+C2H2(+M) 3.8E+17 0.0 1.04E+05

LOW /1.00E+98 -22.25 126321.5/

TROE /1.440547E-01 5.357622E+00 3.283766E+03 6.710101E+09/

CO /1.5/ CO2 /2.0/ H2O /6.0/ H2 /2.0/ CH4 /2.0/

!ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

C5H6+O2 = C5H5+HO2 4.0E+13 0 37150.0

!ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

C5H6+HO2 = C5H5+H2O2 1.1E+4 2.6 12900.0

!ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

C5H6+OH = C5H5+H2O 3.08E+6 2.0 0.0

!ROY AND FRANK, 21ST INTERNATIONAL SYMPOSIUM

!ON SHOCKWAVES, 1997 PPER 1560

C5H6+H = C5H5+H2 7.2E+13 0 3500.0

!ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

C5H6+H = C2H2+AC3H5 7.74E+36 -6.18 32890.0

!ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

C5H6+O = C5H5+OH 4.8E+4 2.71 1100.0

!ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

C5H6+C2H3 = C5H5+C2H4 0.12 4.0 0.0

!EMDEE ET AL.

!J. PHYS. CHEM. 1992, 96, 2151-2161

C5H6+C6H5O = C5H5+C6H5OH 3.16E+11 0.0 8000.0

!ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

C5H6+CH3 = C5H5+CH4 0.18 4.0 0.0

!ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

C5H6+C6H5 = C5H5+C6H6 0.1 4.0 0.0

!WKM

!THIS IS A GLOBAL REACTION INSERTED TO REPRODUCE
!THE BENZENE DATA FROM BUTLER'S RECENT FLOW REACTOR
!STUDY OF CYCLOPENTADIENE. IT SEEMS TO HAVE NO EFFECT
!ON OTHER CONDITIONS.

C5H6+C5H5 = C6H6+C4H5-N	5.0E+9	0.0	0.0
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!LIN J COMPUT CHEM 21 415-425 2000

!C5H5 = H2CCCH+C2H2	1.98E+68	-15.0	124900.0
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!ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

C5H5+O = C4H5-N+CO	3.2E+13	-0.17	440.0
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!ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

C5H5+O = C5H4O+H	5.8E+13	-0.02	20.0
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!ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

C5H5+OH = C5H5OH	6.5E+14	-0.85	-2730.0
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DUP

C5H5+OH = C5H5OH	1.1E+43	-8.76	18730.0
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DUP

C5H5+OH = C5H5OH	1.1E+59	-13.08	33450.0
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DUP

!ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

C5H5+OH = C5H4OH+H	3.5E+57	-12.18	48350.0
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!WKM

!RISTORI ET AL.

!COMBUST. SCI. AND TECH.

!2001. VOL. 167. PP. 223-256

C5H5+OH = C4H6-13+CO	4.0E+14	0.0	4500.0
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!ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

C5H5+HO2 = C5H5O+OH	6.3E+29	-4.69	11650.0
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!WKM

!REDUCED BY 50% TO PROVIDE

!AGREEMENT WITH C5H6 SHOCK TUBE DATA

!ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

C5H5+O2 = C4H4O+HCO	0.60E+19	-2.48	10970.0
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!NOTE C4H4O IS VINYLKETENE.

!ALZUETA ET AL.

!INT J CHEM KINET: 32: 498-522, 2000

C4H4O+H=AC3H5+CO	6.6E+13	-0.02	2740.
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DUP

C4H4O+H=AC3H5+CO DUP	5.9E6	2.0	1300.0
!ALZUETA ET AL. !INT J CHEM KINET: 32: 498-522, 2000			
C4H4O+O=CH2HCO+HCCO	3.E+8	1.45	-860.
!ALZUETA ET AL. !INT J CHEM KINET: 32: 498-522, 2000			
C4H4O+OH=AC3H5+CO2	3.0E+12	0	0
!LIN J COMPUT CHEM 21 415-425 2000			
H2CCCH+C2H2 = C#CC*CCJ	4.11E+72	-18.20	45400.0
!LIN J COMPUT CHEM 21 415-425 2000			
C#CC*CCJ = C5H5	8.0E+13	0.0	34058.3
!LIN J COMPUT CHEM 21 415-425 2000			
C#CC*CCJ+H = C5H6	1.0E+14	0.0	0.0
!LINDSTEDT !C&F 99:551-561 (1994)			
C#CC*CCJ+H = C5H6-L	1.0E+10	0.0	0.0
!LINDSTEDT !C&F 99:551-561 (1994)			
C5H6-L+O = C#CC*CCJ+OH	1.0E+10	0.0	0.0
!LINDSTEDT !C&F 99:551-561 (1994)			
C5H6-L+OH = C#CC*CCJ+H2O	1.0E+10	0.0	0.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000. !PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)			
C5H5OH+H = C5H4OH+H2	3.2E+12	0.0	0.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000. !PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)			
C5H5OH+H = C5H5O+H2	4.0E+13	0.0	6094.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000. !PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)			
C5H5OH+OH = C5H4OH+H2O	5.5E12	0.0	1731.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000. !PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)			
C5H5OH+OH = C5H5O+H2O	1.0E+13	0.0	1697.0

!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
!PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)			
C5H5OH+O = C5H4OH+OH	4.7E+11	0.0	0.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
!PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)			
C5H5OH+O = C5H5O+OH	1.0E+13	0.0	4683.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
!PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)			
C5H5OH+HO2 = C5H4OH+H2O2	3.6E+3	2.55	10531.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
!PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)			
C5H5OH+HO2 = C5H5O+H2O2	1.0E+13	0.0	15800.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
!PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)			
C5H5O = C5H4O+H	2.9E+32	-6.50	21220.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
!PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)			
C5H5O = C4H5-N+CO	1.1E+79	-19.62	66250.0
!BUTLER AND GLASSMAN			
!PROC COMB INSTITUTE 32 (2009) 395-402			
C5H5O = CJ*CC*CC*O	2.0E+13	0.0	14338.0
!ESTIMATED FROM METHODS DESCRIBED IN CURRAN'S N-HEPTANE			
!C&F 114: 149-177 (1998)			
CJ*CC*CC*O = C*CC*CCJ*O	4.3E11	-1.05	4118.0
!WKM			
!ANALOGY TO C2H5+CO = C2H5CO			
C4H5-N+CO = C*CC*CCJ*O	1.51E11	0.0	4810.0
!SAKAI ET AL			
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418			
CJ*CC*CC*O = C2H2+CJ*CC*O	3.00E+13	0.0	43710.0
!SAKAI ET AL			
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418			
CJ*CC*O = C2H3CO	1.40E+09	0.98	32100.0
!SAKAI ET AL			
!PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418			
C2H2+HCO = CJ*CC*O	7.77E+06	1.41	7755.0

!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
C5H4OH+H = C5H5OH	1.0E+14	0.0	0.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
C5H4OH+H = C5H4O+H2	2.1E+13	0.0	54000.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
C5H4OH+O2 = C5H4O+HO2	3.0E+13	0.0	5000.0
!WANG AND BREZINSKY			
!J PHYS CHEM A 102: 1530 1998			
C5H4O = CO+C2H2+C2H2	5.7E+32	-6.76	68500.0
DUP			
C5H4O = CO+C2H2+C2H2	6.2E+41	-7.87	98700.0
DUP			
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
!PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)			
C5H4O+H = C4H5-N+CO	2.1E+61	-13.27	40810.0
!ALZUETA & GLARBORG IJCK 30: 683, 1998.			
C5H4O+O = C4H4+CO2	1.0E13	0.0	2000.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
C5H4O+H = C5H3O+H2	2.0E+12	0.0	8100.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
C5H4O+O = C5H3O+OH	1.4E+13	0.0	1470.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
C5H4O+OH = C5H3O+H2O	1.1E+8	1.42	1450.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
C5H3O+H = C5H4O	1.0E14	0.0	0.0
!CHAOS ET AL.			
!PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007			
C5H3O+O2 => CO2+C2H2+HCCO	9.7E+58	-13.47	38180.0
!CHAOS ET AL.			
!PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007			
C5H3O => C2H2+CO+C2H	2.0E13	0.0	51000.0
!ARENDS ET AL. J PHYS CHEM 97: 7914 1993			
C5H7 = C*CCJC*C	3.2E+15	0.0	39500.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
C5H7+H = C5H6+H2	3.6E+12	0.0	0.0

!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
C5H7+O = C5H6+OH	1.0E+13	0.0	0.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
!PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)			
C5H7+OH = C5H6+H2O	2.4E+13	0.0	0.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
!PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)			
C5H7+O2 = OC5H7O	8.9E+24	-3.80	20000.0
!ZHONG & BOZZELLI J PHYS CHEM A 102: 3537 1998			
C5H6+H = C5H7	2.4E+73	-17.85	31500.0
!ZHONG & BOZZELLI J PHYS CHEM A 102: 3537 1998			
C5H6+H = C*CCJC*C	1.1E+14	-0.16	3100.0
!ZHONG & BOZZELLI J PHYS CHEM A 102: 3537 1998			
C5H6+O = C5H5O+H	8.9E12	-0.15	590.0
DUP			
C5H6+O = C5H5O+H	5.6E12	-0.06	200.0
DUP			
!ZHONG & BOZZELLI J PHYS CHEM A 102: 3537 1998			
C5H6+OH = C*CCJC*COH	1.1E+13	-0.07	870.0
!ZHONG & BOZZELLI J PHYS CHEM A 102: 3537 1998			
C5H6+HO2 = C5H7+O2	1.3E+15	-1.07	9530.0
!ZHONG & BOZZELLI J PHYS CHEM A 102: 3537 1998			
C5H6+HCO = C5H5+CH2O	1.08E+8	1.9	16000.0
!ZHONG & BOZZELLI J PHYS CHEM A 102: 3537 1998			
C5H6+C2H3 = C6H6+CH3	2.1E+67	-16.08	42460.0
!EMDEE ET AL.			
!J. PHYS. CHEM. 1992, 96, 2151-2161			
C5H6+C4H5-I = C5H5+C4H6-13	6.0E+12	0.0	0.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
!PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)			
C*CCJC*C = C*CC*CCJ	5.4E+11	-0.70	60.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
!PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)			
C*CC*CCJ+H = C*CC*CC	2.3E+20	-1.60	3020.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			

!PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)			
C*CC*CC+H = C4H6-13+CH3	5.2E71	-16.38	51000.0
!MARINOV ET AL. COMBUST SCI TECH 116:211 1996			
C*CC*CC+H = C*CC*CCJ+H2	7.0E+6	2.0	5000.0
!MARINOV ET AL. COMBUST SCI TECH 116:211 1996			
C*CC*CC+OH = C*CC*CCJ+H2O	7.0E+6	2.0	0.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
!PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)			
C*CCJC*C+O2 = C2H3CHO+CH2HCO	1.2E36	-7.25	33600.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
!PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)			
C*CC*CCJ+H = C4H5-N+CH3	2.9E+26	-2.18	36770.0
!MARINOV ET AL. COMBUST SCI TECH 116:211 1996			
C*CCJC*C+O = C2H3CHO+C2H3	2.0E+14	0.0	0.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
!PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)			
C*CC*CCJ+OH = C*CC*CCOH	1.5E13	0.0	0.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
!PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)			
C*CC*CCJ+O2 = C*CCJC*O+CH2O	8.2E+10	0.18	9140.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
!PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)			
C*CC*CCOH+H = C4H6-13+CH2OH	2.5E34	-6.12	16250.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
!PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)			
!WKM NOTE			
!HOCO MAY NOT BE THE CORRECT PRODUCT BUT I BELIEVE			
!IT IS THE LOWEST ENERGY STRUCTURE.			
OC5H7O+O2 = OC4H6O+HOCO	6.3E+5	-7.25	33600.0
!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.			
!PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)			
C*CCJC*COH+O2 = HOC*CC*O+CH2HCO	1.2E36	-7.25	33600.0
!WKM			
!ESTIMATE			
!ANALOGY TO IC3H5CHO+R REACTIONS			
HOC*CC*O+OH = HOC*CCJ*O+H2O	2.69E+10	0.76	-340.0
HOC*CC*O+HO2 = HOC*CCJ*O+H2O2	1.00E+12	0.0	11920.0

HOC*CC*O+CH3 = HOC*CCJ*O+CH4	3.98E+12	0.0	8700.0
HOC*CC*O+O = HOC*CCJ*O+OH	7.18E+12	0.0	1389.0
HOC*CC*O+O2 = HOC*CCJ*O+HO2	2.00E+13	0.0	40700.0
HOC*CC*O+H = HOC*CCJ*O+H2	2.60E+12	0.0	2600.0

!WKM

!ANALOGY TO C2H5+CO=C2H5CO

C2H2OH+CO = HOC*CCJ*O	1.51E+11	0.0	4810.0
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!WKM

!ANALOGY TO C3H6+OH

C2H2+OH = C2H2OH	9.93E+11	0.0	-960.0
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!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.

!PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)

OC4H6O+H = OC4H5O+H2	2.3E+10	1.05	3279.0
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!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.

!PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)

OC4H6O+OH = OC4H5O+H2O	3.5E+9	1.18	-447.0
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!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.

!PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)

OC4H5O+O2 = O2CCHOOJ+C2H4	1.6E+45	-9.92	20670.0
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!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.

!PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)

O2CCHOOJ = HOCO+CO2	3.0E13	0.0	4000.0
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!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.

C*CCJC*O = AC3H5+CO	6.1E+5	0.92	-1120.0
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!ALZUETA & GLARBORG IJCK 32: 498-522, 2000.

C*CCJC*O+O2 = C2H3CHO+HOCO	1.2E+36	-7.25	33600.0
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!R. Sivaramakrishnan, R. S. Tranter, K. Brezinsky, Proc. of the Comb. Inst. 30 (2005) 1165-1173

!https://www-

pls.llnl.gov/data/docs/science_and_technology/chemistry/combustion/nbutane_mech.txt

HCOH+OH=HCO+H2O	2.00E+13	0	0	!Marinov
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1996 64

HCOH+H=CH2O+H	2.00E+14	0	0	!Marinov
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1996 65

HCOH+O=CO2+H+H	5.00E+13	0	0	!Marinov
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1996 66

HCOH+O=CO+OH+H	3.00E+13	0	0	!Marinov
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1996 67

HCOH+O2=CO2+H+OH	5.00E+12	0	0
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!(e) 68

HCOH+O2=CO2+H2O !(e) 69	3.00E+13	0	0	
C+O2=CO+O !Miller 1992 110	2.00E+13	0	0	
C+OH=CO+H !Miller 1992 111	5.00E+13	0	0	
C+CH3=C2H2+H !Miller 1992 112	5.00E+13	0	0	
C+CH2=C2H+H !Miller 1992 113	5.00E+13	0	0	
C2H+H2=C2H2+H !Miller 1992 201	4.09E+05	2.39	864.3	
C2H+O=CH+CO !Miller 1992 202	5.00E+13	0	0	
C2H+OH=HCCO+H !Miller 1992 203	2.00E+13	0	0	
C2H+OH=C2+H2O !Miller 1992 204	4.00E+07	2	8000	
C2H+O2=CO+CO+H 1993 205	9.04E+12	0	-457	!Opansky
C2H+C2H2=C4H2+H !Farhat 1993 206	9.64E+13	0	0	
C2H+C2H4=C4H4+H !Tsang 1986 207	1.20E+13	0	0	
HCCO+C2H2=H2CCCH+CO !Miller 1992 208	1.00E+11	0	3000	
HCCO+H=CH2-S+CO !Miller 1992 209	1.00E+14	0	0	
HCCO+O=H+CO+CO 1995 210	8.00E+13	0	0	!Peeters
HCCO+O=CH+CO2 1995 211	2.95E+13	0	1113	!Peeters
HCCO+CH=C2H2+CO !Miller 1992 214	5.00E+13	0	0	
HCCO+HCCO=C2H2+CO+CO !Miller 1992 215	1.00E+13	0	0	
HCCO+OH=C2O+H2O !Miller 1992 216	3.00E+13	0	0	
C2O+H=CH+CO !Miller 1992 217	1.00E+13	0	0	
C2O+O=CO+CO !Miller 1992 218	5.00E+13	0	0	
C2O+OH=CO+CO+H !Miller 1992 219	2.00E+13	0	0	
C2O+O2=CO+CO+O !Miller 1992 220	2.00E+13	0	0	
C2+H2=C2H+H !Miller 1992 221	4.00E+05	2.4	1000	

C2+O2=CO+CO	5.00E+13	0	0	
!Miller 1992 222				
C2+OH=C2O+H	5.00E+13	0	0	
!Miller 1992 223				
CH2+HCCO=C2H3+CO	3.00E+13	0	0	
!Miller 1992 83				
CH2+C2H2=H2CCCH+H	1.20E+13	0	6600	
!Miller 1992 84				
CH2-S+CH2CO=C2H4+CO	1.60E+14	0	0	
!Miller 1992 97				
CH+C2H2=C3H2+H	1.00E+14	0	0	
!Miller 1992 106				
CH+CH2=C2H2+H	4.00E+13	0	0	
!Miller 1992 107				
CH+CH3=C2H3+H	3.00E+13	0	0	
!Miller 1992 108				
CH2-S+C2H2=H2CCCH+H	1.50E+14	0	0	!Canosa-
Mas85 90				
CH2-S+C2H4=AC3H5+H	1.30E+14	0	0	!Canosa-
Mas85 91				
HCCO+O2=HCO+CO+O	9.78E+11	0	850	!Baulch,
1992				
HCCO+O2=CO2+HCO	6.52E+11	0	850	!Baulch,
1992				
!N-PROPYLBENZENE CHEMISTRY				
!				
CPHC3H6+H=PHC3H7	1.00E+14	0	0	
!Estimated				
BPHC3H6+H=PHC3H7	1.00E+14	0	0	
!Estimated				
APHC3H6+H=PHC3H7	1.00E+14	0	0	
!Estimated				
CPHC3H6=C6H5C2H3+CH3	2.00E+13	0	42051	
!Estimated, Dean 1985				
BPHC3H6=C6H5+C3H6	2.00E+13	0	44167	
!Estimated, Dean 1985				
APHC3H6=C6H5CH2+C2H4	2.00E+13	0	12244	
!Estimated, Dean 1985				
!Roughaugh, Barton, Stein, J. Phys. Chem, 85 (1981) 2378 - 2383.				
PHC3H7=C6H5CH2+C2H5	3.00E+15	0	69600	
!*1.5				
!Estimated rate constants				
PHC3H7=C6H5CH2CH2+CH3	8.00E+15	0	87862	
!Estimated, Dean 1985				
PHC3H7=C6H5+NC3H7	8.00E+15	0	102240	
!Estimated, Dean 1985				
!Qi Chen and Gilbert F. Froment J. of Analytical and Applied Pyrolysis 21 (1991) 51-77				

!PHC3H7=C6H5CH2+C2H5 !*1.4 !Estimated from analogous reactions of propane-rxns of abstraction of terminal hydrogens of propane*0.5-a !Same rate constant as reactions of propane+h=ic3h7+h2-b !Estimated from analogous reactions of toluene*(2/3)-c, Look at the paper for more detailed information about the references	2.91E+15	0	68943	
PHC3H7+H=APHC3H6+H2 Tsang-propane-1988	6.63E+05	2.54	6756	!a-
PHC3H7+O=APHC3H6+OH Tsang-propane-1988	9.65E+04	2.68	3716	!a-
PHC3H7+OH=APHC3H6+H2O !a-Cohen-propane-1991	1.22E+07	1.8	934	
PHC3H7+HO2=APHC3H6+H2O2 !a-Tsang-propane-1988	2.38E+04	2.55	16492	
PHC3H7+O2=APHC3H6+HO2 Tsang-propane-1988	1.99E+13	0	50933	!a-
PHC3H7+CH3=APHC3H6+CH4 Tsang-propane-1988	4.52E-01	3.65	7153	!a-
PHC3H7+H=BPHC3H6+H2 Tsang-propane-1988	7.22E+05	2.4	4471	!b-
PHC3H7+O=BPHC3H6+OH Tsang-propane-1988	4.76E+04	2.71	2106	!b-
PHC3H7+OH=BPHC3H6+H2O Cohen-propane-1991	5.45E+06	1.9	-159	!b-
PHC3H7+HO2=BPHC3H6+H2O2 Tsang-propane-1988	9.64E+03	2.60	13909	!b-
PHC3H7+O2=BPHC3H6+HO2 Tsang-propane-1988	3.98E+13	0	47589	!b-
PHC3H7+CH3=BPHC3H6+CH4 Tsang-propane-1988	1.00	3.46	5480	!b-
PHC3H7+H=CPHC3H6+H2 2005	5.31E+02	3.44	3120	!Baulch-
PHC3H7+O=CPHC3H6+OH Ravishankara-JPC-1982	1.97E+13	0	3522	!c-
PHC3H7+OH=CPHC3H6+H2O UIC mxyl	1.63E+05	2.39	-602	!c-
PHC3H7+HO2=CPHC3H6+H2O2 2005	6.23E+04	2.50	14683	!Baulch-
PHC3H7+O2=CPHC3H6+HO2 UIC mxylene-Oxidation-Model	1.74E+07	2.5	44946	!c-
PHC3H7+CH3=CPHC3H6+CH4 UIC mxylene-Oxidation-Model	2.67e-05	5.61	9000	!c-
BPHC3H6=BPHPROPY	2.00E+11	0.0	20000	!Dagaut
BPHPROPY=C6H5C2H3+CH3	1.00E+14	0.0	49675	!Dagaut
BPHC3H6=C6H5C3H5-2+H !Estimated	3.00E+13	0	31586	

!BPHC3H6=BPHPROPY et al.	1.00E+13	0.0	25000 !Litzinger
!BPHPROPY=C6H5C2H3+CH3 et al.	1.00E+14	0.0	25000 !Litzinger
!BPHC3H6=C6H5C3H5-2+H et al.	1.00E+14	0	38000 !Litzinger
BPHC3H6=C6H6+AC3H5 et al.	1.00E+14	0	38000 !Litzinger
!P. Dagaut, A. Ristori, A. E. Bakali and M. Cathonnet, 81 (2002) 173-184			
BPHC3H6+O=C6H5CH2+CH3HCO	2.000E+13	0.0	4000
BPHC3H6+OH=C6H5CH3+CH3HCO	2.000E+13	0.0	4000
BPHC3H6+HO2=>C6H5CH2+CH3HCO+OH	2.000E+13	0.0	4000
CPHC3H6+O=C6H5CHO+C2H5	1.600E+13	0.0	0
CPHC3H6+OH=C6H5CHO+C2H6	1.600E+13	0.0	0
CPHC3H6+HO2=>C6H5CHO+C2H5+OH	5.000E+12	0.0	0
!Same as n-C3H7+O2=C3H6+HO2, J. D. DeSain, S. J. Klippenstein, J. A. Miller, C. A. Taatjes, J. Phys. Chem. A., 107 (2003) 4415-4427			
BPHC3H6+O2=C6H5C3H5+HO2 !*0.5	1.85E+16	-1.63	3418
BPHC3H6+O2=C6H5C3H5-2+HO2	1.5E+12	0.0	5000.0
!A. M. Dean, J. Phys. Chem., 89 (1985) 4601-4608.			
BPHC3H6=C6H5C3H5+H !Estimated	3.00E+13	0	36784
C6H5C3H5=C6H5CH2+C2H3	1.00E+17	0	90547 !Estimated
C6H5C3H5-2=C6H5CHCH+CH3 !Estimated	1.00E+17	0	100067
C6H5C3H5-2=R1C9H9+H !Estimated	3.50E+15	0	107143
!Estimated from analogous C3H6 reactions, from the C0-C8 chemistry of this model			
C6H5C3H5-2+O<=>R1C9H9+OH	5.24E+11	0.7	5884.0!
C6H5C3H5-2+OH<=>R1C9H9+H2O	3.12E+06	2.0	-298.0!
C6H5C3H5-2+HO2<=>R1C9H9+H2O2	2.70E+04	2.5	12340.0!
C6H5C3H5-2+H<=>R1C9H9+H2	1.73E+05	2.5	2490.0!
C6H5C3H5-2+O2<=>R1C9H9+HO2	4.00E+12	0.0	39900.0!
C6H5C3H5-2+CH3<=>R1C9H9+CH4	2.21E+00	3.5	5675.0!
!R. Sivaramakrishnan, R. S. Tranter and K. Brezinsky, J. Phys. Chem. A, 110 (2006) 9400-9404			
R1C9H9=R2C9H9 2002 PCCP Guess A Ea Barrier+RT	1.00E+12	0	5132 !Peeters
R2C9H9=R3C9H9 2002 PCCP Guess A Ea Barrier+RT	1.00E+12	0	33095 !Peeters
R3C9H9=R13C9H9 2002 PCCP Guess A Ea Barrier+RT	1.00E+12	0	26642 !Peeters
R13C9H9=pc-C9H9 2002 PCCP Guess A Ea Barrier+RT	1.00E+12	0	18277 !Peeters
pc-C9H9=i-C9H9 2002 PCCP Guess A Ea Barrier+RT	1.00E+13	0	46719 !Peeters
i-C9H9=n-C9H9 2002 PCCP Guess A Ea Barrier+RT	1.00E+13	0	26642 !Peeters

n-C9H9=R22C9H9	1.00E+11	0	13975	!Peeters
2002 PCCP Guess A Ea Barrier+RT				
R22C9H9=INDENE+H	1.00E+13	0	37158	!Peeters
2002 PCCP Guess A Ea Barrier+RT				
!Estimated from C3H6+H=C2H4+CH3 reaction,R. A. Kalinenko et al., Dokl. Chem., 204 (1972)				
C6H5C3H5+H=C6H5CH2+C2H4	5.42E+12	0	0	
!A-factorx1.1				
!J. Park, L. M. Wang, M. C. Lin, Inter. J. Chem. Kinet., 36 (2004) 49-56.				
C3H8+C6H5=C6H6+NC3H7	1.96E+11	0	3850	
!Y. Choi, J. Park, M. C. Lin, Chem. Phys. Chem., 5 (2004) 661-668				
CH3HCO+C6H5=C6H6+CH2HCO	60.00	3.3	1888	
CH3HCO+C6H5=C6H6+CH3CO	8.80E+03	2.6	179	
!R. Sivaramakrishnan, R. S. Tranter and K. Brezinsky, J. Phys. Chem. A, 110 (2006) 9400-9404				
!phenylacetylene reactions				
!http://web.mit.edu/anish/www/mitsootmodel1atmsymp2004.mec				
!C6H5C2H+H=C6H4C2H+H2	3.23E+07	2.095	15842	!
From Howard 2004 [Mebel et al. 1997, for C6H6+H]				
C6H5C2H+CH3=C6H4C2H+CH4	1.67E+12	0.0	15057	!
From Howard 2004 [Marinov et al. 1996]				
!C6H4C2H+H=C6H5C2H	8.02E+19	-2.011	1968	!
From Howard 2004 [c6h5+h=c6h6]				
C6H5CHCH+H=C6H5C2H+H2	9.57E14	-0.25	720	!
[QRRK-HR, 1 atm]				
C6H5+C2H=C6H5C2H	2.54E17	-1.489	1541	!
[Zhang and McKinnon 1995]				
!I. V. Tokmakov and M. C. Lin, J. Am. Chem. Soc., 125 (2003) 11397-11408				
!C6H5CHCH=>C6H5C2H+H	3.80E+11	0.82	38910	
!Lin, JACS, 2003				
C6H5CCH2=>C6H5C2H+H	1.23E+13	0.55	42580	
!Lin, JACS, 2003				
C6H5CHCH=>C6H5CCH2	4.90E+12	0.45	45740	
!Lin, JACS, 2003				
C6H5CCH2=>C6H5CHCH	6.61E+13	0.14	53120	
!Lin, JACS, 2003				
!P. Frank, J. Herzler, Ber. Bunsenges. Phys. Chem., 96 (1992) 1333 - 1338				
C6H5C2H+H=C6H5+C2H2	2.00E+14	0	9698	
!N. A. Slavinskaya, P. Frank, Combust. Flame, 156 (2009) 1705 - 1722				
INDENE = INDENYL+H	1.10E+15	0	77095.6	
!INDENE+H = INDENYL+H2	5.00E+13	0	0	
!INDENE+H = C6H5CH2+C2H2	3.00E+14	0	45701	
!INDENE+H = C6H5C2H+CH3	4.00E+14	0	45701	
!INDENE+H = C6H6+H2CCCH	2.00E+14	0	48681.5	
C6H5+C6H6 = P2+H	1.10E+23	-2.92	14803.15	
2C6H5 = P2	2.00E+19	-2.05	2881.15	
2C6H5 = P2-+H	2.30E-01	4.62	28811.5	
P2 = P2-+H	1.10E+19	-2.72	113855.1	
P2 = INDENE+C3H2	2.50E+12	0	89415	
P2-+O2 => A2+HCO+CO	2.00E+12	0	7351.9	

P2+H = P2-+H2	2.50E+14	0	15896
P2+OH = P2-+H2O	1.60E+08	1.42	1529.99
C4H5-I+C6H6 => A2+H2+H	5.00E+11	0	2987.41476
2C5H5 => A2+2H	4.30E+13	0	9713.0521
2C5H5 => A2+H2	4.30E+36	-6.3	45373.145
A2+O = CH2CO+C6H5C2H	2.20E+13	0	4500.555
A2+O => INDENYL+CO+H	3.60E+14	0	43898.791
A2+H = A2-+H2	2.50E+14	0	15896
A2+OH = A2-+H2O	2.10E+13	0	4570.1
A2+CH3 = A2-+CH4	2.00E+12	0	14962.11
A2+C2H = A2C2H+H	5.00E+13	0	0
A2-+H = A2	7.80E+13	0	0
A2- + C2H2 = A2C2H + H	1.60E+14	-0.19	19870
A2C2H+H = A2C2H*+H2	2.50E+14	0	15896
A2C2H+OH = A2-+CH2CO	2.18E-04	4.5	-993.5
A2C2H+OH = A2C2H*+H2O	2.10E+13	0	4570.1
INDENYL+H2CCCH => A2C2H+2H	6.00E+11	0	0
C6H5C2H+C6H5 = A3+H	1.10E+23	-2.92	15915.87
C6H4C2H+C6H6= A3+H	1.10E+23	-2.92	15915.87
INDENYL+C5H5 => A3+2H	4.30E+13	0	9713.0521
INDENYL+C5H5 = A3+H2	4.30E+36	-6.3	44767.11
A2-+C4H4 = A3+H	3.30E+33	-5.7	25334.25
A2-+C4H2 = A3-	3.30E+33	-5.7	25334.25
P2-+C2H2 = A3+H	4.64E+06	1.97	7212.81
A2C2H*+C2H2 = A3-	1.10E+62	-14.56	32884.85
A3 = A2+C4H2	1.00E+11	0	89415
A3+O = A3-+OH	2.00E+13	0	14703.8
A3+H = A3-+H2	2.50E+14	0	15896
A3+OH => A2C2H+CH2CO+H	1.30E+13	0	9935
A3+OH = CH2CO+P2-	1.00E+13	0	9935
A3+CH3 = A3-+CH4	2.00E+12	0	14962.11
A3C2H+OH = A3-+CH2CO	2.18E-04	4.5	-993.5
A3-+H = A3	1.00E+14	0	0
C6H4C2H+H(+M) = C6H5C2H(+M)	1.000E+14	.0000	.00
H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/			
LOW / 6.600E+75 -16.30 7000.00 /			
TROE / 1.0000E+00 1.0000E-01 5.8490E+02 6.1130E+03 /			
C4H3-N+C4H2 = C6H4C2H	1.90E+63	-15.25	30401.1
C6H5C2H+O = C6H4C2H+OH	1.10E+13	0	8146.7
C6H5C2H+H = C6H4C2H+H2	2.70E+13	0	9700.534
C6H5C2H+OH = C6H4C2H+H2O	2.10E+13	0	4570.1
!http://creckmodeling.chem.polimi.it/			
!biphenylmethane			
OH+FLUORENE=>P2+CO+H	.1000E+14	.000	7000.0
!C5H5+C6H5C2H=FLUORENE+H	.300E+13	0	23000
!benzofuran			
O+C6H5CHCH=>C8H6O+H	.1000E+14	.000	.0
OH+C6H5CHCH=>C8H6O+H2	.1000E+14	.000	.0

C2H2+C6H5O=>C8H6O+H	.3000E+12	.000	15000.0
C6H5O+C6H5CHCH=>C8H6O+C6H6	.1000E+13	.000	.0
C6H5CH2+CO=>C8H6O+H	.3000E+12	.000	16000.0
C6H5CH2+HCO=>C8H6O+H2	1.00E+14	0	0
C6H5+CH3CO=>C8H6O+H2	1.00E+14	0	0
C6H5O+C6H5O=DIBZFUR+H2O	4.00E+13	0	0
!included from the npb pyrolysis model			
!N.A. Skavinskaya, U. Riedel, S. B. Dworkin, M. J. Thomson, Combust. Flame (2011)			
doi:10.1016/j.combustflame.2011.10.005			
C5H5+C4H3-N => INDENE	3.00E+36	-7.18	8412.958
C5H5+C4H4 => INDENE+H	6.00E+11	0	9995
C6H5+H2CCCH => INDENE	3.86e+11	0	1361
C6H5+AC3H4 => INDENE+H	1.00E+16	0	32984.2
C6H5+PC3H4 => INDENE+H	1.00E+16	0	32984.2
C6H5CH2+C2H2 = INDENE+H	6.00E+11	0	9995
INDENYL+H2CCCH=>A2R5+2H	4.15E+13	0	9713
!A-factor/2			
C6H4C2H+C4H4=A2R5+H	1.60E+16	-1.33	6557
A2R5+H(+M) = A2R5(+M)	1.000E+14	.0000	0.00
CH4/3/ C2H6/3/ AR/0.2/			
LOW / 6.600E+75 -16.30 3.50 /			
TROE / 1.0000E+00 1.0000E-01 5.8500E+02 6.1130E+03 /			
A2R5+H=A2R5+H2	2.50E+14	0	15896
A2R5+C6H6=>BGHIF+H2+H	1.10E+25	-2.92	15916
!rxns of methyl naphthalene			
A2+CH2=A2CH3	2.20E+13	0	8683
A2+CH2-S=A2CH3	4.40E+13	0	8683
A2CH3=A2CH2+H	2.81E+15	0	88819
A2CH3=A2+CH3	1.00E+16	0	96965
A2CH3+H=A2CH2+H2	3.98E+02	3.44	3100
A2CH3+H=A2+CH3	1.20E+13	0	5067
A2CH2+CH2=>A2C2H+H2+H	2.40E+14	0	0
!rxns of methyl anthracene			
A3+CH2=A3CH3	2.20E+13	0	7145
A3+CH2-S=A3CH3	4.2E+13	0	7145
A3CH3=A3CH2+H	2.80E+15	0	88819
A3CH3+H=A3CH2+H2	1.20E+14	0	8345
A3CH3+H=A3+CH3	1.20E+13	0	5067
A3CH3+CH3=A3CH2+CH4	1.58E+12	0	10929
A3CH2+H=A3+CH3	1.00E+16	0	96966
A3CH2+CH2=>A4+H2+H	2.40E+14	0	0
!http://creckmodeling.chem.polimi.it/			
!biphenylmethane			
C6H5+C6H5CH2=C6H5CH2C6H5	.5000E+13	.000	.0
C6H5CH2C6H5=FLUORENE+H2	.1000E+09	.000	32000.0
CH3+FLUORENE=>A3+H2+H	.3000E+12	.000	7600.0
C5H5+C6H5C2H=FLUORENE+H	.300E+13	0	23000
!rxns of diphenylethyne			

CH3+FLUORENE=>C14H10+H2+H	.3000E+12	.000	7600.0	
C14H14=>C14H10+H2+H2	.4000E+08	.000	40000.0	
C6H5+C6H4C2H=C14H10	.5000E+13	.000	.0	
H+C14H10=>H2+C14H9	.4813E+08	2.0	10480.03	
C14H9+C2H2=A4+H	.1000E+13	.000	5000.0	
!R. K. Robinson and R.P. Lindstedt, Combust. Flame 158 (2011) 666-686				
C5H5+CH3=C5H4CH3+H	2.00E+13	0	6214	
C5H4CH3=C5H4CH2+H	1.00E+17	0	51864	
H2CCCH+C2H2=C5H5	6.87E+55	-12.5	42017	
C5H6=C5H5+H	1.61E+16	0.86	89579	
!L. Zhang, J. Cai, T. Zhang, F. Qi, Combust. Flame, 157 (2010) 1686-1697				
C14H12=>A3+H2	2.50E+15	2	84700	
!K. Narayanaswamy, G. Blanquart, H. Pitsch, Combust. Flame 157 (2010) 1879-1898				
C6H5+C4H4=A2+H	1.260e+04	2.610	1434.03	
H2CCCH+H2CCCH = C5H4CH2	8.250e+46	-10.100	16959.85	
C5H4CH2+H=>C4H5-N+C2H2	1.963E+24	-1.992	45912	
C5H4CH2+H=>C4H5-I+C2H2	5.589E+31	-4.213	46143	
C5H5+C5H5=INDENYL+CH3	2.50E+12	0	9560	
!Rate constant same as C6H5C2H5+H=C6H6+C2H5, C. Ellis, M.S. Scott, R. W. Walker, Combust. Flame 132 (2003) 291 -304				
PHC3H7+H=C6H6+NC3H7	1.00E+06	2	944	
!Y. Georgievskii, J. A. Miller, S. J. Klippenstein, Phys. Chem. Chem. Phys., 9 (2007) 4259-4268				
H2CCCH+H2CCCH= HT1245	3.79E+11	0.80	-1029	
!Georgievskii, Y.; Miller, J.A.; Klippenstein, S.J., nist				
H2CCCH+H2CCCH=HD125Y	3.90E+12	0.19	-671	
!Georgievskii, Y.; Miller, J.A.; Klippenstein, S.J., nist				
H2CCCH+H2CCCH=HDY15			6.04E+12	-
0.28 -303 !Georgievskii, Y.; Miller, J.A.; Klippenstein, S.J., nist				
!D. L. Baulch et al., J. Phys. Chem. Ref. Data, 21 (1992) 411-429				
C2H4+H=C2H3+H2	5.42E+14	0	14900	
!A. Comandini, T. Malewicki and K. Brezinsky, "Chemistry of PAHs formation from phenyl radical pyrolysis and phenyl+acetylene reaction", (2011) submitted to Journal of Physical Chemistry				
!C6H6+C6H5 = P2+H	9.55E+11	0.00	4305	
!99PAR/LIN				
P2+C6H5 = m-TERPH+H	6.367E+11	0.00	4305	
!99PAR/LIN As 4/6 of C6H5+C6H6 = c12h10+H				
P2+C6H5 = p-TERPH+H	3.183E+11	0.00	4305	
!99PAR/LIN As 2/6 of C6H5+C6H6 = c12h10+H				
!A. Ergut, S. Granata, J. Jordan, J. Carlson, J. B. Howard, H. Richter, Y. A. Levendis, Combust. Flame, 144 (2006) 757 - 772				
! 2-phenylnaphthalene				
A2->C6H5=A2C6H5-2	1.19E17	-1.16	1990	!
[QRRK-HR, 1 atm]				
A2->C6H6=A2C6H5-2+H	2.22E83	-20.79	46890	!
[Park et al. 1999]				
A2+C6H5=A2C6H5-2+H	2.22E83	-20.79	46890	!
[Park et al. 1999]				

END

N-Propylbenzene Oxidation Model Thermochemistry File

!R.Sivaramakrishnan, R. S. Tranter and K. Brezinsky, Proc. of the Combust. Inst., 30 (2005) 1165-1173

THERMO

```
300.000 1000.000 5000.000
HE      L10/90HE 1 0 0 0G 200.000 6000.000 1000. 1
2.50000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2
-7.45375000E+02 9.28723974E-01 2.50000000E+00 0.00000000E+00 0.00000000E+00 3
0.00000000E+00 0.00000000E+00-7.45375000E+02 9.28723974E-01 0.00000000E+00 4
AR      120186AR 1      G 0300.00 5000.00 1000.00 1
0.02500000E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2
-0.07453750E+04 0.04366001E+02 0.02500000E+02 0.00000000E+00 0.00000000E+00 3
0.00000000E+00 0.00000000E+00-0.07453750E+04 0.04366001E+02 4
N2      121286N 2      G 0300.00 5000.00 1000.00 1
0.02926640E+02 0.01487977E-01-0.05684761E-05 0.01009704E-08-0.06753351E-13 2
-0.09227977E+04 0.05980528E+02 0.03298677E+02 0.01408240E-01-0.03963222E-04 3
0.05641515E-07-0.02444855E-10-0.01020900E+05 0.03950372E+02 4
!C5H3   20387C 5H 3      G 0300.00 5000.00 1000.00 1
! 0.10787622E+02 0.09539619E-01-0.03206744E-04 0.04733323E-08-0.02512135E-12 2
! 0.06392904E+06-0.03005444E+03 0.04328720E+02 0.02352480E+00-0.05856723E-04 3
!-0.12154494E-07 0.07726478E-10 0.06588531E+06 0.04173258E+02 4
!C5H2   20587C 5H 2      G 0300.00 5000.00 1000.00 1
! 0.01132917E+03 0.07424057E-01-0.02628189E-04 0.04082541E-08-0.02301333E-12 2
! 0.07878706E+06-0.03617117E+03 0.03062322E+02 0.02709998E+00-0.01009170E-03 3
!-0.01272745E-06 0.09167219E-10 0.08114969E+06 0.07071078E+02 4
H2O     20387H 2O 1      G 0300.00 5000.00 1000.00 1
0.02672146E+02 0.03056293E-01-0.08730260E-05 0.01200996E-08-0.06391618E-13 2
-0.02989921E+06 0.06862817E+02 0.03386842E+02 0.03474982E-01-0.06354696E-04 3
0.06968581E-07-0.02506588E-10-0.03020811E+06 0.02590233E+02 4
C2      121286C 2      G 0300.00 5000.00 1000.00 1
0.04135979E+02 0.06531618E-03 0.01837099E-05-0.05295085E-09 0.04712137E-13 2
0.09967272E+06 0.07472923E+01 0.06996045E+02-0.07400602E-01 0.03234704E-04 3
0.04802535E-07-0.03295918E-10 0.09897487E+06-0.01386227E+03 4
C2O     121286C 2O 1      G 0300.00 5000.00 1000.00 1
0.04849809E+02 0.02947585E-01-0.01090729E-04 0.01792562E-08-0.01115758E-12 2
0.03282055E+06-0.06453226E+01 0.03368851E+02 0.08241803E-01-0.08765145E-04 3
0.05569262E-07-0.01540009E-10 0.03317081E+06 0.06713314E+02 4
CH2HCO  110393O 1H 3C 2  G 0300.00 5000.00 1000.00 1
0.05975670E+02 0.08130591E-01-0.02743624E-04 0.04070304E-08-0.02176017E-12 2
0.04903218E+04-0.05045251E+02 0.03409062E+02 0.01073857E+00 0.01891492E-04 3
-0.07158583E-07 0.02867385E-10 0.01521477E+05 0.09558290E+02 4
HCOH    MAR94 C 1H 2O 1 0G 300. 5000. 1398. 1
9.18749272E 00 1.52011152E-03-6.27603516E-07 1.09727989E-10-6.89655128E-15 2
7.81364593E 03-2.73434214E 01-2.82157421E 00 3.57331702E-02-3.80861580E-05 3
1.86205951E-08-3.45957838E-12 1.12956672E 04 3.48487757E 01 4
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!R. Sivaramakrishnan, R. S. Tranter and K. Brezinsky, 5 (2003) 2807 - 2817

NE REF ELEMENT L10/90NE 100 0 0 0G 200.000 6000.000 1000. 1
0.25000000E 01 0.00000000E 00 0.00000000E 00 0.00000000E 00 0.00000000E 00 2
-0.74537500E 03 0.33553227E 01 0.25000000E 01 0.00000000E 00 0.00000000E 00 3
0.00000000E 00-0.74537498E 03 0.33553227E 01 0.00000000E 00 0.00000000E+00 4
C9H9 C 9H 9 G 200.000 6000.000 1000.00 1
0.16551020E+02 0.31836757E-01-0.11523691E-04 0.18714361E-08-0.11255478E-12 2
0.16983296E+05-0.65703805E+02 0.41988226E-01 0.42045925E-01 0.56902995E-04 3
-0.99573313E-07 0.39205372E-10 0.23076451E+05 0.27899469E+02 4
C9H8 INDENE T 9/96C 9H 8 0 0G 200.000 6000.000 1000.00 1
0.17318671E+02 0.28982768E-01-0.10605059E-04 0.17334553E-08-0.10467919E-12 2
0.11151429E+05-0.71555323E+02-0.68190289E+00 0.41658733E-01 0.70741234E-04 3
-0.13430875E-06 0.59915845E-10 0.17705036E+05 0.29781396E+02 0.19741190E+05 4
C6H4C2H C 8H 5 G 300.000 5000.000 1403.00 1
1.88370382E+01 1.52445522E-02-5.22469596E-06 8.12518874E-10-4.72045178E-14 2
5.96821996E+04-7.49107592E+01-1.49929738E+00 7.01891496E-02-6.29429910E-05 3
2.85073827E-08-5.11137313E-12 6.59494823E+04 3.15838359E+01 4

!P. Dagaut, A. Ristori, A. E. Bakali, M. Cathonnet, Fuel 81(2002) 173-184

PHC3H7 C 9H 120 00 0G 300.00 3000.00 1000.00 1
0.19564560E+02 0.3371875E-01-0.11279970E-04 0.17806490E-08-0.10900860E-12 2
-0.86688460E+04 -0.7905852E+02-0.42383000E+01 0.90064150E-01-0.53314080E-04 3
0.98838910E-08 0.1259661E-11-0.13268630E+04 0.46994210E+02 4
APHC3H6 C 9H 110 00 0G 300.0 3000.0 1000.0 1
0.21741480E+02 0.26909920E-01-0.79001150E-05 0.11369460E-08-0.65350950E-13 2
0.15090430E+05-0.88689430E+02-0.51094210E+01 0.99100460E-01-0.81408620E-04 3
0.36663080E-07-0.74230540E-11 0.22938900E+05 0.51351110E+02 4
BPHC3H6 C 9H 110 00 0G 300.0 3000.0 1000.0 1
0.21129850E+02 0.27425010E-01-0.80787270E-05 0.11662760E-08-0.67219100E-13 2
0.14768510E+05-0.85102500E+02-0.42891350E+01 0.94219390E-01-0.73481920E-04 3
0.30863700E-07-0.57239250E-11 0.22298360E+05 0.47907890E+02 4
CPHC3H6 C 9H 110 00 0G 300.0 3000.0 1000.0 1
0.20351020E+02 0.28741720E-01-0.86354620E-05 0.12621560E-08-0.73240880E-13 2
0.80655060E+04-0.81773010E+02-0.37883710E+01 0.89749920E-01-0.64624140E-04 3
0.24373790E-07-0.40718430E-11 0.15385500E+05 0.45257910E+02 4
BPHPROPY C 9H 110 00 0G 300.0 3000.0 1000.0 1
0.18773470E+02 0.32017490E-01-0.10167760E-04 0.15489960E-08-0.92642370E-13 2
0.14424040E+05-0.72622580E+02-0.61953190E+01 0.10511650E+00-0.89499430E-04 3
0.40374020E-07-0.77179490E-11 0.21106050E+05 0.55387230E+02 4

!H and S calculated frm NIST Grp additivity based estimates. Frequencies frm usinG B3LYP/6-31G(d)

!Fitted usinG FITDAT chemkin 3.7

C6H5C3H5-2 0C 9H 10 G 200.000 5000.000 1000.00 1
0.14911709E+02 0.39374648E-01-0.15955676E-04 0.29514932E-08-0.20469208E-12 2
0.61265907E+04-0.53958597E+02 0.10396146E+01 0.52422991E-01 0.28131859E-04 3
-0.68880230E-07 0.28363247E-10 0.11023011E+05 0.23576247E+02 4
C6H5C3H5 0C 9H 10 G 200.000 5000.000 1000.00 1
0.15082078E+02 0.39159079E-01-0.15855395E-04 0.29312998E-08-0.20321009E-12 2
0.86541175E+04-0.53323089E+02-0.14481733E+00 0.57569978E-01 0.20273280E-04 3

-0.63651166E-07 0.27066577E-10 0.13824331E+05 0.30762050E+02 4
!Thermochemistry taken from SERDP PAH model 2007
FLUORENE HR11/99 BLYP C 13H 10 0 OG 300.000 5000.000 1400.000 01
3.04476803E+01 3.11178654E-02-1.07640759E-05 1.68444388E-09-9.82875496E-14 2
5.92347405E+03-1.45855799E+02-1.14291780E+01 1.40625771E-01-1.21919889E-04 3
5.33286885E-08-9.28204948E-12 1.91832070E+04 7.47141338E+01 4
BENZYL 5/ 7/97 THERMC 13H 12 0 OG 300.000 5000.000 1397.000 21
3.13943394E+01 3.37145350E-02-1.14863908E-05 1.78018669E-09-1.03206535E-13 2
3.59782041E+03-1.45511248E+02-1.11231775E+01 1.41604302E-01-1.16912225E-04 3
4.87422559E-08-8.10889354E-12 1.73288023E+04 7.95009869E+01 4
!S. Dooley et al., Combust. Flame, 157 (2010) 2333 - 2339
!ThermOCHemiStry data fOr C4 and Toluene meCHaniSmS
!Wayne K. MetCalfe, StepHen DOOley and FrederiCk L. Dryer, PrinCetOn UniverSity 2009.
!tHermO
!0300.00 1000.00 5000.00
! frOm Gri meCHaniSm
H 120186H 1 G 0300.00 5000.00 1000.00 1
0.02500000e+02 0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00 2
0.02547163e+06-0.04601176e+01 0.02500000e+02 0.00000000e+00 0.00000000e+00 3
0.00000000e+00 0.00000000e+00 0.02547163e+06-0.04601176e+01 4
H2 121286H 2 G 0300.00 5000.00 1000.00 1
0.02991423e+02 0.07000644e-02-0.05633829e-06-0.09231578e-10 0.01582752e-13 2
-0.08350340e+04-0.01355110e+02 0.03298124e+02 0.08249442e-02-0.08143015e-05 3
-0.09475434e-09 0.04134872e-11-0.01012521e+05-0.03294094e+02 4
O 120186O 1 G 0300.00 5000.00 1000.00 1
0.02542060e+02-0.02755062e-03-0.03102803e-07 0.04551067e-10-0.04368052e-14 2
0.02923080e+06 0.04920308e+02 0.02946429e+02-0.01638166e-01 0.02421032e-04 3
-0.01602843e-07 0.03890696e-11 0.02914764e+06 0.02963995e+02 4
O2 121386O 2 G 0300.00 5000.00 1000.00 1
0.03697578e+02 0.06135197e-02-0.01258842e-05 0.01775281e-09-0.01136435e-13 2
-0.01233930e+05 0.03189166e+02 0.03212936e+02 0.01127486e-01-0.05756150e-05 3
0.01313877e-07-0.08768554e-11-0.01005249e+05 0.06034738e+02 4
OH S 9/01O 1H 1 0 OG 200.000 6000.000 1000. 1
2.86472886e+00 1.05650448e-03-2.59082758e-07 3.05218674e-11-1.33195876e-15 2
3.68362875e+03 5.70164073e+00 4.12530561e+00-3.22544939e-03 6.52764691e-06 3
-5.79853643e-09 2.06237379e-12 3.34630913e+03-6.90432960e-01 4.51532273e+03 4
H2O 20387H 2O 1 G 0300.00 5000.00 1000.00 1
0.02672146e+02 0.03056293e-01-0.08730260e-05 0.01200996e-08-0.06391618e-13 2
-0.02989921e+06 0.06862817e+02 0.03386842e+02 0.03474982e-01-0.06354696e-04 3
0.06968581e-07-0.02506588e-10-0.03020811e+06 0.02590233e+02 4
N2 121286n 2 G 0300.00 5000.00 1000.00 1
0.02926640e+02 0.01487977e-01-0.05684761e-05 0.01009704e-08-0.06753351e-13 2
-0.09227977e+04 0.05980528e+02 0.03298677e+02 0.01408240e-01-0.03963222e-04 3
0.05641515e-07-0.02444855e-10-0.01020900e+05 0.03950372e+02 4
HO2 15/89H 1O 2 00 OG 200.000 3500.000 1000.000 1
4.01721090e+00 2.23982013e-03-6.33658150e-07 1.14246370e-10-1.07908535e-14 2
1.11856713e+02 3.78510215e+00 4.30179801e+00-4.74912051e-03 2.11582891e-05 3
-2.42763894e-08 9.29225124e-12 2.94808040e+02 3.71666245e+00 1.00021620e+04 4

H2O2 120186H 2O 2 G 0300.00 5000.00 1000.00 1
 0.04573167e+02 0.04336136e-01-0.01474689e-04 0.02348904e-08-0.01431654e-12 2
 -0.01800696e+06 0.05011370e+01 0.03388754e+02 0.06569226e-01-0.01485013e-05 3
 -0.04625806e-07 0.02471515e-10-0.01766315e+06 0.06785363e+02 4
 AR 120186AR 1 G 0300.00 5000.00 1000.00 1
 0.02500000e+02 0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00 2
 -0.07453750e+04 0.04366001e+02 0.02500000e+02 0.00000000e+00 0.00000000e+00 3
 0.00000000e+00 0.00000000e+00-0.07453750e+04 0.04366001e+02 4
 CH2O niSt/98 C 1H 2O 1 OG 300.000 4000.000 1200.00 1
 0.51481905e+01 0.28678016e-02-0.23782633e-06-0.16111303e-09 0.28566735e-13 2
 -0.16230173e+05-0.51213813e+01 0.26962612e+01 0.49261423e-02 0.82826494e-06 3
 -0.55038196e-09-0.39610326e-12-0.14970793e+05 0.94697599e+01 4
 CO 121286C 1O 1 G 0300.00 5000.00 1000.00 1
 0.03025078e+02 0.01442689e-01-0.05630828e-05 0.01018581e-08-0.06910952e-13 2
 -0.01426835e+06 0.06108218e+02 0.03262452e+02 0.01511941e-01-0.03881755e-04 3
 0.05581944e-07-0.02474951e-10-0.01431054e+06 0.04848897e+02 4
 CO2 121286C 1O 2 G 0300.00 5000.00 1000.00 1
 0.04453623e+02 0.03140169e-01-0.01278411e-04 0.02393997e-08-0.01669033e-12 2
 -0.04896696e+06-0.09553959e+01 0.02275725e+02 0.09922072e-01-0.01040911e-03 3
 0.06866687e-07-0.02117280e-10-0.04837314e+06 0.01018849e+03 4
 HCO 121286H 1C 1O 1 G 0300.00 5000.00 1000.00 1
 0.03557271e+02 0.03345573e-01-0.01335006e-04 0.02470573e-08-0.01713851e-12 2
 0.03916324e+05 0.05552299e+02 0.02898330e+02 0.06199147e-01-0.09623084e-04 3
 0.01089825e-06-0.04574885e-10 0.04159922e+05 0.08983614e+02 4
 HO2CHO 6/26/95 tHermC 1H 2O 3 OG 300.000 5000.000 1378.00 21
 9.87503878e+00 4.64663708e-03-1.67230522e-06 2.68624413e-10-1.59595232e-14 2
 -3.80502496e+04-2.24939155e+01 2.42464726e+00 2.19706380e-02-1.68705546e-05 3
 6.25612194e-09-9.11645843e-13-3.54828006e+04 1.75027796e+01 4
 O2CHO 6/26/95 tHermC 1H 1O 3 OG 300.000 5000.000 1368.00 11
 7.24075139e+00 4.63312951e-03-1.63693995e-06 2.59706693e-10-1.52964699e-14 2
 -1.87027618e+04-6.49547212e+00 3.96059309e+00 1.06002279e-02-5.25713351e-06 3
 1.01716726e-09-2.87487602e-14-1.73599383e+04 1.17807483e+01 4
 !wkm
 !HOCHO iS Called HCOOH in pu meCH SO puttinG in tHeir CHemiStry and tHermO
 HCOOH 7/ 1/99 tHermC 1H 2O 2 OG 300.000 5000.000 1376.000 11
 6.68733013e+00 5.14289368e-03-1.82238513e-06 2.89719163e-10-1.70892199e-14 2
 -4.83995400e+04-1.13104798e+01 1.43548185e+00 1.63363016e-02-1.06257421e-05 3
 3.32132977e-09-4.02176103e-13-4.64616504e+04 1.72885798e+01 4
 !HOCHO 9/27/ 5 tHermC 1H 2O 2 OG 300.000 5000.000 1419.000 11
 ! 7.67134440e+00 4.43426373e-03-1.60867436e-06 2.59770020e-10-1.54899704e-14 2
 !-4.89708660e+04-1.73024418e+01 1.28069021e+00 1.52887758e-02-5.64150476e-06 3
 !-1.22968799e-09 8.14273233e-13-4.64347524e+04 1.83142081e+01 4
 HOCO 9/27/ 5 tHermC 1H 1O 2 OG 300.000 5000.000 1549.000 11
 6.94282268e+00 2.37391844e-03-8.67074662e-07 1.40644617e-10-8.41268695e-15 2
 -2.50292163e+04-1.14792361e+01 8.98154532e-01 1.67269019e-02-1.33663562e-05 3
 4.83071199e-09-6.38718748e-13-2.30262021e+04 2.07803865e+01 4
 !!!
 !wkm reCalCulated uSinG tHerm aS tHere waS a larGe diSaGreement in tHe Hf

```

!valueS uSed by nuiG and pu
!pu = -38.24
!nui = -30.36
!new value = -32.30
!prObably nOt an impOrtant SpeCieS but at leaSt aware Of tHe OriGinS.
!
! SpeCieS
! HOCHO
!tHermO eStimatiOn fOr mOleCule
! HOCHO CO2H2
! unitS:kCal
! GrOuP 2
! Gr # - GrOuP id - quantity
! 1 - O/CO/H - 1
! 2 - CO/H/O - 1
! Hf S Cp 300 400 500 600 800 1000 1500
! -90.20 59.40 10.83 12.87 14.62 15.98 18.40 20.00 .00
! Cpinf = 24.84
! nrOtOrS: 1
! Symmetry 1
! CreatiOn date: 9/16/ 8
! endSpeCieS
!
!
! SpeCieS
! OCHO
!tHermO eStimatiOn fOr radiCal
! OCHO OCHO
! radiCal baSed upOn parent HOCHO
! parent fOrmula CO2H2
!parent Symmetry 1
! unitS:kCal
! GrOuP 3
! Gr # - GrOuP id - quantity
! 1 - O/CO/H - 1
! 2 - CO/H/O - 1
! 3 - aCidH - 1
! Hf S Cp 300 400 500 600 800 1000 1500
! -32.30 60.19 9.52 11.00 12.30 13.29 15.12 16.26 .00
! Cpinf = 19.87
! Symmetry 1
!r ln(2) HaS been added tO S tO aCCOunt
! fOr unpaired eleCtrOn
! bOnd 110.00
! CreatiOn date: 9/16/ 8
! endSpeCieS
!
OCHO 9/16/ 8 tHermC 1H 1O 2 0G 300.000 5000.000 1376.000 01
328

```

5.69424313e+00 3.80254685e-03-1.34588655e-06 2.13806333e-10-1.26050130e-14 2
 -1.86996507e+04-4.44435092e+00 1.92396001e+00 1.15312995e-02-6.96484769e-06 3
 1.86741565e-09-1.61493244e-13-1.72839008e+04 1.61852783e+01 4
 !!!
 HOCH2O2H 4/ 9/98 tHermC 1H 4O 3 OG 300.000 5000.000 1422.000 31
 1.16303827e+01 7.15133688e-03-2.39035030e-06 3.65772791e-10-2.10199524e-14 2
 -4.31079242e+04-3.24276725e+01 1.85716693e+00 3.23153132e-02-2.69928902e-05 3
 1.11694484e-08-1.81284103e-12-4.00314471e+04 1.90917729e+01 4
 HOCH2O2 4/ 9/98 tHermC 1H 3O 3 OG 300.000 5000.000 1412.000 21
 9.04545938e+00 7.15223373e-03-2.37005676e-06 3.60083481e-10-2.05750228e-14 2
 -2.49414886e+04-1.74210530e+01 2.85441621e+00 2.33663535e-02-1.88115990e-05 3
 7.96709515e-09-1.36346618e-12-2.29866196e+04 1.51730565e+01 4
 OCH2O2H 4/ 9/98 tHermC 1H 3O 3 OG 300.000 5000.000 1420.000 21
 1.15398246e+01 5.34291432e-03-1.81878917e-06 2.81968625e-10-1.63584348e-14 2
 -1.68237489e+04-3.20700633e+01 1.93823075e+00 3.01465730e-02-2.61053152e-05 3
 1.09463562e-08-1.78312692e-12-1.38166625e+04 1.85042002e+01 4
 !!!
 !wkm
 !taken frOm nuiG
 HOCH2O 2/16/99 tHermC 1H 3O 2 OG 300.000 5000.000 1452.000 11
 6.39521515e+00 7.43673043e-03-2.50422354e-06 3.84879712e-10-2.21778689e-14 2
 -2.41108840e+04-6.63865583e+00 4.11183145e+00 7.53850697e-03 3.77337370e-06 3
 -5.38746005e-09 1.45615887e-12-2.28023001e+04 7.46807254e+00 4
 !!!
 !wkm
 !taken frOm pu dme
 CH3OH 121686C 1H 4O 1 G 0300.00 5000.00 1000.00 1
 0.04029061e+02 0.09376593e-01-0.03050254e-04 0.04358793e-08-0.02224723e-12 2
 -0.02615791e+06 0.02378196e+02 0.02660115e+02 0.07341508e-01 0.07170051e-04 3
 -0.08793194e-07 0.02390570e-10-0.02535348e+06 0.01123263e+03 4
 !!!
 !wkm reCalCulated uSinG tHerm aS tHere waS a larGe diSaGreement in tHe Hf
 !valueS uSed by nuiG and pu
 !pu = -4.25
 !nui = -2.90
 !new value = -3.80
 !
 ! SpeCieS
 ! CH3OH
 !tHermO eStimatiOn fOr mOleCule
 ! CH3OH CH3OH
 ! unitS:kCal
 ! GrOupS 2
 ! Gr # - GrOup id - quantity
 ! 1 - C/H3/O - 1
 ! 2 - O/C/H - 1
 ! Hf S Cp 300 400 500 600 800 1000 1500
 ! -47.90 57.30 10.49 12.34 14.22 16.02 19.05 21.38 25.02

```

!      Cpinf = 30.80
! nrOtOrS: 1
! Symmetry      3
! CreatiOn date: 9/16/ 8
! endSpeCieS
!
!
! SpeCieS
! CH2OH
!tHermO eStimatiOn fOr radiCal
! CH2OH                      CH2OH
! radiCal baSed upOn parent CH3OH
! parent fOrmula              CH3OH
!parent Symmetry      3
! unitS:kCal
! GrOupS 3
! Gr # - GrOup id - quantity
! 1 - C/H3/O      - 1
! 2 - O/C/H      - 1
! 3 - CjOH      - 1
! Hf S Cp 300 400 500 600 800 1000 1500
! -3.80 59.03 11.77 13.27 14.42 15.47 17.22 18.61 20.85
!      Cpinf = 24.84
! nrOtOrS: 1
! Symmetry      2
!r ln(2) HaS been added tO S tO aCCOunt
! fOr unpaired eleCtrOn
! bOnd 96.20
! delta bOnd enerGy = -10.250
! CreatiOn date: 9/16/ 8
! endSpeCieS
!
CH2OH 9/16/ 8 tHermC 1H 3O 1 OG 300.000 5000.000 1401.000 11
5.86215864e+00 5.05364867e-03-1.62043757e-06 2.40631137e-10-1.35277830e-14 2
-4.23416585e+03-5.89849777e+00 2.49772010e+00 1.43138410e-02-1.16464935e-05 3
5.22575348e-09-9.57928395e-13-3.20031010e+03 1.16828031e+01 4
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!wkm
!taken frOm pu dme
CH3O 121686C 1H 3O 1 G 0300.00 3000.00 1000.00 1
0.03770800e+02 0.07871497e-01-0.02656384e-04 0.03944431e-08-0.02112616e-12 2
0.01278325e+04 0.02929575e+02 0.02106204e+02 0.07216595e-01 0.05338472e-04 3
-0.07377636e-07 0.02075611e-10 0.09786011e+04 0.01315218e+03 4
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!wkm
!taken frOm nuiG C4
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
CH3O2H 1/14/ 5 tHermC 1H 4O 2 OG 300.000 5000.000 1367.000 21

```

8.80409289e+00 8.09427218e-03-2.85843274e-06 4.53369754e-10-2.66980707e-14 2
 -1.98512174e+04-2.17000591e+01 2.83880024e+00 1.86096249e-02-8.48165412e-06 3
 1.00387451e-09 1.71612429e-13-1.74033753e+04 1.16092433e+01 4
 CH3O2 1/14/ 5 tHermC 1H 3O 2 OG 300.000 5000.000 1365.000 11
 6.34718801e+00 7.92089358e-03-2.76601913e-06 4.35360631e-10-2.54984762e-14 2
 -1.83436055e+03-7.42552545e+00 3.80497590e+00 9.80784660e-03-3.90940624e-07 3
 -2.23072602e-09 6.43310820e-13-4.55625796e+02 7.81789100e+00 4
 CH2O2H 1/14/ 5 tHermC 1H 3O 2 OG 300.000 5000.000 1357.000 21
 9.10784249e+00 5.27260434e-03-1.88170543e-06 3.00561364e-10-1.77865959e-14 2
 3.77440183e+03-2.11741044e+01 4.47228333e+00 1.33401095e-02-5.92919725e-06 3
 4.44481025e-10 2.12699899e-13 5.67413711e+03 4.72608208e+00 4
 CH4 29/11/04 H 4C 1 0 OG 300.000 5000.000 1462.000 1
 4.09617653e+00 7.44330845e-03-2.63871900e-06 4.19577604e-10-2.47508050e-14 2
 -1.13835704e+04-4.67561383e+00 3.72113020e+00-2.50293289e-03 1.90246534e-05 3
 -1.46871253e-08 3.43791152e-12-1.01424099e+04 1.22776596e+00 4
 CH3 C 1H 3 0 OG 300.000 5000.000 1389.000 01
 3.51281376e+00 5.11412613e-03-1.67632050e-06 2.52495174e-10-1.43302923e-14 2
 1.61238027e+04 1.62436112e+00 3.43858162e+00 4.07752664e-03 3.19830994e-07 3
 -9.47669390e-10 2.21828166e-13 1.63164018e+04 2.52807406e+00 4
 CH2 120186C 1H 2 G 0250.00 4000.00 1000.00 1
 0.03636408e+02 0.01933057e-01-0.01687016e-05-0.01009899e-08 0.01808256e-12 2
 0.04534134e+06 0.02156561e+02 0.03762237e+02 0.01159819e-01 0.02489585e-05 3
 0.08800836e-08-0.07332435e-11 0.04536791e+06 0.01712578e+02 4
 CH2-S 31287C 1H 2 G 0300.00 4000.00 1000.00 1
 0.03552889e+02 0.02066788e-01-0.01914116e-05-0.01104673e-08 0.02021350e-12 2
 0.04984975e+06 0.01686570e+02 0.03971265e+02-0.01699089e-02 0.01025369e-04 3
 0.02492551e-07-0.01981266e-10 0.04989368e+06 0.05753207e+00 4
 CH 121286C 1H 1 G 0300.00 5000.00 1000.00 1
 0.02196223e+02 0.02340381e-01-0.07058201e-05 0.09007582e-09-0.03855040e-13 2
 0.07086723e+06 0.09178373e+02 0.03200202e+02 0.02072876e-01-0.05134431e-04 3
 0.05733890e-07-0.01955533e-10 0.07045259e+06 0.03331588e+02 4
 C C 1 G 0300.00 5000.00 1000.00 1
 0.02602087e+02-0.01787081e-02 0.09087041e-06-0.01149933e-09 0.03310844e-14 2
 0.08542154e+06 0.04195177e+02 0.02498585e+02 0.08085777e-03-0.02697697e-05 3
 0.03040729e-08-0.01106652e-11 0.08545878e+06 0.04753459e+02 4
 C2H6 8/ 4/ 4 tHermC 2H 6 0 OG 300.000 5000.000 1383.000 11
 6.05972630e+00 1.30382837e-02-4.48103942e-06 6.97762095e-10-4.05606353e-14 2
 -1.35751226e+04-1.28608001e+01 4.78623203e-02 2.40569127e-02-1.15155912e-05 3
 2.48666238e-09-1.78343944e-13-1.10923014e+04 2.06544071e+01 4
 !!!
 !wkm
 !taken frOm pu dme
 C2H5 t12/91C 2H 5 0 OG 200.000 6000.000 1000. 1
 0.42878814e+01 0.12433893e-01-0.44139119e-05 0.70654102e-09-0.42035136e-13 2
 0.12056455e+05 0.84602583e+00 0.43058580e+01-0.41833638e-02 0.49707270e-04 3
 -0.59905874e-07 0.23048478e-10 0.12841714e+05 0.47100236e+01 0.14271225e+05 4
 C2H4 11/91C 2H 4 00 OG 200.000 3500.000 1000.000 1
 2.03611116e+00 1.46454151e-02-6.71077915e-06 1.47222923e-09-1.25706061e-13 2

4.93988614e+03 1.03053693e+01 3.95920148e+00-7.57052247e-03 5.70990292e-05 3
 -6.91588753e-08 2.69884373e-11 5.08977593e+03 4.09733096e+00 1.05186890e+04 4
 C2H3 12/92C 2H 3 00 00G 200.000 3500.000 1000.000 1
 3.01672400e+00 1.03302292e-02-4.68082349e-06 1.01763288e-09-8.62607041e-14 2
 3.46128739e+04 7.78732378e+00 3.21246645e+00 1.51479162e-03 2.59209412e-05 3
 -3.57657847e-08 1.47150873e-11 3.48598468e+04 8.51054025e+00 1.05750490e+04 4
 C2H2 11/91C 2H 2 00 00G 200.000 3500.000 1000.000 1
 4.14756964e+00 5.96166664e-03-2.37294852e-06 4.67412171e-10-3.61235213e-14 2
 2.59359992e+04-1.23028121e+00 8.08681094e-01 2.33615629e-02-3.55171815e-05 3
 2.80152437e-08-8.50072974e-12 2.64289807e+04 1.39397051e+01 1.00058390e+04 4
 C2H 11/91C 2H 1 00 00G 200.000 3500.000 1000.000 1
 3.16780652e+00 4.75221902e-03-1.83787077e-06 3.04190252e-10-1.77232770e-14 2
 6.71210650e+04 6.63589475e+00 2.88965733e+00 1.34099611e-02-2.84769501e-05 3
 2.94791045e-08-1.09331511e-11 6.68393932e+04 6.22296438e+00 1.04544720e+04 4
 CH3HCO 8/10/ 4 tHermC 2H 4O 1 0G 300.000 5000.000 1377.000 11
 6.98518866e+00 9.67897787e-03-3.31841954e-06 5.16025901e-10-2.99725903e-14 2
 -2.39807279e+04-1.27484852e+01 1.77060035e+00 1.84475161e-02-7.24138162e-06 3
 2.34364561e-10 3.35543891e-13-2.18078850e+04 1.65023437e+01 4
 CH3CO t9/92C 2H 3O 1 0G 200.000 6000.0 1000.0 1
 0.59447731e+01 0.78667205e-02-0.28865882e-05 0.47270875e-09-0.28599861e-13 2
 -0.37873075e+04-0.50136751e+01 0.41634257e+01-0.23261610e-03 0.34267820e-04 3
 -0.44105227e-07 0.17275612e-10-0.26574529e+04 0.73468280e+01-0.12027167e+04 4
 CH3CO t9/92C 2H 3O 1 0G 200.000 6000.0 1000.0 1
 0.59447731e+01 0.78667205e-02-0.28865882e-05 0.47270875e-09-0.28599861e-13 2
 -0.37873075e+04-0.50136751e+01 0.41634257e+01-0.23261610e-03 0.34267820e-04 3
 -0.44105227e-07 0.17275612e-10-0.26574529e+04 0.73468280e+01-0.12027167e+04 4
 !!!
 !wkm
 !taken fOrm nuiG C4
 CH2CHO 8/10/ 4 tHermC 2H 3O 1 0G 300.000 5000.000 1388.000 11
 7.54145790e+00 6.82297125e-03-2.36938607e-06 3.71633517e-10-2.17160048e-14 2
 -2.61437239e+03-1.62602766e+01 1.47616956e+00 2.08974186e-02-1.50123552e-05 3
 5.62967382e-09-8.76624470e-13-4.82050510e+02 1.63756465e+01 4
 !!!
 !wkm
 !taken frOm pu dme
 CH2CO 15/90C 2H 2O 1 00G 200.000 3500.000 1000.000 1
 4.51129732e+00 9.00359745e-03-4.16939635e-06 9.23345882e-10-7.94838201e-14 2
 -7.55105311e+03 6.32247205e-01 2.13583630e+00 1.81188721e-02-1.73947474e-05 3
 9.34397568e-09-2.01457615e-12-7.04291804e+03 1.22156480e+01 1.17977430e+04 4
 HCCO SriC91H 1C 2O 1 G 0300.00 4000.00 1000.00 1
 0.56282058e+01 0.40853401e-02-0.15934547e-05 0.28626052e-09-0.19407832e-13 2
 0.19327215e+05-0.39302595e+01 0.22517214e+01 0.17655021e-01-0.23729101e-04 3
 0.17275759e-07-0.50664811e-11 0.20059449e+05 0.12490417e+02 4
 !!!
 !wkm takinG HCCOH frOm pu fOr nOw but i Have majOr dOubTS abOut tHe value.
 !GOinG tO try CalCulate it uSinG GauSSian and atOmizatiOn methOd fOr a ballpark
 !fiGure.

HCCOH Sri91C 2O 1H 20 0G 300.000 5000.000 1000.0 1
 0.59238291e+01 0.67923600e-02-0.25658564e-05 0.44987841e-09-0.29940101e-13 2
 0.72646260e+04-0.76017742e+01 0.12423733e+01 0.31072201e-01-0.50866864e-04 3
 0.43137131e-07-0.14014594e-10 0.80316143e+04 0.13874319e+02 4
 !!!
 !wkm
 ! evertHinG elSe taken frOm nuiG C4 aS C2-C4 iS all nuiG CHemiStry.
 CH3CO3H 6/26/95 tHermC 2H 4O 3 0G 300.000 5000.000 1391.000 31
 1.25060485e+01 9.47789695e-03-3.30402246e-06 5.19630793e-10-3.04233568e-14 2
 -4.59856703e+04-3.79195947e+01 2.24135876e+00 3.37963514e-02-2.53887482e-05 3
 9.67583587e-09-1.49266157e-12-4.24677831e+04 1.70668133e+01 4
 CH3CO3 4/ 3/ 0 tHermC 2H 3O 3 0G 300.000 5000.000 1391.000 21
 1.12522498e+01 8.33652672e-03-2.89014530e-06 4.52781734e-10-2.64354456e-14 2
 -2.60238584e+04-2.96370457e+01 3.60373432e+00 2.70080341e-02-2.08293438e-05 3
 8.50541104e-09-1.43846110e-12-2.34205171e+04 1.12014914e+01 4
 CH3CO2 2/14/95 tHermC 2H 3O 2 0G 300.000 5000.000 1395.000 11
 8.54059736e+00 8.32951214e-03-2.84722010e-06 4.41927196e-10-2.56373394e-14 2
 -2.97290678e+04-2.03883545e+01 1.37440768e+00 2.49115604e-02-1.74308894e-05 3
 6.24799508e-09-9.09516835e-13-2.72330150e+04 1.81405454e+01 4
 C2H5OH 8/ 9/ 4 tHermC 2H 6O 1 0G 300.000 5000.000 1395.000 21
 8.31742137e+00 1.29603294e-02-4.39286497e-06 6.77734995e-10-3.91448231e-14 2
 -3.25219715e+04-1.96502783e+01 1.79106094e-01 3.09060081e-02-1.93596697e-05 3
 6.31830859e-09-8.53166875e-13-2.95670605e+04 2.44715919e+01 4
 PC2H4OH 8/ 9/ 4 tHermC 2H 5O 1 0G 300.000 5000.000 1396.000 21
 7.88509591e+00 1.08287795e-02-3.66829683e-06 5.65734300e-10-3.26673351e-14 2
 -7.44974622e+03-1.44673770e+01 9.90023426e-01 2.61564272e-02-1.65928300e-05 3
 5.50525131e-09-7.57520667e-13-4.96032283e+03 2.28675716e+01 4
 SC2H4OH 8/ 9/ 4 tHermC 2H 5O 1 0G 300.000 5000.000 1397.000 21
 8.34980768e+00 1.03718068e-02-3.49683481e-06 5.37524748e-10-3.09661005e-14 2
 -1.10556188e+04-1.81354112e+01 1.61103852e+00 2.63511867e-02-1.82941500e-05 3
 6.91243160e-09-1.10384057e-12-8.71494725e+03 1.80114775e+01 4
 C2H5O 8/ 9/ 4 tHermC 2H 5O 1 0G 300.000 5000.000 1393.000 11
 8.23717244e+00 1.10885879e-02-3.78808372e-06 5.87613473e-10-3.40712889e-14 2
 -6.22948597e+03-1.93190543e+01 2.87429022e-01 2.86500918e-02-1.83857008e-05 3
 6.03096179e-09-8.04562643e-13-3.35717377e+03 2.37513898e+01 4
 O2C2H4OH 2/14/95 tHermC 2H 5O 3 0G 300.000 5000.000 1392.000 31
 1.07432659e+01 1.30957787e-02-4.45370088e-06 6.88548738e-10-3.98230113e-14 2
 -2.55911274e+04-2.33254953e+01 4.11839445e+00 2.72240632e-02-1.60824430e-05 3
 5.17033408e-09-7.31610168e-13-2.30857785e+04 1.28482112e+01 4
 C2H5O2H 1/14/ 5 tHermC 2H 6O 2 0G 300.000 5000.000 1391.000 31
 1.12305737e+01 1.20482120e-02-3.96730201e-06 6.00754632e-10-3.42657803e-14 2
 -2.47977531e+04-3.25607232e+01 1.57329011e+00 3.52379996e-02-2.53203993e-05 3
 9.56802476e-09-1.48167375e-12-2.15278368e+04 1.90472032e+01 4
 C2H5O2 1/14/ 5 tHermC 2H 5O 2 0G 300.000 5000.000 1387.000 21
 8.77641329e+00 1.18767163e-02-3.87683050e-06 5.83210754e-10-3.31006724e-14 2
 -6.78748703e+03-1.83119972e+01 2.58630333e+00 2.61836362e-02-1.68306193e-05 3
 6.08749295e-09-9.57302040e-13-4.58588992e+03 1.50486289e+01 4
 C2H4O2H 1/14/ 5 tHermC 2H 5O 2 0G 300.000 5000.000 1397.000 31

1.05228954e+01 9.48091381e-03-3.55727763e-06 6.41445994e-10-4.21232247e-14 2
 1.55718322e+03-2.31413632e+01 3.46916874e+00 2.71188626e-02-2.08022550e-05 3
 8.44284845e-09-1.40756215e-12 3.89688270e+03 1.43400726e+01 4
 CH3CHO2H 1/14/ 5 tHermC 2H 5O 2 OG 300.000 5000.000 1385.000 31
 1.06284708e+01 1.01662327e-02-3.34915963e-06 5.07257146e-10-2.89352540e-14 2
 -2.15391230e+03-2.60363030e+01 3.91433011e+00 2.52722102e-02-1.62112291e-05 3
 5.45591592e-09-7.57965290e-13 2.38044573e+02 1.02327238e+01 4
 C2H4O1-2 9/ 1/ 0 tHermC 2H 4O 1 OG 300.000 5000.000 1399.000 01
 6.99485763e+00 1.00772459e-02-3.45220932e-06 5.36571216e-10-3.11563543e-14 2
 -1.04091344e+04-1.59857976e+01-1.44361790e+00 2.91837107e-02-1.96805054e-05 3
 6.67472575e-09-9.02139342e-13-7.43433507e+03 2.95212453e+01 4
 C2H3O1-2 4/ 3/ 0 tHermC 2H 3O 1 OG 300.000 5000.000 1492.000 01
 6.88486471e+00 6.94720501e-03-2.23214698e-06 3.32190767e-10-1.87124555e-14 2
 1.26442200e+04-1.23842570e+01-1.62965122e+00 2.93455486e-02-2.43737550e-05 3
 1.00522325e-08-1.61259036e-12 1.52459425e+04 3.22782741e+01 4
 CH3COCH3 8/30/ 4 tHermC 3H 6O 1 OG 300.000 5000.000 1382.000 21
 9.62674379e+00 1.45519245e-02-4.97749457e-06 7.72794591e-10-4.48367165e-14 2
 -3.11862263e+04-2.61613449e+01 1.24527408e+00 2.99760255e-02-1.40026661e-05 3
 2.16453512e-09 1.27637295e-13-2.78348727e+04 2.03682615e+01 4
 CH3COCH2 8/30/ 4 tHermC 3H 5O 1 OG 300.000 5000.000 1388.000 21
 1.08892477e+01 1.11540675e-02-3.85516785e-06 6.02834048e-10-3.51533449e-14 2
 -1.00741464e+04-3.18043322e+01 1.22337251e+00 3.24546742e-02-2.13542518e-05 3
 6.96777735e-09-8.99160299e-13-6.59419324e+03 2.05537233e+01 4
 CH3COCH2O2 2/14/95 C 3H 5O 3 OG 300.000 5000.000 1379.00 31
 1.27690342e+01 1.42554828e-02-4.92821461e-06 7.70448921e-10-4.49110534e-14 2
 -2.34798669e+04-3.27155799e+01 5.95535468e+00 2.70255205e-02-1.37385031e-05 3
 3.53735851e-09-4.03922557e-13-2.06679464e+04 5.21436049e+00 4
 CH3COCH2O2H 2/14/95 C 3H 6O 3 OG 300.000 5000.000 1381.00 41
 1.52372810e+01 1.44114651e-02-5.01290009e-06 7.87071229e-10-4.60225784e-14 2
 -4.27564444e+04-4.77383784e+01 4.94789761e+00 3.60474432e-02-2.21719933e-05 3
 6.98296874e-09-9.21269260e-13-3.88687178e+04 8.49926130e+00 4
 CH3COCH2O 4/ 3/ 0 tHermC 3H 5O 2 OG 300.000 5000.000 1370.000 21
 1.14637586e+01 1.32124342e-02-4.56580495e-06 7.13897538e-10-4.16281047e-14 2
 -2.23833017e+04-3.15127868e+01 3.72927689e+00 2.63943697e-02-1.09796486e-05 3
 8.58185303e-10 3.39474590e-13-1.91551565e+04 1.18505335e+01 4
 C2H3CHO 6/26/95 tHermC 3H 4O 1 OG 300.000 5000.000 1393.000 11
 1.04184959e+01 9.48963321e-03-3.29310529e-06 5.16279203e-10-3.01587291e-14 2
 -1.49630281e+04-3.07235061e+01 2.92355162e-01 3.54321417e-02-2.94936324e-05 3
 1.28100124e-08-2.26144108e-12-1.16521584e+04 2.28878280e+01 4
 C2H3CO 4/ 3/ 0 tHermC 3H 3O 1 OG 300.000 5000.000 1402.000 01
 9.37467676e+00 7.91296900e-03-2.67198280e-06 4.11115430e-10-2.36978981e-14 2
 1.92969514e+03-2.40892696e+01 1.36242013e+00 3.15273972e-02-3.00218935e-05 3
 1.48167112e-08-2.87971530e-12 4.25770215e+03 1.72626546e+01 4
 C2H5CHO 8/10/ 4 tHermC 3H 6O 1 OG 300.000 5000.000 1375.000 21
 8.87216223e+00 2.01710762e-02-8.06487647e-06 1.37617784e-09-8.48922325e-14 2
 -2.83848527e+04-2.35069163e+01 5.93107530e+00 8.87943855e-03 2.03764325e-05 3
 -1.80149348e-08 4.14085655e-12-2.51377751e+04-5.87019974e-01 4
 C2H5CO 8/10/ 4 tHermC 3H 5O 1 OG 300.000 5000.000 1362.000 21

1.00147418e+01 1.61527961e-02-6.62976122e-06 1.15290667e-09-7.21263458e-14 2
 -1.00430305e+04-2.88570933e+01 8.35352246e+00-4.08739727e-03 3.64217954e-05 3
 -2.72457713e-08 6.06440266e-12-6.58577307e+03-1.05948346e+01 4
 CH2CH2CHO 8/10/ 4 tHermC 3H 5O 1 OG 300.000 5000.000 1363.000 21
 9.96855598e+00 1.61917946e-02-6.64161740e-06 1.15444520e-09-7.21981790e-14 2
 -4.16450354e+03-2.73971573e+01 8.36272659e+00-3.90712606e-03 3.59751257e-05 3
 -2.69209237e-08 5.98920261e-12-7.55243244e+02-9.53140102e+00 4
 CH3CHCHO 8/10/ 4 tHermC 3H 5O 1 OG 300.000 5000.000 1253.000 21
 8.27772090e+00 1.95687188e-02-8.47575089e-06 1.53249728e-09-9.86441542e-14 2
 -8.34456062e+03-2.17652483e+01-2.72811212e+00 3.80354483e-02-1.96782132e-05 3
 5.09554570e-09-7.28789092e-13-3.51122739e+03 4.04496677e+01 4
 CH3OCH3 7/20/98 tHermC 2H 6O 1 OG 300.000 5000.000 1368.000 21
 8.27745836e+00 1.32135539e-02-4.53264362e-06 7.05316507e-10-4.09933283e-14 2
 -2.61982700e+04-2.15190894e+01 1.50763450e+00 2.39914228e-02-8.68910500e-06 3
 -9.66835762e-11 4.89319361e-13-2.32810894e+04 1.67317297e+01 4
 CH3OCH2 7/20/98 tHermC 2H 5O 1 OG 300.000 5000.000 1376.000 21
 8.17137842e+00 1.10086181e-02-3.82352277e-06 5.99637202e-10-3.50317513e-14 2
 -3.41941605e+03-1.78650856e+01 2.91327415e+00 2.03364659e-02-9.59712342e-06 3
 2.07478525e-09-1.71343362e-13-1.18844240e+03 1.16066817e+01 4
 CH3OCH2O2 7/20/98 tHermC 2H 5O 3 OG 300.000 5000.000 1389.000 31
 1.24249729e+01 1.18705986e-02-4.07906532e-06 6.35310809e-10-3.69427867e-14 2
 -2.29679238e+04-3.53740145e+01 2.21029612e+00 3.68877454e-02-2.82561555e-05 3
 1.15730533e-08-1.97130470e-12-1.94940940e+04 1.91463601e+01 4
 CH2OCH2O2H 7/20/98 tHermC 2H 5O 3 OG 300.000 5000.000 1393.000 41
 1.51191783e+01 9.23718883e-03-3.19127505e-06 4.99114678e-10-2.91162488e-14 2
 -1.84114867e+04-4.85706618e+01 2.52895507e+00 4.24128290e-02-3.73406386e-05 3
 1.66639333e-08-2.96443312e-12-1.44293306e+04 1.76899251e+01 4
 CH3OCH2O2H 7/20/98 tHermC 2H 6O 3 OG 300.000 5000.000 1392.000 41
 1.49370964e+01 1.19465829e-02-4.12746359e-06 6.45422590e-10-3.76427939e-14 2
 -4.11001068e+04-4.99552737e+01 1.19855761e+00 4.59060764e-02-3.66252420e-05 3
 1.49318970e-08-2.46057445e-12-3.65363161e+04 2.31339904e+01 4
 CH3OCH2O 2/ 9/96 tHermC 2H 5O 2 OG 300.000 5000.000 2012.000 21
 8.60261845e+00 1.35772195e-02-4.84661602e-06 7.77766193e-10-4.62633624e-14 2
 -2.13762444e+04-1.75775023e+01 3.25889339e+00 2.22146359e-02-7.78556340e-06 3
 -2.41484158e-10 4.51914496e-13-1.92377212e+04 1.23680069e+01 4
 O2CH2OCH2O2H 7/20/98 trmC 2H 5O 5 OG 300.000 5000.000 1402.000 51
 1.92038046e+01 1.04394841e-02-3.60582939e-06 5.63792843e-10-3.28807214e-14 2
 -3.79207055e+04-6.51847273e+01 1.99640551e+00 5.83226232e-02-5.53259778e-05 3
 2.59810540e-08-4.77141005e-12-3.27628742e+04 2.44215005e+01 4
 HO2CH2OCHO 8/31/99 tHermC 2H 4O 4 OG 300.000 5000.000 1387.000 41
 1.64584298e+01 8.52683511e-03-3.04113500e-06 4.85596908e-10-2.87316334e-14 2
 -6.23959608e+04-5.38924139e+01 3.47935703e+00 4.02952392e-02-3.30109296e-05 3
 1.34360117e-08-2.18601580e-12-5.80629934e+04 1.52521392e+01 4
 OCH2OCHO 4/ 9/98 tHermC 2H 3O 3 OG 300.000 5000.000 1475.000 21
 1.20233916e+01 8.11262659e-03-2.91356462e-06 4.67340384e-10-2.77375525e-14 2
 -4.33647231e+04-3.33691809e+01 5.19690837e+00 1.58839723e-02 3.53540547e-07 3
 -6.10456923e-09 1.94661801e-12-4.02242792e+04 6.11645828e+00 4
 HOCH2OCO 8/31/99 tHermC 2H 3O 3 OG 300.000 5000.000 1603.000 31

1.13737391e+01 8.17663898e-03-2.92034021e-06 4.66695616e-10-2.76276823e-14 2
 -4.65575743e+04-2.86035265e+01 6.08180801e+00 1.28768359e-02 2.04419418e-06 3
 -6.10154921e-09 1.79820559e-12-4.39526183e+04 2.54054449e+00 4
 CH3OCHO 4/15/ 8 tHermC 2H 4O 2 OG 300.000 5000.000 1452.000 21
 1.06569185e+01 9.38112723e-03-3.37677206e-06 5.42455596e-10-3.22295330e-14 2
 -4.84651758e+04-3.27579443e+01 2.43526200e+00 1.81948325e-02 1.91236590e-06 3
 -8.44248945e-09 2.61758910e-12-4.46514732e+04 1.49522265e+01 4
 CH3OCO 4/15/ 8 tHermC 2H 3O 2 OG 300.000 5000.000 1423.000 21
 1.02053021e+01 7.12269668e-03-2.57594255e-06 4.15104358e-10-2.47168227e-14 2
 -2.46870635e+04-2.86407262e+01 2.83313145e+00 1.53447505e-02 1.89583962e-06 3
 -7.70200413e-09 2.41564410e-12-2.13431832e+04 1.39524183e+01 4
 CH2OCHO 4/15/ 8 tHermC 2H 3O 2 OG 300.000 5000.000 1442.000 21
 1.00960096e+01 7.19887066e-03-2.59813465e-06 4.18110812e-10-2.48723387e-14 2
 -2.36389018e+04-2.71144175e+01 2.31031671e+00 1.80474065e-02-2.71519637e-06 3
 -4.60918579e-09 1.70037078e-12-2.02910878e+04 1.71549722e+01 4
 He 120186He 1 G 0300.00 5000.00 1000.00 1
 0.02500000e+02 0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00 2
 -0.07453750e+04 0.09153489e+01 0.02500000e+02 0.00000000e+00 0.00000000e+00 3
 0.00000000e+00 0.00000000e+00-0.07453750e+04 0.09153488e+01 4
 C3H8 8/ 4/ 4 tHermC 3H 8 0 OG 300.000 5000.000 1387.000 21
 9.31450083e+00 1.73577154e-02-5.94222386e-06 9.22939762e-10-5.35576604e-14 2
 -1.77234234e+04-2.89241517e+01-3.08230087e-01 3.65331801e-02-1.97610926e-05 3
 5.15283344e-09-5.06336649e-13-1.39792198e+04 2.40478733e+01 4
 NC3H7 8/ 4/ 4 tHermC 3H 7 0 OG 300.000 5000.000 1386.000 21
 8.88635047e+00 1.52273279e-02-5.21905860e-06 8.11259208e-10-4.71028059e-14 2
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 4.45927887e-09-4.36675398e-13 1.06314565e+04 2.32670929e+01 4
 IC3H7 8/ 4/ 4 tHermC 3H 7 0 OG 300.000 5000.000 1373.000 21
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 -3.24354603e-09 1.23539044e-12 9.20752889e+03 1.83848082e+01 4
 C3H6 10/23/ 5 tHermC 3H 6 0 OG 300.000 5000.000 1388.000 11
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 3.88814209e-09-3.37890352e-13 1.17760132e+03 2.19003736e+01 4
 !C3H5-a 10/23/ 5 tHermC 3H 5 0 OG 300.000 5000.000 1397.000 01
 ! 8.45883958e+00 1.12695483e-02-3.83792864e-06 5.94059119e-10-3.43918030e-14 2
 ! 1.64683289e+04-2.32704266e+01-5.29131958e-01 3.34559100e-02-2.53401027e-05 3
 ! 1.02865754e-08-1.73258340e-12 1.94941423e+04 2.46172315e+01 4
 !C3H5-t 10/23/ 5 tHermC 3H 5 0 OG 300.000 5000.000 1382.000 11
 ! 7.37492443e+00 1.17510061e-02-4.00021283e-06 6.18947395e-10-3.58215018e-14 2
 ! 2.73982108e+04-1.43478655e+01 2.17916644e+00 2.03826623e-02-7.91413834e-06 3
 ! 4.76906187e-10 2.70398536e-13 2.96002535e+04 1.48785684e+01 4
 !C3H5-S 10/23/ 5 tHermC 3H 5 0 OG 300.000 5000.000 1390.000 11
 ! 7.88765879e+00 1.13012591e-02-3.84213130e-06 5.93982677e-10-3.43567175e-14 2
 ! 2.83484913e+04-1.74291589e+01 1.32807335e+00 2.53107914e-02-1.51530439e-05 3
 ! 4.74345565e-09-6.24666084e-13 3.07981100e+04 1.83328787e+01 4
 !C3H4-a 101993H 4C 3 G 0300.00 4000.00 1400.00 1

! 0.09776256e+02 0.05302138e-01-0.03701118e-05-0.03026386e-08 0.05089581e-12 2
 ! 0.01954972e+06-0.03077061e+03 0.02539831e+02 0.01633437e+00-0.01764950e-04 3
 !-0.04647365e-07 0.01729131e-10 0.02251243e+06 0.09935702e+02 4
 !C3H4-p 101993H 4C 3 G 0300.00 4000.00 1400.00 1
 ! 0.09768102e+02 0.05219151e-01-0.03753140e-05-0.02992191e-08 0.05107878e-12 2
 ! 0.01860277e+06-0.03020678e+03 0.03029730e+02 0.01498961e+00-0.01398500e-04 3
 !-0.03969619e-07 0.01388217e-10 0.02148408e+06 0.08004594e+02 4
 !C3H3 82489C 3H 3 G 0300.00 4000.00 1000.00 1
 ! 0.08831047e+02 0.04357195e-01-0.04109067e-05-0.02368723e-08 0.04376520e-12 2
 ! 0.03847420e+06-0.02177919e+03 0.04754200e+02 0.01108028e+00 0.02793323e-05 3
 !-0.05479212e-07 0.01949629e-10 0.03988883e+06 0.05854549e+01 4
 C3H2 102193X THERMC 3H 2O 0 OG 150.000 4000.000 1000.000 11
 0.07670981e+02 0.02748749e-01-0.04370943e-05-0.06455599e-09 0.01663887e-12 2
 0.06259722e+06-0.01236890e+03 0.03166714e+02 0.02482572e+00-0.04591637e-03 3
 0.04268019e-06-0.01482152e-09 0.06350421e+06 0.08869446e+02 4
 C3H5O 7/20/95 THERMC 3H 5O 1 OG 300.000 5000.000 1380.000 11
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 6.26560810e+03-2.77655042e+01 1.19822582e+00 3.05579837e-02-1.80630276e-05 3
 4.86150033e-09-4.19854562e-13 9.58217784e+03 2.15566221e+01 4
 C3H6OOH1-3 7/19/ 0 tHermC 3H 7O 2 OG 300.000 5000.000 1384.000 41
 1.46881564e+01 1.49941200e-02-5.24056505e-06 8.25462711e-10-4.83758952e-14 2
 -4.77342863e+03-4.77984492e+01 1.88331465e+00 4.40156051e-02-3.07858462e-05 3
 1.13214862e-08-1.75323184e-12-1.68779168e+02 2.14040621e+01 4
 C3H6OOH1-2 7/19/ 0 tHermC 3H 7O 2 OG 300.000 5000.000 1402.000 41
 1.24605763e+01 1.58889526e-02-5.32742106e-06 8.15818791e-10-4.68723250e-14 2
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 C3H6OOH2-1 7/19/ 0 tHermC 3H 7O 2 OG 300.000 5000.000 1407.000 41
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 1.72381453e-08-3.07968979e-12-1.89377918e+03 2.00178282e+01 4
 C3H6OOH2-2 7/19/ 0 tHermC 3H 7O 2 OG 300.000 5000.000 1407.000 41
 1.42163221e+01 1.43382450e-02-4.78004477e-06 7.29133134e-10-4.17761973e-14 2
 -5.67381620e+03-4.35770997e+01 2.09193950e+00 4.69220394e-02-3.90280831e-05 3
 1.72381453e-08-3.07968979e-12-1.89377918e+03 2.00178282e+01 4
 C3H6OOH1-2O2 7/19/ 0 trmC 3H 7O 4 OG 300.000 5000.000 1386.000 51
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 2.05591557e-08-3.68787387e-12-2.08829371e+04 2.01547955e+01 4
 C3H6OOH1-3O2 7/19/ 0 trmC 3H 7O 4 OG 300.000 5000.000 1382.000 51
 1.85916698e+01 1.65328553e-02-5.81343626e-06 9.19396939e-10-5.40320702e-14 2
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 1.67542220e-08-2.89288326e-12-1.85473645e+04 1.86305431e+01 4
 C3H6OOH2-1O2 7/19/ 0 trmC 3H 7O 4 OG 300.000 5000.000 1386.000 51
 1.91759159e+01 1.59857013e-02-5.61306378e-06 8.86880495e-10-5.20877040e-14 2
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 NC3H7O 8/ 9/ 4 tHermC 3H 7O 1 OG 300.000 5000.000 1398.000 21

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 IC3H7O 8/ 9/ 4 tHermC 3H 7O 1 OG 300.000 5000.000 1393.000 21
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 NC3H7O2H 7/19/ 0 tHermC 3H 8O 2 OG 300.000 5000.000 1385.000 41
 1.50895501e+01 1.71714707e-02-5.98498879e-06 9.40964412e-10-5.50728381e-14 2
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 IC3H7O2H 7/19/ 0 tHermC 3H 8O 2 OG 300.000 5000.000 1389.000 41
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 NC3H7O2 7/19/ 0 tHermC 3H 7O 2 OG 300.000 5000.000 1384.000 31
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 IC3H7O2 7/19/ 0 tHermC 3H 7O 2 OG 300.000 5000.000 1388.000 31
 1.32493493e+01 1.64082190e-02-5.67432062e-06 8.87336340e-10-5.17361535e-14 2
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 1.29687136e-08-2.23370569e-12-1.02587980e+04 2.02336490e+01 4
 C3H6O1-3 1/22/95 tHermC 3H 6O 1 OG 300.000 5000.000 2035.000 41
 1.02363953e+01 1.50514705e-02-5.63636534e-06 9.32463455e-10-5.66102441e-14 2
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 6.62981208e-09-5.31193325e-13-1.00990375e+04 3.67181804e+01 4
 C3H6O1-2 1/22/95 tHermC 3H 6O 1 OG 300.000 5000.000 1379.00 41
 1.19825289e+01 1.23964696e-02-4.39113813e-06 6.97911182e-10-4.11585127e-14 2
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 C3KET12 7/19/ 0 tHermC 3H 6O 3 OG 300.000 5000.000 1388.000 41
 1.70756225e+01 1.31013491e-02-4.61949408e-06 7.31991329e-10-4.30788679e-14 2
 -4.17008637e+04-5.95778952e+01 1.10507238e+00 5.27396706e-02-4.31805774e-05 3
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 C3KET13 7/19/ 0 tHermC 3H 6O 3 OG 300.000 5000.000 1379.000 41
 1.58927479e+01 1.40990923e-02-4.96118851e-06 7.84992198e-10-4.61488928e-14 2
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 C3KET21 7/19/ 0 tHermC 3H 6O 3 OG 300.000 5000.000 1371.000 41
 1.56377776e+01 1.44059342e-02-5.08808082e-06 8.07076119e-10-4.75295650e-14 2
 -4.30657975e+04-5.13105869e+01 4.55686367e+00 3.57076837e-02-1.94712054e-05 3
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 C3H51-2,3OOH 8/26/3 tHrmC 3H 7O 4 OG 300.000 5000.000 1386.000 61
 2.12378169e+01 1.39519596e-02-4.94539222e-06 7.86381389e-10-4.63925564e-14 2
 -1.92864584e+04-7.69636561e+01 2.55619708e+00 6.13504487e-02-5.23205391e-05 3
 2.28208029e-08-4.02231508e-12-1.31353414e+04 2.21043799e+01 4
 C3H52-1,3OOH 8/26/3 tHrmC 3H 7O 4 OG 300.000 5000.000 1379.000 61

2.02817964e+01 1.48155431e-02-5.25503386e-06 8.35963453e-10-4.93308915e-14 2
 -1.80085066e+04-7.22688262e+01 4.12253742e+00 5.19553611e-02-3.83733727e-05 3
 1.45851637e-08-2.29820536e-12-1.22759164e+04 1.48367359e+01 4
 C3H6OH 1/ 7/98 tHermC 3H 7O 1 OG 300.000 5000.000 1674.000 31
 9.31287816e+00 1.67579212e-02-5.75555480e-06 9.00584362e-10-5.26566836e-14 2
 -1.20169635e+04-1.95011064e+01 1.20494302e+00 3.30857885e-02-1.63893637e-05 3
 3.18103918e-09-6.84229288e-14-9.12961720e+03 2.47155202e+01 4
 HOC3H6O2 1/ 7/98 tHermC 3H 7O 3 OG 300.000 5000.000 1397.000 41
 1.42691004e+01 1.71837825e-02-5.83419536e-06 9.00994191e-10-5.20716210e-14 2
 -3.14501750e+04-4.15295035e+01 3.06954289e+00 4.43105640e-02-3.18636260e-05 3
 1.26409287e-08-2.12751901e-12-2.75893676e+04 1.83891218e+01 4
 CH3CHCO 03/03/95 tHermC 3H 4O 1 OG 300.000 5000.000 1400.00 41
 1.00219123e+01 9.56966300e-03-3.26221644e-06 5.05231706e-10-2.92593257e-14 2
 -1.42482738e+04-2.77829973e+01 1.48380119e+00 3.22203013e-02-2.70250033e-05 3
 1.20499164e-08-2.18365931e-12-1.15276540e+04 1.71552068e+01 4
 AC3H5OOH 7/20/98 tHermC 3H 6O 2 OG 300.000 5000.000 1394.000 31
 1.36837693e+01 1.33968049e-02-4.61533631e-06 7.19988958e-10-4.19109988e-14 2
 -1.33165248e+04-4.31904193e+01 2.43934647e+00 4.02070638e-02-2.95322679e-05 3
 1.14715600e-08-1.85170511e-12-9.43679906e+03 1.70549969e+01 4
 C2H3OOH 4/18/ 8 tHermC 2H 4O 2 OG 300.000 5000.000 1397.000 21
 1.15749951e+01 8.09909174e-03-2.81808668e-06 4.42697954e-10-2.58998042e-14 2
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 C4H10 8/ 4/ 4 tHermC 4H 10 0 OG 300.000 5000.000 1392.000 31
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 PC4H9 8/ 4/ 4 tHermC 4H 9 0 OG 300.000 5000.000 1391.000 31
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 3.22550473e+03-3.87719384e+01 3.20730933e-01 4.34654454e-02-2.40584970e-05 3
 6.28245308e-09-5.80113166e-13 7.71490893e+03 2.57301085e+01 4
 SC4H9 8/ 4/ 4 tHermC 4H 9 0 OG 300.000 5000.000 1381.000 31
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 1.96382429e+03-3.61626672e+01 8.49159986e-01 3.82085320e-02-1.49626797e-05 3
 2.04499211e-10 8.24254437e-13 6.38832956e+03 2.44466606e+01 4
 C4H8-1 6/29/ 4 tHermC 4H 8 0 OG 300.000 5000.000 1391.000 21
 1.13456574e+01 1.80843428e-02-6.17276514e-06 9.56925815e-10-5.54586212e-14 2
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 C4H8-2 6/29/ 4 tHermC 4H 8 0 OG 300.000 5000.000 1384.000 21
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 C4H71-1 4/ 2/97 tHermC 4H 7 0 OG 300.000 5000.000 1393.000 21
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 C4H71-2 4/ 2/97 tHermC 4H 7 0 OG 300.000 5000.000 1389.000 21

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 C4H71-3 4/ 2/97 tHermC 4H 7 0 0G 300.000 5000.000 1392.000 11
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 C4H71-4 4/ 2/97 tHermC 4H 7 0 0G 300.000 5000.000 1392.000 21
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 3.35089369e-10 4.95669524e-13 2.50864168e+04 1.52219548e+01 4
 !C4H6 4/ 4/ 0 tHermC 4H 6 0 0G 300.000 5000.000 1398.000 11
 ! 1.11633789e+01 1.37163965e-02-4.69715783e-06 7.29693836e-10-4.23486203e-14 2
 ! 7.79039770e+03-3.69847949e+01-1.43095121e+00 4.78706062e-02-4.15446800e-05 3
 ! 1.91549552e-08-3.57158507e-12 1.17551314e+04 2.90825833e+01 4
 PC4H9O2H 7/19/ 0 tHermC 4H 10O 2 0G 300.000 5000.000 1387.000 51
 1.82687454e+01 2.16940079e-02-7.54629828e-06 1.18484806e-09-6.92818498e-14 2
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 SC4H9O2H 7/19/ 0 tHermC 4H 10O 2 0G 300.000 5000.000 1390.000 51
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 PC4H9O2 7/19/ 0 tHermC 4H 9O 2 0G 300.000 5000.000 1385.000 41
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 SC4H9O2 7/19/ 0 tHermC 4H 9O 2 0G 300.000 5000.000 1389.000 41
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 PC4H9O 8/ 9/ 4 tHermC 4H 9O 1 0G 300.000 5000.000 1403.000 31
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 C4H8OOH1-2O2 7/19/0 trmC 4H 9O 4 OG 300.000 5000.000 1387.000 61
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 C4H8OOH1-3O2 7/19/0 trmC 4H 9O 4 OG 300.000 5000.000 1387.000 61
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 C4H8OOH1-4O2 7/19/0 trmC 4H 9O 4 OG 300.000 5000.000 1383.000 61
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 C4H8OOH2-3O2 7/19/0 trmC 4H 9O 4 OG 300.000 5000.000 1389.000 61
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 NC4KET13 7/19/0 tHermC 4H 8O 3 OG 300.000 5000.000 1386.000 51
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 NC4KET14 7/19/0 tHermC 4H 8O 3 OG 300.000 5000.000 1382.000 51

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 NC4KET21 7/19/ 0 tHermC 4H 8O 3 OG 300.000 5000.000 1376.000 51
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 C2H5COCH3 4/ 3/ 0 tHermC 4H 8O 1 OG 300.000 5000.000 1381.000 31
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 C2H3COCH3 6/19/95 tHermC 4H 6O 1 OG 300.000 5000.000 1386.00 21
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 CH2CHOOHCOCH3 6/27/95 C 4H 7O 3 OG 300.000 5000.000 1394.00 51
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 NC3H7CHO 9/27/95 tHermC 4H 8O 1 OG 300.000 5000.000 1378.00 31
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 C3H6CHO-1 9/27/95 tHermC 4H 7O 1 OG 300.000 5000.000 1379.000 31
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 5.80472681e-09-6.09688236e-13-2.49714183e+03 1.75750933e+01 4
 C3H6CHO-2 11/15/95 tHermC 4H 7O 1 OG 300.000 5000.000 1682.000 31
 1.11942816e+01 1.81806772e-02-6.35916662e-06 1.00727333e-09-5.93943618e-14 2
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 1.67282048e-09 2.62011555e-13-3.79034324e+03 1.74324072e+01 4
 C3H6CHO-3 11/15/95 tHermC 4H 7O 1 OG 300.000 5000.000 1387.000 31
 1.34301738e+01 1.62250792e-02-5.60631713e-06 8.76356273e-10-5.10864241e-14 2
 -1.13561098e+04-4.47371262e+01 1.35168659e+00 4.23714083e-02-2.69123192e-05 3
 8.70132567e-09-1.15287455e-12-6.91166610e+03 2.09381509e+01 4
 C2H5CHCO 9/27/95 tHermC 4H 6O 1 OG 300.000 5000.000 1400.00 21
 1.34100537e+01 1.38766678e-02-4.74130143e-06 7.35504188e-10-4.26457752e-14 2
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 SC3H5CHO 11/15/95 tHerC 4H 6O 1 OG 300.000 5000.000 1390.000 21
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 SC3H5CO 11/15/95 tHermC 4H 5O 1 OG 300.000 5000.000 1392.000 21
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 IC4H7 10/23/ 5 tHermC 4H 7 0 OG 300.000 5000.000 1393.000 11
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 TC4H9O2 7/19/0 tHermC 4H 9O 2 OG 300.000 5000.000 1388.000 41
 1.67061556e+01 2.07327780e-02-7.17596169e-06 1.12282473e-09-6.54941386e-14 2
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 TC4H8O2H-I 7/19/0 tHermC 4H 9O 2 OG 300.000 5000.000 1405.000 51
 1.78060253e+01 1.84952716e-02-6.21268423e-06 9.52753962e-10-5.48010330e-14 2
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 IC4H9O 8/9/4 tHermC 4H 9O 1 OG 300.000 5000.000 1393.000 31
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 IC4H9O2H 7/19/0 tHermC 4H 10O 2 OG 300.000 5000.000 1388.000 51
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 TC4H9O2H 7/19/0 tHermC 4H 10O 2 OG 300.000 5000.000 1390.000 51
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 IC4H7O 4/3/0 tHermC 4H 7O 1 OG 300.000 5000.000 1386.000 21
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 IC3H7CHO 2/22/96 tHermC 4H 8O 1 OG 300.000 5000.000 1391.000 31
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 IC3H7CO 2/22/96 tHermC 4H 7O 1 OG 300.000 5000.000 1390.000 31
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 TC4H8OOH-IO2 7/19/0 trmC 4H 9O 4 OG 300.000 5000.000 1386.000 61
 2.26382889e+01 2.03246143e-02-7.12390770e-06 1.12425028e-09-6.59732993e-14 2
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 IC4H8OOH-IO2 7/19/0 trmC 4H 9O 4 OG 300.000 5000.000 1385.000 61
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 2.56759171e-08-4.61678643e-12-2.55622378e+04 2.07846231e+01 4
 IC4KETII 7/19/0 tHermC 4H 8O 3 OG 300.000 5000.000 1387.000 51
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 IC4H7OH 4/8/97 tHermC 4H 8O 1 OG 300.000 5000.000 1384.000 31
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 IC4H6OH 8/19/95 tHermC 4H 7O 1 OG 300.000 5000.000 1390.000 31

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 IC3H5CHO 7/19/95 tHermC 4H 6O 1 OG 300.000 5000.000 1396.000 21
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 IC4H7OOH 7/19/95 tHermC 4H 8O 2 OG 300.000 5000.000 1392.00 41
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 TC3H6OH 8/9/4 tHermC 3H 7O 1 OG 300.000 5000.000 1392.000 31
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 TC3H6O2HCO 8/2/95 tHermC 4H 7O 3 OG 300.000 5000.000 1387.00 51
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 IC3H5O2HCHO 8/2/95 tHermC 4H 7O 3 OG 300.000 5000.000 1387.00 51
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 TC4H8CHO 9/ 7/95 tHermC 5H 9O 1 OG 300.000 5000.000 1397.00 41
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 O2HC4H8CO 9/ 7/95 tHermC 5H 9O 3 OG 300.000 5000.000 1394.00 61
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 !!!
 !wkm
 !tOluene
 C6H5CH2OO 3/ 4/94 tHe.mC 7H 7O 2 OG 300.000 5000.000 1389.000 21
 2.18946260e+01 2.02701494e-02-7.14525361e-06 1.13208570e-09-6.66220534e-14 2
 3.93272947e+03-8.95685129e+01-3.77863659e+00 8.29484718e-02-6.64288143e-05 3
 2.69504875e-08-4.41844689e-12 1.25603231e+04 4.73269747e+01 4
 BZCOOH 3/ 4/94 tHe.mC 7H 8O 2 OG 300.000 5000.000 1390.000 31
 2.21951256e+01 2.19901041e-02-7.70452728e-06 1.21574282e-09-7.13427270e-14 2
 -1.43966742e+04-9.07483698e+01-3.39515159e+00 8.45306884e-02-6.70634097e-05 3
 2.72113250e-08-4.48289693e-12-5.78730853e+03 4.57078979e+01 4
 C6H5CH3 16/87C 7H 8 0 OG 200.000 6000.000 1000. 1
 0.12940034e+02 0.26691287e-01-0.96838505e-05 0.15738629e-08-0.94663601e-13 2
 -0.69764908e+03-0.46728785e+02 0.16152663e+01 0.21099438e-01 0.85366018e-04 3
 -0.13261066e-06 0.55956604e-10 0.40756300e+04 0.20282210e+02 0.60135835e+04 4
 C6H5CH2 iu3/03C 7.H 7. 0. 0.G 250.000 6000.000 1000. 1
 0.14723052e+02 0.23034244e-01-0.84847359e-05 0.13916962e-08-0.84247967e-13 2
 0.17990189e+05-0.55950989e+02-0.12303836e+01 0.48986376e-01 0.13815518e-04 3
 -0.62587233e-07 0.31595731e-10 0.23192877e+05 0.30555495e+02 0.25016622e+05 4
 C6H5CH2O 4/14/94 tHe.mC 7H 7O 1 OG 300.000 5000.000 1392.000 1
 1.78843033e+01 2.09011735e-02-7.21832713e-06 1.12839851e-09-6.57955260e-14 2
 4.93182818e+03-7.01304667e+01-4.77736690e+00 7.51049308e-02-5.68532831e-05 3
 2.18290029e-08-3.38134298e-12 1.26234438e+04 5.10429366e+01 4
 C6H5CH2OH 3/ 8/90 C 7H 8O 1 OG 300.000 5000.000 1396.000 21
 1.81575155e+01 2.26620146e-02-7.79454113e-06 1.21491074e-09-7.06883434e-14 2
 -2.13319736e+04-7.19512787e+01-3.72475901e+00 7.42375044e-02-5.41481788e-05 3
 2.01178934e-08-3.02199053e-12-1.38224993e+04 4.53342817e+01 4
 C6H5CHO 5/16/90 tHermC 7H 6O 1 OG 300.000 5000.000 1386.000 11
 1.74024893e+01 1.89508317e-02-6.58694307e-06 1.03413046e-09-6.04793155e-14 2

-1.31418522e+04-6.83371315e+01-2.37082285e+00 6.28843128e-02-4.26460754e-05 3
 1.39416083e-08-1.74474949e-12-6.11656186e+03 3.85478773e+01 4
 C6H5CO tHerm C 7H 5O 1 OG 300.000 5000.000 1392.000 11
 1.75116258e+01 1.62650511e-02-5.65051892e-06 8.86922680e-10-5.18657990e-14 2
 4.67641545e+03-6.70531966e+01-1.56729686e+00 5.99817511e-02-4.29153585e-05 3
 1.48666854e-08-1.98938453e-12 1.12873830e+04 3.55490009e+01 4
 C6H5C2H5 C 8H 10 0 OG 300.000 5000.000 1397.000 21
 2.02816724e+01 2.59464082e-02-8.92667064e-06 1.39161163e-09-8.09786280e-14 2
 -6.88695837e+03-8.65892579e+01-5.93600077e+00 8.94618416e-02-6.81230510e-05 3
 2.66103734e-08-4.21398102e-12 1.94317497e+03 5.33309542e+01 4
 C6H5C2H3 trC tableS C 8H 8 0 OG 300.000 5000.000 1400.000 11
 1.94675525e+01 2.19916239e-02-7.56672249e-06 1.17967158e-09-6.86483959e-14 2
 8.16106600e+03-8.19394370e+01-5.75443698e+00 8.70398896e-02-7.28533682e-05 3
 3.12720079e-08-5.39379278e-12 1.62673706e+04 5.12775455e+01 4
 C6H5OH 14/84C 6H 6O 1 OG 300.000 5000.000 1000. 1
 0.14912073e+02 0.18378135e-01-0.61983128e-05 0.91983221e-09-0.49209565e-13 2
 -0.18375199e+05-0.55924103e+02-0.16956539e+01 0.52271299e-01-0.72024050e-05 3
 -0.35859603e-07 0.20449073e-10-0.13284121e+05 0.32542160e+02-0.11594207e+05 4
 C6H5O t05/02C 6.H 5.O 1. 0.G 200.000 6000.000 1000. 1
 1.37221720e+01 1.74688771e-02-6.35504520e-06 1.03492308e-09-6.23410504e-14 2
 2.87274751e+02-4.88181680e+01-4.66204455e-01 4.13443975e-02 1.32412991e-05 3
 -5.72872769e-08 2.89763707e-11 4.77858391e+03 2.76990274e+01 6.49467016e+03 4
 C6H6 G 6/01C 6.H 6. 0. 0.G 200.000 6000.000 1000. 1
 1.10809576e+01 2.07176746e-02-7.52145991e-06 1.22320984e-09-7.36091279e-14 2
 4.30641035e+03-4.00413310e+01 5.04818632e-01 1.85020642e-02 7.38345881e-05 3
 -1.18135741e-07 5.07210429e-11 8.55247913e+03 2.16412893e+01 9.96811598e+03 4
 C6H5 t04/02C 6.H 5. 0. 0.G 200.000 6000.000 1000. 1
 1.08444762e+01 1.73212473e-02-6.29233249e-06 1.02369961e-09-6.16216828e-14 2
 3.55598475e+04-3.53735134e+01 2.10306633e-01 2.04745507e-02 5.89743006e-05 3
 -1.01534255e-07 4.47105660e-11 3.95468722e+04 2.52910455e+01 4.08610970e+04 4
 P-C6H4O2 ak0405C 6H 4O 2 OG 270.000 3000.000 1370.00 1
 1.23423732e+01 2.40612690e-02-1.16565184e-05 2.71393504e-09-2.47643065e-13 2
 -2.06185312e+04-4.08244024e+01-2.43170113e+00 6.87937608e-02-6.41382837e-05 3
 3.08126855e-08-5.99832072e-12-1.65696994e+04 3.48309430e+01 4
 P-C6H3O2 ak0505C 6H 3O 2 OG 270.000 3000.000 1290.00 1
 1.22963699e+01 2.15055142e-02-1.07516136e-05 2.57528163e-09-2.41023652e-13 2
 1.15428998e+04-3.72584002e+01-1.57852347e+00 6.55376473e-02-6.50308721e-05 3
 3.32026554e-08-6.86665555e-12 1.51750093e+04 3.31518638e+01 4
 O-C6H4O2 ak0405C 6H 4O 2 OG 270.000 3000.000 1370.00 1
 1.23614349e+01 2.40491397e-02-1.16529057e-05 2.71332785e-09-2.47593219e-13 2
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 3.06903009e-08-5.97357785e-12-1.26704431e+04 3.53724482e+01 4
 O-C6H3O2-1 ak0505C 6H 3O 2 OG 270.000 3000.000 1290.00 1
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 1.64502545e+04-3.72569775e+01-1.39018425e+00 6.50294183e-02-6.44290980e-05 3
 3.28694438e-08-6.79612734e-12 2.00503639e+04 3.24858445e+01 4
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 1.24848239e+01 2.12013845e-02-1.05559891e-05 2.51850992e-09-2.34851853e-13 2

1.52130566e+04-3.81453848e+01-1.37357372e+00 6.49450451e-02-6.41934438e-05 3
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 C5H5 tak0505C 5H 5 0 0G 298.150 3500.000 969.35 1
 1.33675715e+00 3.24793912e-02-1.67587774e-05 4.03514137e-09-3.70739036e-13 2
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 9.04628776e-08-2.80999747e-11 3.01769405e+04 3.67153636e+01 4
 C5H6 t1/90C 5H 6 0 0G 200.000 6000.000 1000. 1
 0.99757848e+01 0.18905543e-01-0.68411461e-05 0.11099340e-08-0.66680236e-13 2
 0.11081693e+05-0.32209454e+02 0.86108957e+00 0.14804031e-01 0.72108895e-04 3
 -0.11338055e-06 0.48689972e-10 0.14801755e+05 0.21353453e+02 0.16152485e+05 4
 C5H5OH 5/2/91 tHe.mC 5H 6O 1 0G 300.000 5000.000 1398.000 11
 1.53433477e+01 1.50754059e-02-5.13553582e-06 7.95807816e-10-4.61311517e-14 2
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 2.46858526e-08-4.26820696e-12-5.75581338e+03 4.47962850e+01 4!!
 C5H4O t8/99C 5.H 4.O 1. 0.G 200.000 6000.000 1000. 1
 1.00806824e+01 1.61143465e-02-5.83314509e-06 9.46759320e-10-5.68972206e-14 2
 1.94364771e+03-2.94521623e+01 2.64576497e-01 3.34873827e-02 1.67738470e-06 3
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 C5H5O 5/16/90 tHermC 5H 5O 1 0G 300.000 5000.000 1392.000 01
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 C5H4OH t8/99C 5.H 5.O 1. 0.G 200.000 6000.000 1000. 1
 1.33741248e+01 1.51996469e-02-5.45685046e-06 8.80944866e-10-5.27493258e-14 2
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 -2.92983743e-08 1.90820619e-11 6.37364803e+03 3.08073591e+01 8.00114499e+03 4
 C4H5-n t05/04C 4.H 5. 0. 0.G 200.000 6000.000 1000. 1
 8.11183574e+00 1.42276370e-02-5.02419535e-06 8.00816580e-10-4.75459802e-14 2
 4.00134524e+04-1.52704514e+01 3.28605952e+00 1.43352325e-02 2.78456642e-05 3
 -4.84612551e-08 2.10628469e-11 4.19222504e+04 1.26653969e+01 4.36993353e+04 4
 C4H5-i t05/04C 4.H 5. 0. 0.G 200.000 6000.000 1000. 1
 8.58761100e+00 1.42683804e-02-5.04812095e-06 8.06555355e-10-4.79335634e-14 2
 3.40836919e+04-1.96196761e+01 2.00881066e+00 2.50340684e-02 4.47930427e-06 3
 -2.63989791e-08 1.34432880e-11 3.62069792e+04 1.59913722e+01 3.79123436e+04 4
 C4H4 t06/04C 4.H 4. 0. 0.G 200.000 6000.000 1000. 1
 7.98456038e+00 1.20558816e-02-4.23587475e-06 6.73646140e-10-3.99059864e-14 2
 3.11993029e+04-1.67958975e+01 1.37368786e+00 2.88801256e-02-1.46863874e-05 3
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 C4H3-N t06/04C 4.H 3. 0. 0.G 200.000 6000.000 1000. 1
 8.44631306e+00 9.07291526e-03-3.18681201e-06 5.06725048e-10-3.00149855e-14 2
 6.20007365e+04-1.77938854e+01 5.54263934e-01 3.86185425e-02-4.70818280e-05 3
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 C4H3-I t06/04C 4.H 3. 0. 0.G 200.000 6000.000 1000. 1
 8.51181244e+00 9.03337808e-03-3.17602594e-06 5.05276458e-10-2.99379699e-14 2
 5.71046116e+04-1.51017769e+01 3.37964170e+00 2.70498840e-02-2.90761572e-05 3
 1.83027765e-08-4.81164203e-12 5.83688723e+04 1.05464883e+01 6.03558069e+04 4
 ! tHiS pOlynOmial HaS diSCOntinuitieS in Cp!!!
 !C5H3O 0C 5H 3O 1 G 0300.00 5000.00 1000.00 1

! 1.38663664e+01 7.63013012e-03-1.30630630e-06 0.00000000e+00 0.00000000e+00 2
 ! 3.00500624e+04-4.65791272e+01-2.97887884e+00 5.38346630e-02-4.06051040e-05 3
 ! 2.18196545e-08-3.88019537e-12 3.33238398e+04 3.71809786e+01 4
 C5H3O tak0905C 5H 3O 1 OG 300.000 3500.000 1500.00 1
 1.19961781e+01 1.34287065e-02-5.90045309e-06 1.22553862e-09-9.86114716e-14 2
 2.89592010e+04-4.07548249e+01-3.03242604e+00 5.43937201e-02-4.95018348e-05 3
 2.25523751e-08-4.10727920e-12 3.35644081e+04 3.78374823e+01 4
 CH2CHCHCO 12/27/94 tHermC 4H 4O 1 OG 300.000 5000.000 1401.000 11
 1.32918890e+01 9.42783712e-03-3.23329764e-06 5.02853718e-10-2.92089737e-14 2
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 2.57383902e-08-5.04416081e-12-8.53247629e+02 2.43466973e+01 4
 C5H3O tak0905C 5H 3O 1 Og 300.000 3500.000 1500.00 1
 1.19961781e+01 1.34287065e-02-5.90045309e-06 1.22553862e-09-9.86114716e-14 2
 2.89592010e+04-4.07548249e+01-3.03242604e+00 5.43937201e-02-4.95018348e-05 3
 2.25523751e-08-4.10727920e-12 3.35644081e+04 3.78374823e+01 4
 H2C4O 120189H 2C 4O 1 G 0300.00 4000.00 1000.00 1
 0.01026888e+03 0.04896164e-01-0.04885081e-05-0.02708566e-08 0.05107013e-12 2
 0.02346903e+06-0.02815985e+03 0.04810971e+02 0.01313999e+00 0.09865073e-05 3
 -0.06120720e-07 0.01640003e-10 0.02545803e+06 0.02113424e+02 4
 C4H2 121686C 4H 2 G 0300.00 5000.00 1000.00 1
 0.09031407e+02 0.06047253e-01-0.01948789e-04 0.02754863e-08-0.01385608e-12 2
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 C5H7 1/22/ 9 wkm C 5H 7 0 OG 300.000 5000.000 1377.000 31
 1.36630213e+01 1.68061358e-02-5.98746539e-06 9.55341072e-10-5.64951981e-14 2
 1.27238941e+04-5.46331286e+01-6.75118368e+00 6.06461693e-02-4.01260152e-05 3
 1.22051562e-08-1.33459844e-12 2.01365277e+04 5.62694938e+01 4
 C*CCJC*C 3/1/95 z&b C 5H 7 0 Og 300.000 5000.000 1388.000 21
 1.40879309e+01 1.62398907e-02-5.64768950e-06 8.86857524e-10-5.18698993e-14 2
 1.76798698e+04-5.13735038e+01-2.94595603e+00 5.68783623e-02-4.31336497e-05 3
 1.68169537e-08-2.67926433e-12 2.35156925e+04 3.98188778e+01 4
 OC5H7O 1/22/ 9 wkm C 5H 7O 2 OG 300.000 5000.000 1375.000 31
 1.65416953e+01 1.86677673e-02-6.44836048e-06 1.00787611e-09-5.87521858e-14 2
 -2.82017168e+04-5.47258181e+01 4.88394767e+00 4.03401300e-02-1.97774150e-05 3
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 C*CCJC*COH 10/6/95 z&b C 5H 7O 1 OG 300.000 5000.000 1397.000 31
 1.67465815e+01 1.58357240e-02-5.44954706e-06 8.49881387e-10-4.94743246e-14 2
 -4.30972870e+03-6.19378748e+01-2.91175436e+00 6.69362484e-02-5.71603047e-05 3
 2.48753749e-08-4.33243894e-12 1.96441523e+03 4.17454344e+01 4
 C*CC*CCJ z&b C 5H 7 0 OG 300.000 5000.000 1386.000 21
 1.47302883e+01 1.59030900e-02-5.57729508e-06 8.80604825e-10-5.16963733e-14 2
 1.74050791e+04-5.42670706e+01-1.60087476e+00 5.38764703e-02-3.96302225e-05 3
 1.49599474e-08-2.31995284e-12 2.31199746e+04 3.35492960e+01 4
 C*CC*CC 3/1/95 z&b C 5H 8 0 OG 300.000 5000.000 1395.000 21
 1.41303131e+01 1.81877961e-02-6.19208788e-06 9.58333792e-10-5.54785472e-14 2
 2.25907168e+03-5.11705577e+01-1.19376866e+00 5.65474329e-02-4.39472481e-05 3
 1.82341266e-08-3.12226566e-12 7.36084709e+03 3.02808980e+01 4
 C*CC*CCOH 1/23/ 9 wkm C 5H 8O 1 OG 300.000 5000.000 1396.000 31

1.63079670e+01 1.79957763e-02-6.03115896e-06 9.23992259e-10-5.31254053e-14 2
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 C*CCJC*O z&b C 4H 5O 1 OG 300.000 5000.000 1385.000 11
 1.22833215e+01 1.26428506e-02-4.31034879e-06 6.68415867e-10-3.87693974e-14 2
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 1.11441978e-08-1.63863920e-12 6.28635090e+03 3.00860103e+01 4
 OC4H6O 1/23/ 9 wkm C 4H 6O 2 OG 300.000 5000.000 1382.000 31
 1.41894774e+01 1.53345510e-02-5.24594862e-06 8.14655154e-10-4.72759368e-14 2
 -4.10001835e+04-4.43771751e+01 4.21628848e+00 3.57422725e-02-2.04226185e-05 3
 5.63821367e-09-5.88888993e-13-3.72055911e+04 1.02814620e+01 4
 OC4H5O 1/23/ 9 wkm C 4H 5O 2 OG 300.000 5000.000 1388.000 21
 1.32138775e+01 1.37339051e-02-4.62639517e-06 7.10941370e-10-4.09538499e-14 2
 -2.16535271e+04-3.64185255e+01 4.60550978e+00 3.30498712e-02-2.13102363e-05 3
 7.37021089e-09-1.08289438e-12-1.85460831e+04 1.01599453e+01 4
 HOC*CC*O 1/26/ 9 wkm C 3H 4O 2 OG 300.000 5000.000 1413.000 21
 1.66505478e+01 6.11745137e-03-2.09080785e-06 3.24985683e-10-1.88875073e-14 2
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 3.39430425e-08-6.48917648e-12-3.31367523e+04 3.18162860e+01 4
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 1.52720985e+01 5.02586331e-03-1.68408578e-06 2.58390706e-10-1.48849424e-14 2
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 2.68392951e-08-5.13094510e-12-1.58814562e+04 1.94817133e+01 4
 C2H3OH 1/26/ 9 wkm C 2H 4O 1 OG 300.000 5000.000 1417.000 11
 1.04816132e+01 6.26095577e-03-2.04502899e-06 3.07801996e-10-1.74769743e-14 2
 -1.93125540e+04-3.35156461e+01-2.38349747e+00 4.62915479e-02-4.93008726e-05 3
 2.50913014e-08-4.85108587e-12-1.59107891e+04 3.19236375e+01 4
 C2H2OH 1/26/ 9 wkm C 2H 3O 1 OG 300.000 5000.000 1470.000 11
 6.93453102e+00 7.23098468e-03-1.99956432e-06 1.43274685e-10 5.18910992e-15 2
 1.28905371e+04-1.02350453e+01 1.43806872e+00 2.93422585e-02-2.90685031e-05 3
 1.38331994e-08-2.56485091e-12 1.32889028e+04 1.50985534e+01 4
 CH2CHCHO burCat C 3H 4O 1 OG 300.000 5000.000 1396.000 01
 8.88726664e+00 1.03444470e-02-3.39254807e-06 5.11212534e-10-2.90229900e-14 2
 -1.16437988e+04-1.85698464e+01 7.26547054e+00 1.29751321e-02-4.99309402e-06 3
 1.03242966e-09-1.21031241e-13-1.08889964e+04-9.32398463e+00 4
 CH2CHCO burCat C 3H 3O 1 OG 300.000 5000.000 1399.000 01
 8.05879513e+00 8.41574111e-03-2.71140677e-06 4.03456779e-10-2.26972095e-14 2
 7.63082562e+03-1.26580575e+01 6.79715602e+00 1.06999686e-02-4.36180712e-06 3
 1.03285546e-09-1.34218501e-13 8.18362689e+03-5.56756773e+00 4
 O2CCHOOJ z&b C 2H 1O 4 OG 300.000 5000.000 1682.000 01
 1.09910849e+01 7.46985861e-03-2.75568271e-06 4.51353051e-10-2.72108652e-14 2
 -3.51335323e+04-2.11652231e+01 8.91497688e+00 8.60571847e-03 5.24416766e-07 3
 -2.79301331e-09 7.62963051e-13-3.40867754e+04-8.72978273e+00 4
 HOCO 11/ 6/ 6 tHermC 1H 1O 2 OG 300.000 5000.000 1376.000 11
 6.36686103e+00 2.83426573e-03-1.01859095e-06 1.63464108e-10-9.70543480e-15 2
 -2.64094764e+04-7.85498782e+00 2.11627189e+00 1.23644489e-02-8.92040916e-06 3
 3.02782004e-09-3.90274859e-13-2.49122464e+04 1.50843574e+01 4
 C#CC*CCJ Glar C 5H 5 0 OG 300.000 5000.000 1396.000 11

1.41230912e+01 1.14233190e-02-3.95851276e-06 6.20128961e-10-3.62097887e-14 2
 4.25158384e+04-5.02942871e+01-6.16143558e-01 5.06466579e-02-4.48561743e-05 3
 2.02459419e-08-3.64542145e-12 4.71532377e+04 2.71623299e+01 4
 CJ*CC*CC*O 2/ 5/ 9 tHermC 5H 5O 1 OG 300.000 5000.000 1396.000 21
 1.62360823e+01 1.18297101e-02-4.11454219e-06 6.46026823e-10-3.77767639e-14 2
 1.93499885e+04-5.83498817e+01-5.06628841e-01 6.04671965e-02-5.97396749e-05 3
 2.96804228e-08-5.76240010e-12 2.42765544e+04 2.82994148e+01 4
 C*CC*CCJ*O 2/ 5/ 9 tHermC 5H 5O 1 OG 300.000 5000.000 1399.000 11
 1.53178248e+01 1.27352911e-02-4.35882964e-06 6.76912763e-10-3.92771371e-14 2
 7.60582726e+03-5.43599625e+01-2.18492198e-01 5.92100223e-02-5.89241174e-05 3
 2.97411920e-08-5.85244770e-12 1.20600764e+04 2.55968530e+01 4
 C5H6-L 2/ 5/ 9 tHermC 5H 6 0 OG 300.000 5000.000 1372.000 21
 1.29600892e+01 1.48953758e-02-5.23622902e-06 8.27916389e-10-4.86464523e-14 2
 2.38180800e+04-4.25312093e+01 3.58448213e+00 3.24459626e-02-1.70150991e-05 3
 4.22715914e-09-4.18452556e-13 2.76514681e+04 9.60644208e+00 4
 C4H6-12 a 8/83C 4H 6 0 OG 300. 3000. 1000.0 1
 0.1781557e 02 -0.4257502e-02 0.1051185e-04 -0.4473844e-08 0.5848138e-12 2
 0.1267342e 05 -0.6982662e 02 0.1023467e 01 0.3495919e-01 -0.2200905e-04 3
 0.6942272e-08 -0.7879187e-12 0.1811799e 05 0.1975066e 02 0.1950807e+05 4
 C4H6-2 a 8/83C 4H 6 0 OG 300. 3000. 1000.0 1
 9.0338133e+00 8.2124510e-03 7.1753952e-06 -5.8834334e-09 1.0343915e-12 2
 1.4335068e+04 -2.0985762e+01 2.1373338e+00 2.6486229e-02 -9.0568711e-06 3
 -5.5386397e-19 2.1281884e-22 1.5710902e+04 1.3529426e+01 1.7488676e+04 4
 L-C6H4 h6w/94C 6H 4 0 Og 300.000 3000.000 1000.000 1
 0.12715182e+02 0.13839662e-01-0.43765440e-05 0.31541636e-09 0.46619026e-13 2
 0.57031148e+05-0.39464600e+02 0.29590225e+00 0.58053318e-01-0.67766756e-04 3
 0.43376762e-07-0.11418864e-10 0.60001371e+05 0.22318970e+02 4
 C-C6H4 h6w/94C 6H 4 0 Og 300.000 3000.000 1000.000 1
 0.13849209e+02 0.78807920e-02 0.18243836e-05-0.21169166e-08 0.37459977e-12 2
 0.47446340e+05-0.50404953e+02-0.30991268e+01 0.54030564e-01-0.40839004e-04 3
 0.10738837e-07 0.98078490e-12 0.52205711e+05 0.37415207e+02 4
 !C6H5C2H3 Hw /94C 8H 8 0 OG 300.000 3000.000 1
 ! 0.11303213e+02 0.33709887e-01-0.13208885e-04 0.21140962e-08-0.87311377e-13 2
 ! 0.11725388e+05-0.34737919e+02-0.38678493e+01 0.67947865e-01-0.25230333e-04 3
 !-0.18017145e-07 0.12998470e-10 0.16200269e+05 0.45271770e+02 4
 C6H5C2H Hw /94C 8H 6 0 OG 300.000 3000.000 1000.0 1
 0.24090759e+02 0.78232400e-03 0.11453964e-04-0.61620504e-08 0.93346685e-12 2
 0.27429445e+05-0.10499631e+03-0.52645016e+01 0.84511042e-01-0.76597848e-04 3
 0.33216978e-07-0.47673063e-11 0.35566242e+05 0.46378815e+02 4
 C4H6O25 t 3/97C 4H 6O 1 OG 200.000 5000.000 1000.0 1
 8.60658242e+00 2.08310051e-02-8.42229481e-06 1.56717640e-09-1.09391202e-13 2
 -1.76177415e+04-2.32464750e+01 2.67053463e+00 4.92586420e-03 8.86967406e-05 3
 -1.26219194e-07 5.23991321e-11-1.46572472e+04 1.45722395e+01-1.30831522e+04 4
 C4H6O23 t 3/97C 4H 6O 1 OG 200.000 5000.000 1000.0 1
 8.60658242e+00 2.08310051e-02-8.42229481e-06 1.56717640e-09-1.09391202e-13 2
 -1.32392815e+04-2.32464750e+01 2.67053463e+00 4.92586420e-03 8.86967406e-05 3
 -1.26219194e-07 5.23991321e-11-1.02787872e+04 1.45722395e+01-1.30831522e+04 4
 C6H2 p 1/93C 6H 2 0 Og 300.000 3000.000 1000.000 1

0.13226281e+02 0.73904302e-02-0.22715381e-05 0.25875217e-09-0.55356741e-14 2
 0.80565258e+05-0.41201176e+02-0.15932624e+01 0.80530145e-01-0.14800649e-03 3
 0.13300031e-06-0.45332313e-10 0.83273227e+05 0.27980873e+02 4
 C6H3 H6W/94C 6H 3 G 300.000 3000.000 1000.000 1
 0.58188343E+01 0.27933408E-01-0.17825427E-04 0.53702536E-08-0.61707627E-12 2
 0.85188250E+05-0.92147827E+00 0.11790619E+01 0.55547360E-01-0.73076168E-04 3
 0.52076736E-07-0.15046964E-10 0.85647312E+05 0.19179199E+02 4
 C2H3CHOCH2 a 8/83C 4H 6O 1 OG 300. 3000. 1000.0 1
 -4.72093360e+00 3.91413780e-02-6.52872650e-06-7.68209500e-09 2.51473310e-12 2
 1.75352252e+03 5.17190420e+01 7.97985440e-01 3.44034320e-02-1.24598510e-05 3
 -5.18062790e-18 1.99359540e-21-6.48927540e+02 2.18896980e+01 1.00654250e+03 4
 CH3CHCHCHO t 5/92C 4H 6O 1 OG 298.150 3000.0 1000.0 1
 1.98794540e+01-2.09130550e-02 4.45360508e-05-2.60374870e-08 4.86836120e-12 2
 -1.95278768e+04-6.87200320e+01-1.55577660e+00 4.09640630e-02-1.69868810e-05 3
 -6.00928140e-18 2.31368530e-21-1.41394920e+04 3.74707580e+01-1.29340710e+04 4
 CH3CHCHCO t03/97C 4H 5O 1 OG 200.000 6000.000 1000.0 1
 8.90967920e+00 1.34364140e-02-7.62977390e-07-1.69114810e-09 2.95540440e-13 2
 1.48898740e+03-1.79662460e+01-1.08199860e+00 3.64929760e-02-1.52255950e-05 3
 -5.62607170e-18 2.16113750e-21 3.56713230e+03 3.27142550e+01 4.73074990e+03 4
 CH2CHCHCHO t03/97C 4H 5O 1 OG 200.000 6000.000 1000.0 1
 8.90967920e+00 1.34364140e-02-7.62977390e-07-1.69114810e-09 2.95540440e-13 2
 1.48898740e+03-1.79662460e+01-1.08199860e+00 3.64929760e-02-1.52255950e-05 3
 -5.62607170e-18 2.16113750e-21 3.56713230e+03 3.27142550e+01 4.73074990e+03 4
 CC3H4 t12/81C 3H 4 0 OG 300.000 5000.000 1000.000 1
 0.66999931e+01 0.10357372e-01-0.34551167e-05 0.50652949e-09-0.26682276e-13 2
 0.30199051e+05-0.13378770e+02-0.24621047e-01 0.23197215e-01-0.18474357e-05 3
 -0.15927593e-07 0.86846155e-11 0.32334137e+05 0.22729762e+02 0.3332728 e+05 4
 H2CC 112/89H 2C 2 0 OG 200.000 6000.000 1000.000 1
 0.42780340e+01 0.47562804e-02-0.16301009e-05 0.25462806e-09-0.14886379e-13 2
 0.48316688e+05 0.64023701e+00 0.32815483e+01 0.69764791e-02-0.23855244e-05 3
 -0.12104432e-08 0.98189545e-12 0.48621794e+05 0.59203910e+01 0.49887266e+05 4
 C4H5-2 h6w/94C 4H 5 0 OG 300.000 3000.000 1000.000 1
 1.45381710e+01-8.56770560e-03 2.35595240e-05-1.36763790e-08 2.44369270e-12 2
 3.32590950e+04-4.53694970e+01 2.96962800e+00 2.44422450e-02-9.12514240e-06 3
 -4.24668710e-18 1.63047280e-21 3.55033160e+04 1.20360510e+01 3.73930550e+04 4
 C4H4O t03/97C 4H 4O 1 OG 200.000 6000.0 1000.0 1
 9.38935003e+00 1.40291241e-02-5.07755110e-06 8.24137332e-10-4.95319963e-14 2
 -8.68241814e+03-2.79162920e+01 8.47469463e-01 1.31773796e-02 5.99735901e-05 3
 -9.71562904e-08 4.22733796e-11-5.36785445e+03 2.14945172e+01-4.17166616e+03 4
 !C4H7 am1/94C 4H 7 0 OG 300.000 3000.000 1000.000 1
 ! 0.11963392e+02 0.11425305e-01 0.78948909e-06-0.19858872e-08 0.36873645e-12 2
 ! 0.16962977e+05-0.37542908e+02 0.28698254e+00 0.36964495e-01-0.86277441e-05 3
 AC3H4 18/89C 3H 4 0 OG 200.000 6000.000 1000.000 1
 0.63168722e+01 0.11133728e-01-0.39629378e-05 0.63564238e-09-0.37875540e-13 2
 0.20117495e+05-0.10995766e+02 0.26130445e+01 0.12122575e-01 0.18539880e-04 3
 -0.34525149e-07 0.15335079e-10 0.21541567e+05 0.10226139e+02 0.22962267e+05 4
 PC3H4 t 2/90H 4C 3 0 OG 200.000 6000.000 1000.000 1
 0.60252400e+01 0.11336542e-01-0.40223391e-05 0.64376063e-09-0.38299635e-13 2

0.19620942e+05-0.86043785e+01 0.26803869e+01 0.15799651e-01 0.25070596e-05 3
 -0.13657623e-07 0.66154285e-11 0.20802374e+05 0.98769351e+01 0.22302059e+05 4
 C4H6-13 H6w/94C 4H 6 0 OG 300.000 3000.000 1000.000 1
 0.88673134e+01 0.14918670e-01-0.31548716e-05-0.41841330e-09 0.15761258e-12 2
 0.91338516e+04-0.23328171e+02 0.11284465e+00 0.34369022e-01-0.11107392e-04 3
 -0.92106660e-08 0.62065179e-11 0.11802270e+05 0.23089996e+02 4
 C4H5-N H6w/94C 4H 5 0 OG 300.000 3000.000 1000.000 1
 0.98501978e+01 0.10779008e-01-0.13672125e-05-0.77200535e-09 0.18366314e-12 2
 0.38840301e+05-0.26001846e+02 0.16305321e+00 0.39830137e-01-0.34000128e-04 3
 0.15147233e-07-0.24665825e-11 0.41429766e+05 0.23536163e+02 4
 C4H5-I H6w/94C 4H 5 0 OG 300.000 3000.000 1000.000 1
 0.10229092e+02 0.94850138e-02-0.90406445e-07-0.12596100e-08 0.24781468e-12 2
 0.34642812e+05-0.28564529e+02-0.19932900e-01 0.38005672e-01-0.27559450e-04 3
 0.77835551e-08 0.40209383e-12 0.37496223e+05 0.24394241e+02 4
 C4H3-N H6w/94C 4H 3 0 OG 300.000 3000.000 1000.000 1
 0.54328279e+01 0.16860981e-01-0.94313109e-05 0.25703895e-08-0.27456309e-12 2
 0.61600680e+05-0.15673981e+01-0.31684113e+00 0.46912100e-01-0.68093810e-04 3
 0.53179921e-07-0.16523005e-10 0.62476199e+05 0.24622559e+02 4
 C4H3-I Ab1/93C 4H 3 0 OG 300.000 3000.000 1000.000 1
 0.90978165e+01 0.92207119e-02-0.33878441e-05 0.49160498e-09-0.14529780e-13 2
 0.56600574e+05-0.19802597e+02 0.20830412e+01 0.40834274e-01-0.62159685e-04 3
 0.51679358e-07-0.17029184e-10 0.58005129e+05 0.13617462e+02 4
 C4H4 H6w/94C 4H 4 0 OG 300.000 3000.000 1000.000 1
 0.66507092e+01 0.16129434e-01-0.71938875e-05 0.14981787e-08-0.11864110e-12 2
 0.31195992e+05-0.97952118e+01-0.19152479e+01 0.52750878e-01-0.71655944e-04 3
 0.55072423e-07-0.17286228e-10 0.32978504e+05 0.31419983e+02 4
 AC3H5 pd5/98C 3H 5 0 OG 300.000 3000.000 1000.000 1
 0.65007877e+01 0.14324731e-01-0.56781632e-05 0.11080801e-08-0.90363887e-13 2
 0.17482449e+05-0.11243050e+02 0.13631835e+01 0.19813821e-01 0.12497060e-04 3
 -0.33355555e-07 0.15846571e-10 0.19245629e+05 0.17173214e+02 4
 PC3H5 pd5/98C 3H 5 0 OG 300.000 3000.000 1000.000 1
 0.54255528e+01 0.15511072e-01-0.56678350e-05 0.79224388e-09-0.16878034e-13 2
 0.27843027e+05-0.33527184e+01 0.17329209e+01 0.22394620e-01-0.51490611e-05 3
 -0.67596466e-08 0.38253211e-11 0.29040498e+05 0.16568878e+02 4
 SC3H5 pd5/98C 3H 5 0 OG 300.000 3000.000 1000.000 1
 0.53725281e+01 0.15780509e-01-0.59922850e-05 0.93089664e-09-0.36550966e-13 2
 0.29614760e+05-0.34186478e+01 0.91372931e+00 0.26432343e-01-0.11758950e-04 3
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 H2CCCH 82489C 3H 3 G 0300.00 4000.00 1000.00 1
 0.08831047E+02 0.04357195E-01-0.04109067E-05-0.02368723E-08 0.04376520E-12 2
 0.03847420E+06-0.02177919E+03 0.04754200E+02 0.01108028E+00 0.02793323E-05 3
 -0.05479212E-07 0.01949629E-10 0.03988883E+06 0.05854549E+01 4
 !H2CCCH t 5/97C 3H 3 0 OG 200.000 6000.000 3000.000 1
 ! 7.14221880e+00 7.61902005e-03-2.67459950e-06 4.24914801e-10-2.51475415e-14 2
 ! 3.89087427e+04-1.25848436e+01 1.35110927e+00 3.27411223e-02-4.73827135e-05 3
 ! 3.76309808e-08-1.18540923e-11 4.01057783e+04 1.52058924e+01 4.16139977e+04 4
 !C3H3 t 5/97C 3H 3 0 OG 200.000 6000.000 1
 ! 7.14221880e+00 7.61902005e-03-2.67459950e-06 4.24914801e-10-2.51475415e-14 2

! 3.89087427e+04-1.25848436e+01 1.35110927e+00 3.27411223e-02-4.73827135e-05 3
 ! 3.76309808e-08-1.18540923e-11 4.01057783e+04 1.52058924e+01 4.16139977e+04 4
 C14H14 3/19/ 9 tHermC 14H 14 0 OG 300.000 5000.000 1397.000 31
 3.45703166e+01 3.81757891e-02-1.30119616e-05 2.01694176e-09-1.16936941e-13 2
 -1.18127204e+02-1.59744284e+02-1.13836981e+01 1.53953882e-01-1.25354767e-04 3
 5.17441987e-08-8.54872684e-12 1.48227672e+04 8.37777034e+01 4
 C14H13 3/19/ 9 tHermC 14H 13 0 OG 300.000 5000.000 1396.000 21
 3.47417341e+01 3.59337719e-02-1.22450631e-05 1.89794621e-09-1.10038037e-13 2
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 4.97625178e-08-8.23851673e-12 3.17775915e+04 7.18644702e+01 4
 C14H13OOH 3/19/ 9 tHermC 14H 14O 2 OG 300.000 5000.000 1395.000 51
 4.01427062e+01 3.93395367e-02-1.37664348e-05 2.17056135e-09-1.27304368e-13 2
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 C14H13OO 3/19/ 9 tHermC 14H 13O 2 OG 300.000 5000.000 1394.000 41
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 4.02968908e+01 3.71210431e-02-1.30088643e-05 2.05309245e-09-1.20495552e-13 2
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 5.95672829e-08-1.03363053e-11 1.94259748e+04 7.06782085e+01 4
 C14H11 3/19/ 9 tHermC 14H 11 0 OG 300.000 5000.000 1395.000 11
 3.27609182e+01 3.39480669e-02-1.17667240e-05 1.84362057e-09-1.07661574e-13 2
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 4.03057402e+01 3.72594407e-02-1.30902950e-05 2.06942373e-09-1.21596482e-13 2
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 P-OC6H5OJ wkm C 6O 2H 5 OG 300.000 5000.000 1400.000 01
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 C6H4CH3 4/ 3/ 9 C 7H 7 0 OG 300.000 5000.000 1392.000 11
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 2.69433208e+01 1.98821379e-02-6.93248136e-06 1.09047819e-09-6.38542299e-14 2
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 C6H5CH2CH2 4/ 7/ 9 C 8H 9 0 OG 300.000 5000.000 1397.000 11
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 C6H4OH 4/ 9/ 9 tHermC 6H 5O 1 OG 300.000 5000.000 1402.000 11
 1.73187560e+01 1.36366984e-02-4.68316332e-06 7.29071204e-10-4.23805358e-14 2
 1.14990276e+04-6.89986593e+01-5.99875435e+00 8.59063379e-02-9.12525636e-05 3
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 HOC6H4OH 4/ 9/ 9 tHermC 6H 6O 2 OG 300.000 5000.000 1405.000 21
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 OC6H4OH 4/ 9/ 9 tHermC 6H 5O 2 OG 300.000 5000.000 1403.000 11
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 rOdC6jdO 4/26/ 0Hadad C 6H 5O 2 OG 300.000 5000.000 1400.000 01
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 0.16770320E-07-0.78580680E-12 0.52592500E+05 0.40587132E+02 4
 C5H5OH 5/ 2/91 tHe.mC 5H 6O 1 0g 300.000 5000.000 1398.000 11
 1.53433477e+01 1.50754059e-02-5.13553582e-06 7.95807816e-10-4.61311517e-14 2
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 !P. Dagaut, A. Ristori, A. E. Bakali and M. Cathonnet, 81 (2002) 173-184
 PXYLENE (CH3PCH3) C 8H 10O 0 0G 300.00 5000.00 1000.00 1
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 !R. Sivaramakrishnan, R. S. Tranter and K. Brezinsky, J. Phys. Chem. A, 110 (2006) 9400-9404
 i-C9H9 C 9H 9 G 200.000 6000.000 1000.00 1
 0.17157630E+02 0.31174366E-01-0.11256170E-04 0.18249879E-08-0.10963670E-12 2
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 0.16896527E+02 0.31437513E-01-0.11384195E-04 0.18534120E-08-0.11189553E-12 2
 0.35672282E+05-0.64033565E+02 0.17801818E+01 0.43749859E-01 0.42376835E-04 3
 -0.82140307E-07 0.32924793E-10 0.41103203E+05 0.20932320E+02 4
 !N. A. Slavinskaya, P. Frank, Combust. Flame, 156 (2009) 1705 - 1722
 n-C8H7 HR11/99BLYP00C 8H 7 0 OG 200.000 6000.000 1000.000 01
 1.80458471E+01 2.21498794E-02-8.05082743E-06 1.30961070E-09-7.88615885E-14 2
 3.87090843E+04-7.17917960E+01-8.85283632E-01 5.61565120E-02 1.16600084E-05 3
 -6.99146159E-08 3.63590274E-11 4.45850990E+04 2.97497087E+01 4.67991499E+04 4
 A1C2H3* C 8H 7 G 300.000 3000.000 1000.00 1
 1.15635990E+01 3.02108100E-02-1.15455930E-05 1.73023200E-09-5.23797650E-14 2
 4.04984920E+04-3.48829650E+01-3.88686850E+00 6.81689610E-02-3.48058750E-05 3
 -5.64102540E-09 8.07147580E-12 4.49413590E+04 4.59431880E+01 4
 A1C2H- C 8H 5 G 300.000 3000.000 1000.00 1
 1.23595010E+01 2.54533570E-02-1.06065540E-05 1.89146030E-09-1.06306220E-13 2

6.09304610E+04-4.09002080E+01-4.44958590E+00 7.69950670E-02-6.66170380E-05 3
 2.50386820E-08-1.97566010E-12 6.52259260E+04 4.44279480E+01 4
 A2 OC 10H 8O OG 0200.00 6000.00 1000.00 1
 1.86129884E+01 3.04494175E-02-1.11224825E-05 1.81615474E-09-1.09601281E-13 2
 8.91578988E+03-8.00230396E+01-1.04919475E+00 4.62970781E-02 7.07591636E-05 3
 -1.38408111E-07 6.20475407E-11 1.59848987E+04 3.02121626E+01 1.81107678E+04 4
 A2- C 10H 7 G 200.000 6000.000 1000.00 1
 1.83535073E+01 2.77474314E-02-1.00885968E-05 1.64229575E-09-9.89002001E-14 2
 3.89261241E+04-7.48978150E+01-1.89559772E+00 5.83077290E-02 2.79388931E-05 3
 -9.14375172E-08 4.46422302E-11 4.55409775E+04 3.52453263E+01 4.76546183E+04 4
 INDENE C 9H 8 G 200.000 6000.000 1000.00 1
 0.17318671E+02 0.28982768E-01-0.10605059E-04 0.17334553E-08-0.10467919E-12 2
 0.11151429E+05-0.71555323E+02-0.68190289E+00 0.41658733E-01 0.70741234E-04 3
 -0.13430875E-06 0.59915845E-10 0.17705036E+05 0.29781396E+02 0.19741190E+05 4
 INDENYL C 9H 7 G 200.000 6000.000 1000.00 1
 0.18554959E+02 0.25035076E-01-0.91457509E-05 0.14934838E-08-0.90133030E-13 2
 0.25721156E+05-0.76300347E+02-0.26698729E+01 0.62177216E-01 0.15067018E-04 3
 -0.79645699E-07 0.40918972E-10 0.32386969E+05 0.37861193E+02 0.34349570E+05 4
 P2 OC 12H 10O OG 0300.00 5000.00 1000.00 1
 0.24289017E 02 0.34006648E-01-0.11722408E-04 0.17729298E-08-0.96812532E-13 2
 0.10287000E 05-0.10802374E 03-0.40739527E 01 0.86973310E-01-0.42353613E-05 3
 -0.64564460E-07 0.34150169E-10 0.19405965E 05 0.44741348E 02 0.21905340E 05 4
 P2- OC 12H 9O OG 0300.00 5000.00 1000.00 1
 0.23851303E 02 0.31960227E-01-0.11076719E-04 0.16847825E-08-0.92641173E-13 2
 0.40171297E 05-0.10270549E 03-0.31376228E 01 0.82217276E-01-0.40171444E-05 3
 -0.60809782E-07 0.32074482E-10 0.48868754E 05 0.42730362E 02 0.51444448E 05 4
 A2C2H* C 12H 7 G 300.000 3000.000 1000.00 1
 1.33715110E+01 4.99657190E-02-2.62269020E-05 6.59494350E-09-6.45885050E-13 2
 6.84904150E+04-4.64872350E+01-6.25389030E+00 1.14753010E-01-1.05430910E-04 3
 4.79127480E-08-7.92157250E-12 7.32491920E+04 5.19412620E+01 4
 A2C2H C 12H 8 G 200.000 6000.000 1000.00 1
 2.34108373E+01 3.12979308E-02-1.13777419E-05 1.85217551E-09-1.11546889E-13 2
 3.49196941E+04-1.00594596E+02-2.59169367E+00 8.63306190E-02-1.76590976E-05 3
 -5.26006488E-08 3.15924760E-11 4.27720678E+04 3.73574503E+01 4.55914299E+04 4
 A3 OC 14H 10O OG 0200.00 6000.00 1000.00 1
 0.26602474E+02 0.39769744E-01-0.14572026E-04 0.23843296E-08-0.14409548E-12 2
 0.12132838E+05-0.12266672E+03-0.33646717E+01 0.85073271E-01 0.37531110E-04 3
 -0.12664499E-06 0.61445705E-10 0.22019878E+05 0.40596218E+02 0.24908263E+05 4
 A3- OC 14H 9O OG 0200.00 3000.00 1000.00 1
 1.30899250E+01 6.54850270E-02-3.46655370E-05 8.77017890E-09-8.62784060E-13 2
 4.64475940E+04-4.75652960E+01-7.67067940E+00 1.23515340E-01-8.47954330E-05 3
 1.59995970E-08 4.76798380E-12 5.19694990E+04 5.90610150E+01 4
 A3C2H OC 16H 10O OG 0300.00 3000.00 1000.00 1
 5.21651460E+01-1.31973180E-02 3.43530560E-05-1.62838920E-08 2.36773620E-12 2
 3.42350550E+04-2.54066510E+02-1.16026740E+01 1.68243940E-01-1.64320300E-04 3
 8.63943800E-08-1.93105670E-11 5.21728360E+04 7.55153660E+01 4
 !Ranzi model, <http://creckmodeling.chem.polimi.it/tot1101NOx.CKT>
 C6H5CH2C6H5 C 13H 12 G 300.00 5000.00 1000.00 1

.185418955E+02 .513343070E-01-.178726910E-04 .207043850E-08 .000000000E+00 2
 .668552054E+04-.690121392E+02-.940899900E+01 .125451300E+00-.822539730E-04 3
 .202856220E-07 .000000000E+00 .144845500E+05 .760677200E+02 4

!UIC NPB PYR MODEL

!K. Narayanswamy, G. Blanquart, H. Pitsch, Comb. and Flame, Vol. 157, Issue 10, Oct 2010, 1879-1898

C5H4CH2 FULVENE G3B3 H 6C 6O 0N 0G 300.000 3000.000 1000.000 1
 2.78194214E+00 4.06322016E-02-2.35029327E-05 6.51056017E-09-6.96809087E-13 2
 2.43155607E+04 7.84215958E+00-5.34007612E+00 7.17283827E-02-6.45824457E-05 3
 2.78691157E-08-3.95001455E-12 2.58936616E+04 4.70844323E+01 4

A2R5 G3B3 H 8C 12O 0N 0G 300.000 3000.000 1000.000 1
 3.65432884E+00 7.52647236E-02-4.54864951E-05 1.29795341E-08-1.41730827E-12 2
 2.65223472E+04 7.23303392E-01-1.05497902E+01 1.25536790E-01-1.03646045E-04 3
 3.52989130E-08-1.64508384E-12 2.94426605E+04 7.02667419E+01 4

!Burcat database

C5H4CH3 C 6H 7 G 200.000 6000.000 1000.00 1
 1.28996538E+01 2.12183240E-02-7.67565006E-06 1.24495899E-09-7.47731827E-14 2
 2.12053775E+04-4.47534535E+01 5.64034275E-01 3.84201803E-02 1.94958520E-05 3
 -5.95545053E-08 2.86869522E-11 2.53304225E+04 2.27464371E+01 4

!1245-hexatetraene

HT1245 HR11/99BLYP00C 6H 6 0 0G 300.000 6000.000 1000.000 1
 1.27627347E+01 1.77516318E-02-6.31267704E-06 1.01181415E-09-6.02595474E-14 2
 4.47746179E+04-3.91868742E+01 1.05462594E+00 5.30359803E-02-4.42294933E-05 3
 1.60203849E-08-7.28253865E-13 4.78609473E+04 2.05280769E+01 4

!12-hexadien-5-yne

HD125Y HR11/99BLYP00C 6H 6 0 0G 200.000 6000.000 1000.000 1
 1.28917993E+01 1.87846596E-02-6.75323481E-06 1.09103560E-09-6.53558491E-14 2
 4.43776462E+04-4.07135109E+01 2.21979932E+00 3.93045111E-02-4.49195341E-06 3
 -2.49701907E-08 1.38867376E-11 4.77608479E+04 1.65546134E+01 4

!15hexadiyne

HDY15 HR11/99BLYP00C 6H 6 0 0G 200.000 6000.000 1000.000 1
 1.27627347E+01 1.77516318E-02-6.31267704E-06 1.01181415E-09-6.02595474E-14 2
 4.47746179E+04-3.91868742E+01 1.05462594E+00 5.30359803E-02-4.42294933E-05 3
 1.60203849E-08-7.28253865E-13 4.78609473E+04 2.05280769E+01 4

!N. A. Slavinskaya, P. Frank, Combust. Flame, 156 (2009) 1705 - 1722

BGHIF HR11/99BLYP00C 18H 10 0 0G 300.000 5000.000 1397.000 1
 4.03484789E+01 3.60369349E-02-1.25974449E-05 1.98535622E-09-1.16421390E-13 2
 2.33917123E+04-2.03794640E+02-1.35024568E+01 1.75273343E-01-1.52006334E-04 3
 6.58323068E-08-1.13175755E-11 4.05739002E+04 8.03624456E+01 4

A2R5- HR 4/99 BLYP00C 12H 7 0 0G 300.000 3000.000 1000.000 1
 1.19534280E+01 5.23860720E-02-2.76952570E-05 6.98583910E-09-6.84938560E-13 2
 5.31995200E+04-4.03924920E+01-7.33802680E+00 1.11965800E-01-9.32829450E-05 3
 3.58663420E-08-4.26602220E-12 5.80597670E+04 5.73507140E+01 4

A2CH3 C 11H 10 G 200.000 6000.000 1000.00 1
 2.17939213E+01 3.60214098E-02-1.33228698E-05 2.19304403E-09-1.33071380E-13 2
 3.16261439E+03-9.48675403E+01-1.03043715E+00 6.03358177E-02 5.45655719E-05 3
 -1.22769251E-07 5.54507327E-11 1.13241014E+04 3.22970611E+01 4

A2CH2 C 11H 9 G 200.000 6000.000 1000.00 1

2.18977539E+01 3.26102636E-02-1.18401218E-05 1.92574628E-09-1.15903442E-13 2
 2.24571098E+04-9.41050741E+01-2.53234304E+00 7.32920338E-02 2.02974707E-05 3
 -9.36547823E-08 4.70753594E-11 3.02906705E+04 3.79638513E+01 4
 A3CH3 C 15H 12 G 300.000 5000.000 2025.00 1
 2.86721901E+01 4.57935671E-02-1.67466881E-05 2.72794395E-09-1.63863026E-13 2
 6.77859249E+03-1.31269124E+02 2.45407326E-01 1.03437006E-01-5.52427842E-05 3
 1.17708807E-08-4.92994185E-13 1.69368456E+04 2.37077261E+01 4
 A3CH2 C 15H 11 G 300.000 5000.000 2030.00 1
 2.95619587E+01 4.24589619E-02-1.55841596E-05 2.54481062E-09-1.53124916E-13 2
 2.56273028E+04-1.36219923E+02 1.33783643E-01 1.04067922E-01-5.92362501E-05 3
 1.43179766E-08-9.91637313E-13 3.59458944E+04 2.35063505E+01 4
 A4 C 16H 10 G 300.000 6000.000 1000.00 1
 0.29910014E+02 0.42668069E-01-0.15733834E-04 0.25851725E-08-0.15667980E-12 2
 0.12786491E+05-0.14186953E+03-0.40420321E+01 0.91549657E-01 0.51443344E-04 3
 -0.15276576E-06 0.73087530E-10 0.24094241E+05 0.43665312E+02 4
 !A. Comandini, T. Malewicki and K. Brezinsky, "Chemistry of PAHs formation from phenyl
 radical pyrolysis and phenyl+acetylene reaction", (2011) submitted to Journal of Physical
 Chemistry
 m-TERPH C 18H 14 G 200.000 6000.000 1000.00 1
 0.33247445E+02 0.54924357E-01-0.19975048E-04 0.32549825E-08-0.19625439E-12 2
 0.20384334E+05-0.15453354E+03-0.57179147E+00 0.87428769E-01 0.85427137E-04 3
 -0.16978568E-06 0.68757044E-10 0.32286809E+05 0.34317865E+02 4
 p-TERPH C 18H 14 G 200.000 6000.000 1000.00 1
 0.33227265E+02 0.54949329E-01-0.19985956E-04 0.32569825E-08-0.19638519E-12 2
 0.20295647E+05-0.15433427E+03-0.64797155E+00 0.87859710E-01 0.84534319E-04 3
 -0.16901376E-06 0.68518943E-10 0.32200223E+05 0.34741802E+02 4
 !A. Ergut, S. Granata, J. Jordan, J. Carlson, J. B. Howard, H. Richter, Y. A. Levendis, Combust.
 Flame, 144 (2006) 757 - 772
 A2C6H5-2 HR 8/99 BLYP C 16H 12 0 0G 300.000 5000.000 1397.000 11
 3.80282037E+01 3.76519528E-02-1.31640724E-05 2.07433637E-09-1.21609502E-13 2
 1.11550764E+04-1.85043277E+02-1.33768307E+01 1.73717213E-01-1.54115598E-04 3
 6.92566084E-08-1.23987608E-11 2.73858799E+04 8.53292167E+01 4
 C14H9 C 14H 9 G 300.00 5000.00 1000.00 1
 .255171870E+02 .393727940E-01-.123155080E-04 .127852800E-08 .000000000E+00 2
 .431324738E+05-.115618425E+03-.909474100E+01 .131333800E+00-.924017290E-04 3
 .240156710E-07 .000000000E+00 .527750200E+05 .639753600E+02 4
 END

1,3,5-Trimethylbenzene Oxidation Model

!1,3,5-Trimethylbenzene includes the m-xylene oxidation model

ELEMENTS H O C AR N NE HE END

SPECIES

H O AR NE HE

MXYLENE O2 CO CO2

CH4 C2H4 C2H6 C2H2

AC3H4 PC3H4 C3H6 C3H8

C4H6-13 C4H4 C4H2 C8H6

C5H6 C5H5-1CH3

C6H6 C6H5CH3 C6H5C2H3

C6H5CHO MCPHHCO MCPHC2H5

BIBENZYL MCSTYREN

C6H5C2H5 C6H2 MDICPCH2

C9H12 DIMETB DIMSTYR

DIMPHHCO DIMPHCH2OH

C18H22 DIMERS238 DIMERS224

DIMERS210 DIMERS196 C2H5C6H4CHO

TETRAMB O-XYL TMB123 PTRIARO178

PTRIARO192 A3 A3CH3 A2R5 A2 A2C2H

INDENE DIMERS182 C6H5CH2C6H5 FLUORENE

TMB124 B124PM B11MB3 A3C2H

MXYLYL RDIMERS196a RPTRIARO178a

RPTRIARO192a

H2CCCH C4H C4H8-1

AC3H5 C2H5 C2H3 C2H CH3 CH2 CH H2 N2

NC3H7 IC3H7 C4H5-N C5H5 C6H5

C6H5CH2 C4H10

PC4H9 SC4H9 SC3H5 C4H8-2 C4H5-I C4H7 PC3H5

C C2 C3H2

C4H6-1 C4H6-12 C5H2 C5H3

CH2-S C12H10 C6H5CHCH

C6H5CCH2 C2H4OH

C6H5CHCH3

C6H5CH2CH2 C6H4C2H

C6H4CH3 MBCPHC2H4

MACPHC2H4 MACSTYRYL MBCSTYRYL MCPCH2OH

CH2CO CH2HCO CH2O CH2OH CH3HCO CH3CO

CH3CHCO CH3O CH3OH H2O2 HCCO

HCCOH HCO HO2 OH CHOCHO CH2CHCHO

CH2CHCO HCOH CHCHCHO HCCCHO HCCCO

H2C4O C2O H2O C6H5O C6H5OH C5H4O C5H4OH C6H5CH2OH

HOC6H4CH3 OC6H4CH3 C6H5CO C6H4O2 OC6H3(CH3)2

HOC6H3(CH3)2 MCPHCO C5H5O phenyl(CH3)2

CH3CHO
 C5H5-1CH3 n-C4H3 i-C4H3
 C5H5-1CH2 c-C6H7 n-C6H7
 C5H4CH3CH2 C5H4(CH3)2
 C6H6CH3 C5H4-1CH3 C5H3(CH3)2
 C7H6f o-C6H4 C6H3
 CH2PCH2 CHOPHCH2
 CHOPCHO Y1P4CHO OY1P4CHO CHOPCO
 C5H5CHO CPDCO
 ETCPD
 CH3C6H4CH2OO C6H5CH2OO
 C6H5CH2OOH C6H5CH2O
 CHD4F1Y25 O1O47D5Y
 POXYMETHYL C5H4CH2
 CH3C6H4CH2OOH CH3C6H4CH2O
 !135-TMB chemistry
 C9H11 C6H3(CH3)2 DIMCHCH3
 DIMCH2CH2 DIMCHCH DIMPHCO
 DIMPHCH2O C9H11OOH C18H22
 C9H11OO CH2C6H4CHO A3- P2-
 A2- A2R5- A2C2H* INDENYL
 END

REACTIONS

!R. Sivaramakrishnan, R. S. Tranter, K. Brezinsky, Combust. Flame 139 (2004) 340-350.

CH3+CH3=C2H6 1992	3.61E+13	0	0	!Baulch
CH4+OH=CH3+H2O 1995 29	4.19E+06	2	2547	!Marinov
CH4+O=CH3+OH 1995 30	6.92E+08	1.56	8485	!Marinov
CH4+HO2=CH3+H2O2 1995 31	1.12E+13	0	24640	!Marinov
CH3+HO2=CH3O+OH !Troe 1993 32	7.00E+12	0	0	
CH3+HO2=CH4+O2 !Marinov 1995 33	3.00E+12	0	0	
CH3+O=CH2O+H 1995 34	8.00E+13	0	0	!Marinov
CH3+O2=CH3O+O !Klatt 1991 35	1.45E+13	0	29209	
CH3+O2=CH2O+OH 1995 36	2.51E+11	0	14640	!Marinov
CH3O+H=CH3+OH !Miller92/10 37	1.00E+13	0	0	
CH2OH+H=CH3+OH !Miller92/10 38	1.00E+13	0	0	

CH ₃ +OH=CH ₂ -S+H ₂ O 1994 39	2.65E+13	0	2186	!Humpfer
CH ₃ +OH=CH ₂ +H ₂ O 1996 40	3.00E+06	2	2500	!Marinov
CH ₃ +OH=HCOH+H ₂ 1994 41	5.48E+13	0	2981	!Humpfer
CH ₃ +OH=CH ₂ O+H ₂ !(b) 42	2.25E+13	0	4300	
CH ₃ OH+OH=CH ₂ OH+H ₂ O !Tsang 1987 48	2.61E+05	2.182	-1344	
CH ₃ OH+OH=CH ₃ O+H ₂ O !Tsang 1987 49	2.62E+06	2.056	916	
CH ₃ OH+O=CH ₂ OH+OH !Tsang 1987 50	3.88E+05	2.5	3080	
CH ₃ OH+H=CH ₂ OH+H ₂ !Tsang 1987 51	1.70E+07	2.1	4868	
CH ₃ OH+H=CH ₃ O+H ₂ !Tsang 1987 52	4.24E+06	2.1	4868	
CH ₃ OH+HO ₂ =CH ₂ OH+H ₂ O ₂ !Tsang 1987 53	9.64E+10	0	12578	
CH ₃ O+M=CH ₂ O+H+M !Choudhury1990 54	5.45E+13	0	13497	
!CH ₂ OH+M=CH ₂ O+H+M !Miller 1992 55	1.00E+14	0	25000	
CH ₃ O+H=CH ₂ O+H ₂ !Miller 1992 56	2.00E+13	0	0	
CH ₂ OH+H=CH ₂ O+H ₂ !Miller 1992 57	2.00E+13	0	0	
CH ₃ O+OH=CH ₂ O+H ₂ O !Miller 1992 58	1.00E+13	0	0	
CH ₂ OH+OH=CH ₂ O+H ₂ O !Miller 1992 59	1.00E+13	0	0	
CH ₃ O+O=CH ₂ O+OH !Miller 1992 60	1.00E+13	0	0	
CH ₂ OH+O=CH ₂ O+OH !Miller 1992 61	1.00E+13	0	0	
CH ₃ O+O ₂ =CH ₂ O+HO ₂ !Miller 1992 62	6.30E+10	0	2600	
CH ₂ OH+O ₂ =CH ₂ O+HO ₂ 1992 63 dup	1.57E+15	-1	0	!Baulch
CH ₂ OH+O ₂ =CH ₂ O+HO ₂ 1992 dup	7.23E+13	0	3577	!Baulch
HCOH+OH=HCO+H ₂ O 1996 64	2.00E+13	0	0	!Marinov
HCOH+H=CH ₂ O+H 1996 65	2.00E+14	0	0	!Marinov

HCOH+O=>CO2+H+H 1996 66	5.00E+13	0	0	!Marinov
HCOH+O=>CO+OH+H 1996 67	3.00E+13	0	0	!Marinov
HCOH+O2=>CO2+H+OH !(e) 68	5.00E+12	0	0	
HCOH+O2=CO2+H2O !(e) 69	3.00E+13	0	0	
CH2+OH=CH+H2O !Miller 1992 71	1.13E+07	2	3000	
CH2+OH=CH2O+H !Miller 1992 72	2.50E+13	0	0	
CH2+CO2=CH2O+CO !Miller 1992 73	1.10E+11	0	1000	
CH2+O=CO+H+H !Miller 1992 74	5.00E+13	0	0	
CH2+O=CO+H2 !Miller 1992 75	3.00E+13	0	0	
CH2+O2=CH2O+O !(f) 76	3.29E+21	-3.3	2868	
CH2+O2=>CO2+H+H !(f) 77	3.29E+21	-3.3	2868	
CH2+O2=CO2+H2 !(f) 78	1.01E+21	-3.3	1508	
CH2+O2=CO+H2O !(f) 79	7.28E+19	-2.54	1809	
CH2+O2=HCO+OH !(f) 80	1.29E+20	-3.3	284	
CH2+HCCO=C2H3+CO !Miller 1992 83	3.00E+13	0	0	
CH2-S+M=CH2+M !Miller 1992 85	1.00E+13	0	0	
H /12.0/ C2H2 /4.0/ H2O/3.0/				
CH2-S+O2=>CO+OH+H !Miller 1992 88	7.00E+13	0	0	
CH2-S+O=>CO+H+H !Miller 1992 92	3.00E+13	0	0	
CH2-S+OH=CH2O+H !Miller 1992 93	3.00E+13	0	0	
CH2-S+CO2=CH2O+CO !Miller 1992 95	3.00E+12	0	0	
CH2-S+CH2CO=C2H4+CO !Miller 1992 97	1.60E+14	0	0	
CH+O2=HCO+O !Miller 1992 98	3.30E+13	0	0	
CH+O=CO+H !Miller 1992 99	5.70E+13	0	0	

CH+OH=HCO+H !Miller 1992 100	3.00E+13	0	0	
CH+OH=C+H2O !Miller 1992 101	4.00E+07	2	3000	
CH+CO2=HCO+CO !Miller 1992 102	3.40E+12	0	690	
CH+H2O=CH2O+H !Miller 1992 104	1.17E+15	-0.75	0	
CH+CH2O=CH2CO+H !Miller 1992 105	9.46E+13	0	-515	
C+O2=CO+O !Miller 1992 110	2.00E+13	0	0	
C+OH=CO+H !Miller 1992 111	5.00E+13	0	0	
CH2O+OH=HCO+H2O !Miller 1992 114	3.43E+09	1.18	-447	
CH2O+H=HCO+H2 !Miller 1992 115	2.19E+08	1.77	3000	
CH2O+O=HCO+OH !Miller 1992 117	1.80E+13	0	3080	
C2H6+O=C2H5+OH !Miller 1992 130	3.00E+07	2	5115	
C2H5+OH=C2H4+H2O 1995 135	4.00E+13	0	0	!Marinov
C2H5+O=CH3+CH2O 1988 136	1.00E+14	0	0	!Herron
C2H5+HO2=>CH3+CH2O+OH 1995 137	3.00E+13	0	0	!Marinov
C2H5+O2=C2H4+HO2 1995 138	3.00E+20	-2.86	6760	!Marinov
C2H4+O=CH3+HCO 1994 141	1.02E+07	1.88	179	!Baulch
C2H4+O=CH2HCO+H 1994 142	3.39E+06	1.88	179	!Baulch
C2H4+H(+M)=C2H5(+M) !Feng 1993 144	1.08E+12	0.454	1822	
low / 1.112E+34 -5.0 4448.0 / troe / 1.0 1.0E-15 95.0 200.0 / H2O /5.0/ H2/2.0/ CO2/3.0/ CO/2.0/				
C2H3+O=CH2CO+H !Miller 1992 148	3.00E+13	0	0	
C2H3+O2=CH2HCO+O !150	3.50E+14	-0.611	5260	
C2H3+O2=C2H2+HO2 !cfm/nmm 1996 151	2.12E-06	6	9484	
C2H3+OH=C2H2+H2O !Miller 1992 152	2.00E+13	0	0	

C2H2+OH=C2H+H2O !Miller 1992 162	3.37E+07	2	14000	
C2H2+OH=HCCOH+H !Miller 1992 163	5.04E+05	2.3	13500	
C2H2+OH=CH2CO+H !Miller 1992 164	2.18E-04	4.5	-1000	
dup				
C2H2+OH=CH2CO+H !Vandooren 1977	2.00E+11	0	0	
dup				
C2H2+OH=CH3+CO !Miller 1992 165	4.83E-04	4	-2000	
HCCOH+H=CH2CO+H !Miller 1992 166	1.00E+13	0	0	
!C2H2+O=CH2+CO !(j) 167	6.12E+06	2	1900	
!C2H2+O=HCCO+H !(j) 168	1.43E+07	2	1900	
!C2H2+O=C2H+OH !Miller 1992 169	3.16E+15	-0.6	15000	
C2H2+O2=HCCO+OH !Miller92/10 171	2.00E+07	1.5	30100	
C2H2+M=C2H+H+M !Miller 1992 172	4.20E+16	0	107000	
C2H2+H(+M)=C2H3(+M) 1995 173	3.11E+11	0.58	2589	!Knyazev
low / 2.25E+40 -7.269 6577.0 / !(k)				
troe /1.0 1.0E-15 675.0 1.0E+15 / H2O /5.0/ H2/2.0/ CO2/3.0/ CO/2.0/				
CH3HCO+OH=CH3CO+H2O 1995 174	5.37E+10	0.73	-1110	!Marinov
CH3HCO+H=CH3CO+H2 1995 175	4.09E+09	1.16	2400	!Marinov
CH3HCO+O=CH3CO+OH 1995 176	5.89E+12	0	1810	!Marinov
CH3HCO+HO2=CH3CO+H2O2 1995 177	1.70E+12	0	10700	!Marinov
CH3HCO+O2=CH3CO+HO2 1995 178	2.00E+13	0.5	42200	!Marinov
CH3HCO+CH3=CH3CO+CH4 1996 179	2.00E-06	5.64	2464	!Marinov
CH2HCO+H=CH2CO+H2 1996 180	4.00E+13	0	0	!Marinov
CH2HCO+O=CH2O+HCO 1996 181	1.00E+14	0	0	!Marinov
CH2HCO+OH=CH2CO+H2O 1996 182	3.00E+13	0	0	!Marinov

CH ₂ HCO+O ₂ =>CH ₂ O+CO+OH 1992 183	3.00E+10	0	0	!Baulch
CH ₂ HCO+CH ₃ =>C ₂ H ₅ +CO+H !(l) 184	4.90E+14	-0.5	0	
CH ₂ HCO=CH ₂ CO+H 1995 185	3.95E+38	-7.649	45115	!Marinov
CHOCHO(+M)=CH ₂ O+CO(+M) 1995 186	4.27E+12	0	50600	!Marinov
low / 8.91E+16 0.0 49200.0 / 1995				!Marinov
CHOCHO=>CO+CO+H ₂ !(m) 187	4.07E+42	-8.5	69278	
CHOCHO+OH=>HCO+CO+H ₂ O 1995 188	1.00E+13	0	0	!Marinov
CHOCHO+O=>HCO+CO+OH 1995 189	7.24E+12	0	1970	!Marinov
CHOCHO+H=CH ₂ O+HCO 1995 190	1.00E+12	0	0	!Marinov
CHOCHO+HO ₂ =>HCO+CO+H ₂ O ₂ 1995 191	1.70E+12	0	10700	!Marinov
CHOCHO+CH ₃ =>HCO+CO+CH ₄ 1995 192	1.74E+12	0	8440	!Marinov
CHOCHO+O ₂ =>HCO+CO+HO ₂ 1995 193	1.00E+14	0	37000	!Marinov
CH ₃ CO(+M)=CH ₃ +CO(+M) 1984 194	3.00E+12	0	16722	!Warnatz
low / 1.20E+15 0.0 12518.0 / 1984				!Warnatz
CH ₂ CO+O=CO ₂ +CH ₂ 1995 195	1.75E+12	0	1350	!Marinov
CH ₂ CO+H=CH ₃ +CO 1984 196	7.00E+12	0	3011	!Warnatz
CH ₂ CO+H=HCCO+H ₂ !(n) 197	2.00E+14	0	8000	
CH ₂ CO+O=HCCO+OH !Miller 1992 198	1.00E+13	0	8000	
CH ₂ CO+OH=HCCO+H ₂ O !Miller 1992 199	1.00E+13	0	2000	
CH ₂ CO+OH=CH ₂ OH+CO 1989 200	3.73E+12	0	-1013	!Brown
CH ₂ CO(+M)=CH ₂ +CO(+M) !Miller 1992	3.00E+14	0	70980	
low / 3.60E+15 0.0 59270.0 / !Miller 1992				
C ₂ H+O=CH+CO !Miller 1992 202	5.00E+13	0	0	
C ₂ H+OH=HCCO+H !Miller 1992 203	2.00E+13	0	0	

C2H+OH=C2+H2O !Miller 1992 204	4.00E+07	2	8000	
C2H+O2=>CO+CO+H 1993 205	9.04E+12	0	-457	!Opansky
HCCO+C2H2=H2CCCH+CO !Miller 1992 208	1.00E+11	0	3000	
HCCO+H=CH2-S+CO !Miller 1992 209	1.00E+14	0	0	
HCCO+O=>H+CO+CO 1995 210	8.00E+13	0	0	!Peeters
HCCO+O=CH+CO2 1995 211	2.95E+13	0	1113	!Peeters
HCCO+O2=>HCO+CO+O 1992	9.78E+11	0	850	!Baulch,
HCCO+O2=CO2+HCO !Bikas et al 2001	8.13E+11	0	855	
HCCO+CH=C2H2+CO !Miller 1992 214	5.00E+13	0	0	
HCCO+HCCO=>C2H2+CO+CO !Miller 1992 215	1.00E+13	0	0	
HCCO+OH=C2O+H2O !Miller 1992 216	3.00E+13	0	0	
HCO+O2 = CO+HO2 !96HSU/MEB	1.204E+10	0.807	-727.00	
C2O+H=CH+CO !Miller 1992 217	1.00E+13	0	0	
C2O+O=CO+CO !Miller 1992 218	5.00E+13	0	0	
C2O+OH=>CO+CO+H !Miller 1992 219	2.00E+13	0	0	
C2O+O2=>CO+CO+O !Miller 1992 220	2.00E+13	0	0	
C2+O2=CO+CO !Miller 1992 222	5.00E+13	0	0	
C2+OH=C2O+H !Miller 1992 223	5.00E+13	0	0	
C3H8(+M)=C2H5+CH3(+M) !Tsang 1988 224	7.90E+22	-1.8	8629	
low / 7.237E+27 -2.88 67448.0 !Al-Alami 1983				
troe /1.0 1.0E-15 1500.0 1.0E+15/ H2O/5.0/ CO2/3.0/ CO/2.0/ H2/2.0/				
C3H8+O2=IC3H7+HO2 !Tsang 1988 225	4.00E+13	0	48610	
C3H8+O2=NC3H7+HO2 !Tsang 1988 226	4.00E+13	0	51360	
C3H8+HO2=NC3H7+H2O2 !Tsang 1988 227	4.76E+04	2.55	16492	

C3H8+HO2=IC3H7+H2O2 !Tsang 1988 228	9.64E+03	2.6	13909	
C3H8+OH=NC3H7+H2O !Cohen 1991 229	3.16E+07	1.8	934	
C3H8+OH=IC3H7+H2O !Cohen 1991 230	7.08E+06	1.9	-159	
C3H8+O=NC3H7+OH !Cohen 1986 231	3.73E+06	2.4	5504	
C3H8+O=IC3H7+OH !Cohen 1986 232	5.48E+05	2.5	3139	
NC3H7(+M)=C2H4+CH3(+M) 1992 243	1.23E+13	-0.1	30202	!Bencsura
low / 5.485E+49 -10.0 35766.0 / 1992				!Bencsura
troe / 2.17 1.0E-15 251.0 1185.0 / H2O /5.0/ H2/2.0/ CO2/3.0/ CO/2.0/ NC3H7+O2=C3H6+HO2 1992 244	3.58E+09	0	-3532	!Dagaut
IC3H7+O2=C3H6+HO2 !(p) 245	6.10E+20	-2.86	7910	
C3H6+H(+M)=IC3H7(+M) 1993 246	5.70E+09	1.16	874	!Seakins
low / 1.64E+54 -11.1 9364.0 / troe / 1.0 1.0E-15 260.0 3000.0 / H2O /5.0/ H2/2.0/ CO2/3.0/ CO/2.0/ C3H6+HO2=AC3H5+H2O2 !Tsang 1991 253	9.64E+03	2.6	13910	
C3H6+OH+O2=>CH3HCO+CH2O+OH 1992 254	3.00E+10	0	-8280	!Dagaut
C3H6+OH=AC3H5+H2O !Tsang 1991 255	3.12E+06	2	-298	
C3H6+OH=SC3H5+H2O !Tsang 1991 256	1.11E+06	2	1451	
C3H6+OH=PC3H5+H2O !Tsang 1991 257	2.11E+06	2	2778	
C3H6+O=>CH3CHCO+H+H !Tsang 1991 258	5.01E+07	1.76	76	
C3H6+O=C2H5+HCO !Tsang 1991 259	1.58E+07	1.76	-1216	
C3H6+O=AC3H5+OH !Tsang 1991 260	5.24E+11	0.7	5884	
C3H6+O=PC3H5+OH !Tsang 1991 261	1.20E+11	0.7	8959	
C3H6+O=SC3H5+OH !Tsang 1991 262	6.03E+10	0.7	7632	
PC3H5+HO2=C3H6+O2 !267	1.50E+12	0	0	

SC3H5+HO2=C3H6+O2 !268	1.00E+12	0	0
AC3H5+HO2=C3H6+O2 !269	3.00E+12	0	0
C3H6+HCO=AC3H5+CH2O !Tsang 1991 273	1.08E+07	1.9	17010
CH3CHCO+OH=CH2CHCO+H2O !(q) 274	4.00E+06	2	0
CH3CHCO+O=CH2CHCO+OH !(q) 275	7.60E+08	1.5	8500
CH3CHCO+H=CH2CHCO+H2 !(q) 275	2.00E+05	2.5	2500
CH3CHCO+H=C2H5+CO !(r) 276	2.00E+13	0	2000
CH3CHCO+O=>CH3+HCO+CO !(s) 277	3.00E+07	2	0
CH2CHCHO+OH=CH2CHCO+H2O !(t) 278	1.00E+13	0	0
CH2CHCHO+O=CH2CHCO+OH !(t) 279	7.24E+12	0	1970
CH2CHCHO+O=>CH2CO+HCO+H !(s) 280	5.01E+07	1.76	76
CH2CHCHO+H=CH2CHCO+H2 !(t) 281	3.98E+13	0	4200
CH2CHCHO+H=C2H4+HCO !(r) 282	2.00E+13	0	3500
CH2CHCHO+O2=CH2CHCO+HO2 !(u) 283	3.00E+13	0	36000
CH2CHCO=C2H3+CO !(v) 284	1.00E+14	0	34000
CH2CHCO+O=C2H3+CO2 !(w) 285	1.00E+14	0	0
AC3H5+O2=CH2CHCHO+OH 1993 285	1.82E+13	-0.41	22859 !Bozzelli
AC3H5+O2=AC3H4+HO2 1993 286	4.99E+15	-1.4	22428 !Bozzelli
AC3H5+O2=CH2HCO+CH2O 1993 287	1.06E+10	0.34	12838 !Bozzelli
AC3H5+O2=>C2H2+CH2O+OH 1993 288	2.78E+25	-4.8	15468 !Bozzelli
AC3H5+HO2=>CH2CHCHO+H+OH !Tsang 1991 289	1.00E+13	0	0
AC3H5+OH=AC3H4+H2O !Tsang 1991 290	1.00E+13	0	0
!AC3H5+O=CH2CHCHO+H !Slagle 1992 292	1.81E+14	0	0
PC3H5+O2=CH3HCO+HCO !(z) 295	1.09E+23	-3.29	3892

PC3H5+O2=>CH3CHCO+H+O !(z) 296	1.60E+15	-0.78	3135	
PC3H5+O=CH3CHCO+H !(aa) 297	1.00E+14	0	0	
PC3H5+OH=PC3H4+H2O !(aa) 299	1.00E+13	0	0	
SC3H5+O2=CH3CO+CH2O !(z) 302	1.09E+22	-3.29	3892	
SC3H5+O=CH2CO+CH3 !(aa) 303	1.00E+14	0	0	
SC3H5+OH=PC3H4+H2O !(aa) 305	2.00E+13	0	0	
AC3H4+O=C2H4+CO !(bb) 307	1.34E+07	1.88	179	
!AC3H4+OH=H2CCCH+H2O !308	2.00E+08	2	1000	
PC3H4+O=C2H4+CO !Warnatz84/(cc) 312	1.50E+13	0	2102	
PC3H4+OH=H2CCCH+H2O !313	4.00E+08	2	1000	
H2CCCH+O2=CH2CO+HCO !Miller 1992 319	3.00E+10	0	2868	
H2CCCH+O=CH2O+C2H !Miller 1992 320	2.00E+13	0	0	
H2CCCH+OH=C3H2+H2O !Miller 1992 322	2.00E+13	0	0	
H2CCCH+H(+M)=AC3H4(+M) !(ff) 327	1.66E+15	-0.37	0	
low / 3.36E+45 -8.52 6293.0 / !Kiefer 1995/(gg)				
H2O/5.0/ H2/2.0/ CO2/3.0/ CO/2.0/ O2/2.0/ C2H2/2.0/ H2CCCH+H(+M)=PC3H4(+M) !(ff) 328	1.66E+15	-0.37	0	
low / 8.78E+45 -8.9 7974.0 / !Kiefer 1995/(gg)				
H2O /5.0/ H2/2.0/ CO2/3.0/ CO/2.0/ O2/2.0/ C2H2/2.0/ C3H2+O2=>HCCO+CO+H !Miller 1992 329	5.00E+13	0	0	
C3H2+OH=C2H2+HCO !Miller 1992 330	5.00E+13	0	0	
CHCHCHO+O2=>C2H2+CO+HO2 331	3.00E+12	0	0	!
CHCHCHO=C2H2+HCO !(ii) 332	1.00E+14	0	33000	
CHCHCHO+H=CH2CHCO+H 1996 333	1.00E+14	0	0	!Marinov
CHCHCHO+OH=HCCCHO+H2O !(aa) 334	1.00E+13	0	0	

CHCHCHO+H=HCCCCHO+H2 !(aa) 335	2.00E+13	0	0
HCCCHO+H=C2H2+HCO !(jj) 336	1.00E+14	0	3000
HCCCHO+OH=HCCCO+H2O !(t) 337	1.00E+13	0	0
HCCCHO+H=HCCCO+H2 !(t) 338	4.00E+13	0	4200
HCCCO+O2=>HCO+CO+CO !(kk) 339	1.40E+09	1	0
HCCCO+H=C2H2+CO !(kk) 340	1.00E+14	0	0
C4H10+O2=PC4H9+HO2 !Pitz 1991 345	2.50E+13	0	49000
C4H10+O2=SC4H9+HO2 !Pitz 1991 346	4.00E+13	0	47600
C4H10+OH=PC4H9+H2O !Pitz 1991 352	4.13E+07	1.73	753
C4H10+OH=SC4H9+H2O !Pitz 1991 353	7.23E+07	1.64	-247
C4H10+O=PC4H9+OH !Pitz 1991 354	1.13E+14	0	7850
C4H10+O=SC4H9+OH !Pitz 1991 355	5.62E+13	0	5200
C4H10+HO2=PC4H9+H2O2 !Pitz 1991 356	1.70E+13	0	20460
C4H10+HO2=SC4H9+H2O2 !Pitz 1991 357	1.12E+13	0	17700
SC4H9(+M)=C3H6+CH3(+M) !358	2.14E+12	0.65	30856
low /6.323e58 -12.85 35567./ H2O/5./ H2/2./ CO2/3./ CO/2./			
C4H8-1+O=NC3H7+HCO !Pitz 1991 368	1.80E+05	2.5	-1029
C4H8-1+O=>CH2CHCHO+CH3+H !Pitz 1991 369	9.67E+04	2.5	-1029
C4H8-1+OH=C4H7+H2O !Pitz 1991 370	2.25E+13	0	2217
C4H8-1+O2=C4H7+HO2 !Pitz 1991 372	4.00E+12	0	33200
C4H8-2+O=IC3H7+HCO !Pitz 1991 376	2.79E+06	2.12	-1775
C4H8-2+OH=C4H7+H2O !Pitz 1991 377	3.90E+13	0	2217
C4H8-2+O=CH3CO+C2H5 1994 378	1.53E+07	1.87	-1476 !Adusei
C4H8-2+O=>CH3+CH3CHCO+H 1994 379	8.22E+06	1.87	-1476 !Adusei

C4H8-2+O2=C4H7+HO2 !Pitz 1991 380	8.00E+13	0	37400	
C4H7+OH=C4H6-13+H2O !Pitz 1991 382	1.00E+13	0	0	
C4H7+O2=C4H6-13+HO2 !Pitz 1991 385	1.00E+09	0	0	
C4H6-13+OH=C4H5-N+H2O !Miller 1992 387	2.00E+07	2	5000	
C4H6-13+OH=C4H5-I+H2O !Miller 1992 388	2.00E+07	2	2000	
C4H6-13+O=HCO+AC3H5 1993 389	6.02E+08	1.45	-858	!Adusei
C4H6-13+O=CH2HCO+C2H3 !Pitz 1991 390	1.00E+12	0	0	
!C4H6-1+OH=C4H5-3MA+H2O !(q) 393	1.00E+07	2	2000	
C4H6-12+OH=C4H5-I+H2O !(q) 395	2.00E+07	2	1000	
!C4H6-12+OH=C4H5-1MA+H2O !(ll) 396	1.00E+07	2	2000	
!C4H6-12+OH=C4H5-3MA+H2O !(ll) 397	2.00E+07	2	2500	
!C4H5-3MA+O2=CH3CHCO+HCO !Slagle 1992 403	4.16E+10	0	2510	
!C4H5-3MA+OH=C4H4+H2O !(mm) 404	3.00E+13	0	0	
!C4H5-1MA+O2=CH3CO+CH2CO 1996 408	4.16E+10	0	2510	!Marinov
!C4H5-1MA+OH=C4H4-123+H2O !(mm) 410	1.00E+13	0	0	
C4H5-N+OH=C4H4+H2O !Miller 1992 412	2.00E+07	2	1000	
C4H5-N+O2=CHCHCHO+CH2O !(qq) 418	1.00E+12	0	0	
!C4H4-123+OH=C4H3-123+H2O !(ss) 420	2.00E+07	2	2000	
!C4H4+OH=C4H3+H2O !Miller 1992 422	7.50E+06	2	5000	
!C4H4+OH=C4H3-123+H2O !Miller 1992 424	1.00E+07	2	2000	
!C4H3+O2=HCCCHO+HCO !(tt) 427	3.00E+12	0	0	
!C4H3-123+O2=CH2CO+HCCO !Miller 1992 428	1.00E+12	0	0	
!C4H3-123+OH=C4H2+H2O !Miller 1992 429	3.00E+13	0	0	
!C4H3-123+O=CH2CO+C2H !Miller 1992 430	2.00E+13	0	0	

!C4H3-123+O=H2C4O+H !Miller 1992 431	2.00E+13	0	0
!C4H2+OH=H2C4O+H !Miller 1992 439	6.66E+12	0	-410
!C4H2+O=C3H2+CO !Miller 1992 440	1.20E+12	0	0
!H2C4O+H=C2H2+HCCO !Miller 1992 441	5.00E+13	0	3000
!H2C4O+OH=CH2CO+HCCO !Miller 1992 442	1.00E+07	2	2000
! *****ebg mechanism *****			
C6H6+O2=C6H5+HO2 !EBG, 1992 444	6.30E+13	0	60000
C6H6+OH=C6H5+H2O !EBG, 1992 445,	2.11E+13	0	4570
!C6H6+O=C6H5O+H !EBG, 1992 446	2.78E+13	0	4910
C6H5O=CO+C5H5 !EBG, 1992 449	2.51E+11	0	43900
C6H5O+H=C6H5OH !EBG, 1992 450	2.50E+14	0	0
C6H5OH+OH=C6H5O+H2O !EBG, 1992 451	6.00E+12	0	0
C6H5OH+H=C6H6+OH !EBG, 1992 452	2.21E+13	0	7910
C6H5OH+H=C6H5O+H2 !EBG, 1992 453	1.15E+14	0	12400
C6H5OH+O=C6H5O+OH !EBG, 1992 454	2.81E+13	0	7352
C2H3+C6H5OH=C2H4+C6H5O !EBG, 1992 455	6.00E+12	0	0
C4H5-N+C6H5OH=C4H6-13+C6H5O !EBG, 1992 456	6.00E+12	0	0
C6H5+C6H5OH=C6H6+C6H5O !EBG, 1992 457	4.91E+12	0	4400
C5H5+O=C4H5-N+CO !EBG, 1992 459	1.00E+14	0	0
C5H6+HO2=C5H5+H2O2 !EBG, 1992 463	1.99E+12	0	11660
C5H6+OH=C5H5+H2O !EBG, 1992 464	3.43E+09	1.18	-447
C5H6+O=C5H5+OH !EBG, 1992 466	1.81E+13	0	3080
C5H6+C6H5O=C5H5+C6H5OH !EBG, 1992 469	3.16E+11	0	8000

C5H4OH=C5H4O+H !EBG, 1992 471	2.10E+13	0	48000
C5H4O=>CO+C2H2+C2H2 !EBG, 1992 472	1.00E+15	0	78000
!C6H5CH3+O2=C6H5CH2+HO2 al. 2005	1.14E+07	2.5	44946 !Baulch et
!C6H5CH3+OH=C6H5CH2+H2O !EBG, 1992 514	1.26E+13	0	2583
!C6H5OH+C6H5CH2=C6H5O+C6H5CH3 !EBG, 1992 520	1.05E+11	0	9500
HOC6H4CH3+C6H5CH2=OC6H4CH3+C6H5CH3 !EBG, 1992 521	1.05E+11	0	9500
!C6H5CH2+O=C6H5+CH2O !EBG, 1992 523	8.00E+13	0	0
!C6H5CH2+HO2=>C6H5CHO+H+OH !Coll Freq. * 0.7575	3.67E+14	0	0
!C6H5CH2+HO2=>C6H5+CH2O+OH !Coll Freq. * 0.2525	1.17E+14	0	0
C6H5CH2+OH=C6H5CH2OH !EBG, 1992 528	6.00E+13	0	0
C6H5CH2OH+O2=>C6H5CHO+HO2+H !EBG, 1992 529	2.00E+14	0	41400
C6H5CH2OH+OH=>C6H5CHO+H2O+H !EBG, 1992 530	8.43E+12	0	2583
C6H5CH2OH+H=>C6H5CHO+H2+H !EBG, 1992 531	8.00E+13	0	8235
C6H5CH2OH+H=C6H6+CH2OH !EBG, 1992 532	1.20E+13	0	5148
C6H5CH2OH+C6H5CH2=>C6H5CHO+C6H5CH3+H !EBG, 1992 533	2.11E+11	0	9500
C6H5CH2OH+C6H5=>C6H5CHO+C6H6+H !EBG, 1992 534	1.40E+12	0	4400
C6H5CHO+O2=C6H5CO+HO2 !EBG, 1992 535	1.02E+13	0	38950
C6H5CHO+OH=C6H5CO+H2O !EBG, 1992 536	1.71E+09	1.18	-447
C6H5CHO+H=C6H5CO+H2 !EBG, 1992 537	5.00E+13	0	4928
C6H5CHO+H=C6H6+HCO !EBG, 1992 538	1.20E+13	0	5148
C6H5CHO+O=C6H5CO+OH !EBG, 1992 539	9.04E+12	0	3080
CH3+C6H5CHO=CH4+C6H5CO !EBG, 1992 541	2.77E+03	2.81	5773
C6H5+C6H5CHO=C6H6+C6H5CO !EBG, 1992 542	7.01E+11	0	4400
C6H5C2H5+OH=>C6H5C2H3+H2O+H !EBG, 1992 543	8.43E+12	0	2583

C6H5C2H5+O2=>C6H5C2H3+HO2+H !EBG, 1992 545	2.00E+14	0	41400	
C6H5C2H5+H=>C6H5C2H3+H2+H !EBG, 1992 544	8.00E+13	0	8235	
C6H5CO=C6H5+CO !EBG, 1992 552	3.98E+14	0	29400	
C4H5-I+C6H5OH=C4H6-13+C6H5O !est from EBG #14 577	6.00E+12	0	0	
C6H5O+O=C6H4O2+H et al., 2000 Int. J. Chem. Kin.	8.50E+13	0	0	!Glarborg
C6H5+O2=C6H4O2+H !Just et al., 1994 Symp. Int. Comb.	3.00E+13	0	8982	
C6H4O2=C5H4O+CO !Just et al., 1994 Symp. Int. Comb.	7.40E+11	0	59020	
!C6H5=n-C4H3+C2H2 !Kiefer et al., 1985, J. Phys. Chem.	1.58E+15	0	82000	
C6H5+O2=C6H5O+O !Just, 1994	2.60E+13	0	6120	
C6H5CH3+O=OC6H4CH3+H !EBG, 1992 517	1.63E+13	0	3418	
!Additions and Modifications to the High Pressure Toluene Oxidation Model, R. Sivaramakrishnan, R. S. Tranter, K. Brezinsky, Combust. Flame 139 (2004) 340-350.				
!R. Sivaramakrishnan, R. S. Tranter, K. Brezinsky, J. Phys. Chem. A 110 (2006) 9388-9399.				
!R. Sivaramakrishnan, R. S. Tranter, K. Brezinsky, J. Phys. Chem. A 110 (2006) 9400-9404.				
CH4+H=CH3+H2 !Miller 1992 28	2.20E+04	3	8750	
CH3+H=CH2+H2 !Miller 1992 43	9.00E+13	0	15100	
H+CH2(+M)<=>CH3(+M) 3.0	6.000E+14	.000	.00	!Grimech
LOW / 1.040E+26 -2.760 1600.00/ TROE/ .5620 91.00 5836.00 8552.00/ H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ !Grimech 3.0				
CH+H2(+M)<=>CH3(+M) LOW/ 4.820E+25 -2.80 590.0 / TROE/ .578 122.0 2535.0 9365.0 / H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ H+CH3(+M)<=>CH4(+M) 3.0	1.970E+12	.430	-370.00	
LOW / 2.620E+33 -4.760 2440.00/ TROE/ .7830 74.00 2941.00 6964.00 / H2/2.00/ H2O/6.00/ CH4/3.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/ CH2+H=CH+H2				
!Miller 1992 70	1.00E+18	-1.56	0	
CH2+CH3=C2H4+H !Miller 1992 81	4.00E+13	0	0	

CH ₂ +CH ₂ =>C ₂ H ₂ +H+H !Miller 1992 82	4.00E+13	0	0	
CH ₂ +C ₂ H ₂ =H ₂ CCCH+H !Miller 1992 84	1.20E+13	0	6600	
CH ₂ -S+CH ₄ =CH ₃ +CH ₃ !Miller 1992 86	4.00E+13	0	0	
CH ₂ -S+C ₂ H ₆ =CH ₃ +C ₂ H ₅ !Miller 1992 87	1.20E+14	0	0	
CH ₂ -S+H ₂ =CH ₃ +H !Miller 1992 89	7.00E+13	0	0	
CH ₂ -S+C ₂ H ₂ =H ₂ CCCH+H Mas85 90	1.50E+14	0	0	!Canosa-
CH ₂ -S+C ₂ H ₄ =AC ₃ H ₅ +H Mas85 91	1.30E+14	0	0	!Canosa-
CH ₂ -S+H=CH+H ₂ !Miller 1992 94	3.00E+13	0	0	
CH ₂ -S+CH ₃ =C ₂ H ₄ +H !Miller 1992 96	2.00E+13	0	0	
CH+H=C+H ₂ !Miller 1992 103	1.50E+14	0	0	
CH+C ₂ H ₂ =C ₃ H ₂ +H !Miller 1992 106	1.00E+14	0	0	
CH+CH ₂ =C ₂ H ₂ +H !Miller 1992 107	4.00E+13	0	0	
CH+CH ₃ =C ₂ H ₃ +H !Miller 1992 108	3.00E+13	0	0	
CH+CH ₄ =C ₂ H ₄ +H !Miller 1992 109	6.00E+13	0	0	
C+CH ₃ =C ₂ H ₂ +H !Miller 1992 112	5.00E+13	0	0	
C+CH ₂ =C ₂ H+H !Miller 1992 113	5.00E+13	0	0	
C ₂ H ₆ +CH ₃ =C ₂ H ₅ +CH ₄ !Miller 1992 128	5.50E-01	4	8300	
C ₂ H ₆ +H=C ₂ H ₅ +H ₂ !Miller 1992 129	5.40E+02	3.5	5210	
C ₂ H ₅ +H=C ₂ H ₄ +H ₂ 1995 132	1.25E+14	0	8000	!Marinov
C ₂ H ₅ +H=CH ₃ +CH ₃ 1984 133	3.00E+13	0	0	!Warnatz
C ₂ H ₅ +H=C ₂ H ₆ 1996 134	1.00E+14	0	0	!Marinov
C ₂ H ₄ +H=C ₂ H ₃ +H ₂ 1990 139	3.36E-07	6	1692	!Dagaut
C ₂ H ₄ +CH ₃ =C ₂ H ₃ +CH ₄ 1995 143	6.62E+00	3.7	9500	!Marinov
C ₂ H ₄ (+M)=C ₂ H ₂ +H ₂ (+M) !145	1.80E+13	0	76000	

low / 1.5e15 0.0 55443. / C2H4(+M)=C2H3+H(+M) !146	2.00E+16	0	110000
low / 1.4e15 0.0 81833. / C2H3+H=C2H2+H2 !Miller 1992 147	4.00E+13	0	0
C2H3+C2H=C2H2+C2H2 !Miller 1992 153	3.00E+13	0	0
C2H3+CH=CH2+C2H2 !Miller 1992 154	5.00E+13	0	0
!C2H3+CH3=AC3H5+H !(i) 155	4.73E+02	3.7	5677
C2H3+CH3=C2H2+CH4 !Fahr 1991 157	2.00E+13	0	0
!C2H3+C2H2=C4H4+H !Miller 1992 158	2.00E+12	0	5000
C2H3+C2H4=C4H6-13+H !Tsang 1986 159	5.00E+11	0	7304
C2H3+C2H3=C4H5-I+H !Fahr 1991 160	7.00E+13	0	0
C2H3+C2H3=C2H4+C2H2 !Fahr 1991 161	1.45E+13	0	0
C2H2+CH3=C2H+CH4 !Tsang 1986 170	1.81E+11	0	17289
C2H+H2=C2H2+H !Miller 1992 201	4.09E+05	2.39	864.3
!C2H+C2H2=C4H2+H !Farhat 1993 206	9.64E+13	0	0
!C2H+C2H4=C4H4+H !Tsang 1986 207	1.20E+13	0	0
C2+H2=C2H+H !Miller 1992 221	4.00E+05	2.4	1000
C3H8+H=IC3H7+H2 !Tsang 1988 233	1.30E+06	2.4	4471
C3H8+H=NC3H7+H2 !Tsang 1988 234	1.33E+06	2.54	6756
C3H8+CH3=NC3H7+CH4 !Tsang 1988 235	9.04E-01	3.65	7153
C3H8+CH3=IC3H7+CH4 !Tsang 1988 236	1.51E+00	3.46	5480
C3H8+C2H3=IC3H7+C2H4 !Tsang 1988 237	1.00E+03	3.1	8830
C3H8+C2H3=NC3H7+C2H4 !Tsang 1988 238	6.00E+02	3.3	10500
C3H8+C2H5=IC3H7+C2H6 !Tsang 1988 239	1.51E+00	3.46	7470
C3H8+C2H5=NC3H7+C2H6 !Tsang 1988 240	9.03E-01	3.65	9140

C3H8+AC3H5=C3H6+NC3H7 !Tsang 1988 241	2.35E+02	3.3	19842	
C3H8+AC3H5=C3H6+IC3H7 !Tsang 1988 242	7.83E+01	3.3	18169	
IC3H7+H=C2H5+CH3 !Tsang 1988 247	5.00E+13	0	0	
NC3H7+H=C2H5+CH3 !Tsang 1988 248	1.00E+14	0	0	
PC3H5+H=C3H6 249	7.00E+13	0	0	!
SC3H5+H=C3H6 !250	5.00E+13	0	0	
C3H6=C2H2+CH4 1992 251	2.50E+12	0	70000	!Hidaka
C3H6=AC3H4+H2 1992 252	3.00E+13	0	80000	!Hidaka
C3H6+H=C2H4+CH3 !Tsang 1991 263	7.23E+12	0	1302	
C3H6+H=AC3H5+H2 !Tsang 1991 264	1.73E+05	2.5	2492	
C3H6+H=SC3H5+H2 !Tsang 1991 265	4.09E+05	2.5	9794	
C3H6+H=PC3H5+H2 !Tsang 1991 266	8.04E+05	2.5	12284	
C3H6+CH3=AC3H5+CH4 !Tsang 1991 270	2.22E+00	3.5	5675	
C3H6+CH3=SC3H5+CH4 !Tsang 1991 271	8.43E-01	3.5	11656	
C3H6+CH3=PC3H5+CH4 !Tsang 1991 272	1.35E+00	3.5	12848	
AC3H5+H=AC3H4+H2 !Tsang 1991 291	5.00E+13	0	0	
AC3H5+H=C3H6 !(y) 292	1.88E+26	-3.6	5468	
AC3H5+CH3=AC3H4+CH4 !Tsang 1991 293	3.02E+12	-0.32	-131	
AC3H5+CH3=C4H8-1 !(y) 294	1.76E+50	-11	18600	
PC3H5+H=PC3H4+H2 !(aa) 298	2.00E+13	0	0	
PC3H5+H=AC3H5+H 1996 300	1.00E+14	0	0	!Marinov
SC3H5+H=AC3H5+H 1996 301	1.00E+14	0	0	!Marinov
SC3H5+H=PC3H4+H2 !(aa) 304	4.00E+13	0	0	
AC3H4+H=H2CCCH+H2 306	2.00E+07	2	5000	!

AC3H4+CH3=H2CCCH+CH4 !309	1.50E+00	3.5	5600	
AC3H4=PC3H4 !310	1.48E+13	0	60401	
PC3H4+H=H2CCCH+H2 !311	2.00E+07	2	5000	
PC3H4+CH3=H2CCCH+CH4 !314	1.50E+00	3.5	5600	
PC3H4+H=CH3+C2H2 !315	5.12E+10	1	2060	
PC3H4+H(+M)=SC3H5(+M) 1972 316 low / 8.45E+39 -7.27 6577.0 / !(dd)	6.50E+12	0	2000	!Wagner
AC3H4+H(+M)=AC3H5(+M) !Tsang 1992 317 low / 5.56E+33 -5.0 4448.0 / !(ee)	1.20E+11	0.69	3007	
AC3H4+H(+M)=SC3H5(+M) 1972 318 low / 1.11E+34 -5.0 4448.0 / !(ee)	8.49E+12	0	2000	!Wagner
H2CCCH+H=C3H2+H2 !Miller 1992 321	5.00E+13	0	3000	
H2CCCH+CH3=C4H6-12 !Wu 1987 323	5.00E+12	0	0	
H2CCCH+CH3=C4H6-1 !Wu 1987 324	5.00E+12	0	0	
!H2CCCH+CH=C4H3+H !Miller 1992 325	7.00E+13	0	0	
!H2CCCH+CH=C4H3-123+H !Miller 1992 326	7.00E+13	0	0	
C4H10=PC4H9+H !Pitz 1991 343	1.00E+14	0	100000	
C4H10=SC4H9+H !Pitz 1991 344	1.00E+14	0	100000	
C4H10+AC3H5=PC4H9+C3H6 !Pitz 1991 347	7.94E+11	0	20500	
C4H10+AC3H5=SC4H9+C3H6 !Pitz 1991 348	3.16E+11	0	16400	
C4H10+CH3=PC4H9+CH4 !349	5.00E+11	0	13600	
C4H10+CH3=SC4H9+CH4 !350	4.30E+11	0	10500	
C4H10+H=PC4H9+H2 !351	2.84E+05	2.54	6050	
C4H10+H=SC4H9+H2 !352	5.68E+05	2.4	3765	

SC4H9=C4H8-1+H !Pitz 1991 359	2.00E+13	0	40400
SC4H9=C4H8-2+H !Pitz 1991 360	5.01E+12	0	37900
PC4H9(+M)=C2H5+C2H4(+M) !361	1.06E+13	0	27828
low / 1.897e55 -11.91 32263./ H2/2.0/			
!PC4H9=C2H5+C2H4 !Pitz 1991 362	2.50E+13	0	28800
PC4H9=C4H8-1+H !Pitz 1991 363	1.26E+13	0	38600
C4H8-1=C2H3+C2H5 !Pitz 1991 364	1.00E+19	-1	96770
!C4H8-1=H+C4H7 !Pitz 1991 365	4.11E+18	-1	97350
C4H8-1+CH3=C4H7+CH4 !Pitz 1991 366	1.00E+11	0	7300
C4H8-1+H=C4H7+H2 !Pitz 1991 367	5.00E+13	0	3900
C4H8-1+AC3H5=C4H7+C3H6 !Pitz 1991 371	7.90E+10	0	12400
!C4H8-2=H+C4H7 !Pitz 1991 373	4.11E+18	-1	97350
C4H8-2+CH3=C4H7+CH4 !Pitz 1991 374	1.00E+11	0	8200
C4H8-2+H=C4H7+H2 !Pitz 1991 375	5.00E+13	0	3800
C4H7=C4H6-13+H !Pitz 1991 381	1.00E+14	0	55000
C4H7+CH3=C4H6-13+CH4 !Pitz 1991 383	8.00E+12	0	0
C4H7+AC3H5=C3H6+C4H6-13 !Pitz 1991 384	6.31E+12	0	0
C4H7+H=C4H6-13+H2 !Pitz 1991 386	3.16E+13	0	0
C4H6-13+H=C4H5-N+H2 !Miller 1992 391	3.00E+07	2	13000
C4H6-13+H=C4H5-I+H2 !Miller 1992 392	3.00E+07	2	6000
C4H6-1+H=C2H5+C2H2 !(jj) 394	1.00E+14	0	3000
C4H6-12+H=C4H5-I+H2 !(q) 398	5.00E+07	2	5000
!C4H6-12+H=C4H5-1MA+H2 !(ll) 399	1.50E+07	2	6000
!C4H6-12+H=C4H5-3MA+H2 !(ll) 400	3.00E+07	2	6500

C4H6-12+H=CH3+AC3H4 !(r) 401	2.00E+13	0	2000	
!C4H5-3MA+H=CH3+H2CCCH 1996 402	1.00E+14	0	0	!Marinov
C4H5-I+H=CH3+H2CCCH !(nn) 405	1.00E+14	0	0	
!C4H5-I+H=C4H5-1MA+H !(nn) 406	3.00E+13	0	0	
!C4H5-1MA+H=CH3+H2CCCH 1996 407	1.00E+14	0	0	!Marinov
!C4H5-1MA+H=C4H4-123+H2 !(mm) 409	1.00E+14	0	8000	
C4H5-N+H=C4H5-I+H !411	1.00E+14	0	0	
C4H5-N+H=C4H4+H2 !Miller 1992 413	3.00E+07	2	1000	
!C4H5-3MA(+M)=C4H4+H(+M) !(pp) 414	1.00E+13	0	49000	
!low / 2.00E+14 0.0 41000.0 / !(pp)				
!(+M)=C4H4-123+H(+M) !415	1.00E+13	0	56000	
!low / 2.00E14 0.0 48000.0/ C4H5-I(+M)=C4H4+H(+M) !Miller 1992 416	1.00E+14	0	50000	
low / 2.00E+15 0.0 42000.0 / !Miller 1992				
!C4H4-123+H=C4H3-123+H2 !(ss) 421	3.00E+07	2	6000	
!C4H4+H=C4H3+H2 !Miller 1992 423	2.00E+07	2	15000	
!C4H3+H=C4H3-123+H !Miller 1992 426	1.00E+14	0	0	
!C4H3-123+H=C4H2+H2 !Miller 1992 432	5.00E+13	0	0	
!C4H3-123+CH2=AC3H4+C2H !Miller 1992 433	2.00E+13	0	0	
!C4H3-123(+M)=C4H2+H(+M) !Miller 1992 434	1.00E+14	0	55000	
!low / 2.00E+15 0.0 48000.0 / !Miller 1992				
!C4H3(+M)=C4H2+H(+M) !Miller 1992 435	1.00E+14	0	36000	
!low / 1.00E+14 0.0 30000.0 / !Miller 1992				
!C4H2+CH2=C5H3+H !Miller 1992 435	1.30E+13	0	4326	

!C4H2+CH=C5H2+H !Miller 1992 436	1.00E+14	0	0	
!C4H2+CH2-S=C5H3+H !Miller 1992 437	3.00E+13	0	0	
!C4H2+C2H=C6H2+H 1996 438	9.60E+13	0	0	!Marinov
! *****ebg mechanism *****				
C6H6+H=C6H5+H2 1971	3.98E+14	0	7190	!Asaba,
C5H5+H=C5H6 !EBG, 1992 458	1.00E+14	0	0	
C5H6+H=C5H5+H2 !EBG, 1992 465	2.19E+08	1.8	3000	
C5H6+C2H3=C5H5+C2H4 !EBG, 1992 467	6.00E+12	0	0	
C5H6+C4H5-N=C5H5+C4H6-13 !EBG, 1992 468	6.00E+12	0	0	
H+C6H5CH2=C6H5CH3 !Harding and Klippenstein 2007 Fit 1027-1897 K	7.23E+13	0.062	-44	
REV/ 1.524E+16 -0.04 93499/ Marina 51.5 Rev Fitted 1027-1897 K				!Benzyl
CH3+C6H5=C6H5CH3 !Harding and Klippenstein 2007 Fit 1027-1897 K	2.22E+14	-0.283	-191	
REV/ 4.621E+25 -2.53 104483/ Hf298K for C6H5 78.00 Fitted 1027-1897 K				!Phenyl
CH3+C6H5CH3=CH4+C6H5CH2 !Estimated	4.00e-05	5.61504	9000	
C6H5+C6H5CH3=C6H6+C6H5CH2 1996	7.94E+13	0	11935	!Hippler,
C6H5CH2+C6H5CH2=BIBENZYL !EBG, 1992 526	2.51E+11	0.4	0	
C6H5C2H5=C6H5CH2+CH3 IJCK, 1986	8.91E+15	0	74720	!Kiefer,
C6H5C2H5+H=C6H5CHCH3+H2 !Baulch, 2005	265.012	3.44	1004	
C4H5-I=C4H5-N !L&L, 1995 573	2.00E+13	0	53500	
C5H6+C4H5-I=C5H5+C4H6-13 !est from EBG #26 578	6.00E+12	0	0	
C4H5-I+C6H5CH3=C4H6-13+C6H5CH2 !est from EBG #14 579	6.00E+12	0	0	
C6H5CH2=C4H4+H2CCCH !Colket and Seery, 1994 Symp. Int. Comb	2.00E+14	0	83600	
C6H5CH2=C2H2+C5H5 !Colket and Seery, 1994 Symp. Int. Comb.	6.03E+13	0	70000	
!H2CCCH+H2CCCH=C6H6 !Fernandes et al., Proc. Combust. Inst. 2005	1.00E+13	0	0	

!n-C4H3+C2H3=C6H6	2.87E+14	0	817	
!Dagaut et al., 2002, Phys. Chem. Chem. Phys.				
C5H5=C2H2+H2CCCH	6.31E+13	-0.075	62300	!Tarnter
et al., 1998 Symp. Int. Comb				
!C6H5(+M)=C6H4+H(+M)	4.30E+12	0.62	77300	
!Wang, 28th				
!!low / 1.00E+84 -18.87 90100.0 /				
!Wang 1992				
!troe / 0.902 696.0 358.0 3856.0 /				
!C4H2+C2H2=C6H4	1.40E+07	1.45	25410	
!Wang, 28th				
!C6H5=LC6H5	1.000E+15	0.000	67000.00	
!LL, 1996				
C6H6+C6H5=C12H10+H	3.16E+12	0	8510	
!Fahr and Stein, 1989				
!C6H5+C6H5=C12H10	2.00E+19	-2.1	2900	
!WAng and Frenklach, 1997				
!PhenylAcetylene Reactions				
C6H5+C2H2=C8H6+H	1.00E+13	0	7648.2	
!Heckmann 1996				
C6H5+C2H2=C6H5CHCH	2.69E+06	2.05	3720	
!Lin, JACS, 2003				
C6H5+C2H2=C6H5CCH2	2.04E+10	0.70	27500	
!Lin, JACS, 2003				
C8H6+H=C6H4C2H+H2	3.23E+07	2.095	15842	!
From Howard 2004 [Mebel et al. 1997, for C6H6+H]				
C8H6+CH3=C6H4C2H+CH4	1.67E+12	0.0	15057	!
From Howard 2004 [Marinov et al. 1996]				
C6H4C2H+H=C8H6	8.02E+19	-2.011	1968	!
From Howard 2004 [c6h5+h=c6h6]				
C6H5CHCH+H=C8H6+H2	9.57E14	-0.25	720	!
[QRRK-HR, 1 atm]				
C6H5+C2H=C8H6	2.54E17	-1.489	1541	!
[Zhang and McKinnon 1995]				
C6H5CHCH=>C8H6+H	3.80E+11	0.82	38910	
!Lin, JACS, 2003				
C6H5CCH2=>C8H6+H	1.23E+13	0.55	42580	
!Lin, JACS, 2003				
C6H5CHCH=>C6H5CCH2	4.90E+12	0.45	45740	
!Lin, JACS, 2003				
C6H5CCH2=>C6H5CHCH	6.61E+13	0.14	53120	
!Lin, JACS, 2003				
!Styrene Reactions				
C6H5+C2H4=C6H5C2H3+H	1.50E+45	-8.65	42422	
!Lin JPC 2004, 100 atm 1000-2500K Rate				
C6H5+C2H4=C6H6+C2H3	9.44E-03	4.47	4470	
!Lin, JPC, 2004				

C6H5+C2H4=C6H5CH2CH2 !Lin ,JPC, 2004	4.04E+03	2.64	1459	
C6H5CH2CH2=C6H5C2H3+H !Lin, JPC, 2004	3.79E+06	1.991	32106	
C6H5CH2CH2=C6H5CHCH3 !Lin, JPC, 2004	5.95E+05	2.074	29582	
C6H5CHCH3=C6H5C2H3+H !Lin, JPC, 2004	3.74E+08	1.550	44609	
C4H4+C4H4=C6H5C2H3 !Lundgard and Heicklen, IJCK 1984	1.50E+14	0.00	38000	
C6H5CHCH+H=C6H5C2H3 [QRRK-HR, 1 atm]	1.54E13	-0.99	-6880	!
C6H5C2H3+H=C6H5CHCH+H2 [Knyazev et al. 1996a for C2H4+H]	5.07E07	1.93	12951	!
!Ethylbenzene Reactions				
C6H5+C2H6=C6H6+C2H5 !Lin, IJCK 2001	2.09E+11	0	4440	
C6H5C2H5+H=C6H5CH2CH2+H2 2005	234.897	1.90	6637	!Baulch,
C6H5C2H5+H=C6H6+C2H5 2005	5.78e+13	0	8088	!Baulch,
C6H5C2H5+C6H5CH2=C6H5CH3+C6H5CHCH3 to Toluene 492, Hippler, 1996	7.94E+13	0	11935	!Similar
C6H5C2H5=>C6H5CHCH3+H Markgraf and Troe, JPC, 1988	2.51E+15	0.00	81262	!Muller-
C6H5CHCH3+H=>C6H5C2H5 !calculated using CHEMREV	1.17E+14	-2.117	-5290	
!S. Gail, P. Dagaut, Combust. Sci. Technol. 179 (2007) 813-844.				
HOC6H4CH3+ H= C6H5OH +CH3 !arbitraire,Dagaut MXYLENE model	1.150E+13	0.0	8500.0	
!R. Sivaramakrishnan, A. Comandini, R. S. Tranter, K. Brezinsky, S. G. Davis, H. Wang, Proc. Combust. Inst. 31 (2007) 429-437.				
H+H+H2 = H2+H2 H2CO Mech 2007	9.000E+16	-0.600	0.00	!GRI3.0,
H+H+M = H2+M * 1.78, H2CO Mech 2007	1.780E+18	-1.000	0.00	!GRI3.0
H2/0.0/ H2O/0.0/ CO2/0.0/ AR/0.63/HE/0.63/				
H2O2+OH = HO2+H2O !95HIP/NEU H2CO Mech 2007	2.000E+12	0.000	427.00	
DUPLICATE				
H2O2+OH = HO2+H2O !Refit95HIP/NEU H2CO Mech 2007	2.670E+41	-7.000	37600.00	
DUPLICATE				
!2.2E14 MAX K				
H2O2+O = OH+HO2 !86TSA/HAM H2CO Mech 2007	9.630E+06	2.000	3970.00	
H2O2+H = OH+H2O !86TSA/HAM H2CO Mech 2007	2.410E+13	0.000	3970.00	

H2O2+H = HO2+H2	6.050E+06	2.000	5200.00	
!GRI3.0 * 0.50 H2CO Mech 2007				
HO2+OH = O2+H2O	1.410E+18	-1.760	59.61	
!Term 1, This Work H2CO Mech 2007				
DUPLICATE				
HO2+OH = O2+H2O	1.120E+85	-22.300	26900.00	
!Term 2, This Work H2CO Mech 2007				
DUPLICATE				
HO2+OH = O2+H2O	5.370E+70	-16.720	32900.75	
!Term 3, This Work H2CO Mech 2007				
DUPLICATE				
HO2+OH = O2+H2O	1.000E+136	-40.000	34800.30	
!Term 4, This Work H2CO Mech 2007				
DUPLICATE				
HO2+OH = O2+H2O	2.510E+12	2.000	40000.30	
!Term 5, This Work H2CO Mech 2007				
DUPLICATE				
HO2+O = OH+O2	4.000E+13	0.000	0.00	!GRI3.0 *
2.00 H2CO Mech 2007				
HO2+H = O+H2O	3.970E+12	0.000	671.00	
!GRI3.0				
HO2+H = OH+OH	7.485E+13	0.000	295.00	
!99MUE/KIM * 1.06				
!HO2+H=OH+OH	1.69E+14	0	875	!Baulch
!HO2+H = O+H2O	3.970E+12	0.000	671.00	!GRI3.0
H2CO Mech 2007				
OH+OH(+M) = H2O2(+M)	1.110E+14	-0.370	0.00	
!88ZEL/EWI * 1.50 H2CO Mech 2007				
LOW / 2.010E+17 -0.584 -2293.00/				
!Fit 88ZEL/EWI and 92BAU/COBH2CO Mech 2007				
TROE/ 0.7346 94.00 1756.00 5182.00 /				
!H2O=6xN2 88ZEL/EWIH2CO Mech 2007				
H2/2.0/ H2O/6.00/ CO/1.75/ CO2/3.6/ AR/0.7/ HE/0.7/				
H2+O2 = HO2+H	5.916E+05	2.433	53502.00	
!00MIC/SUT * 0.80, H2CO Mech 2007				
O+H+M = OH+M	9.428E+18	-1.000	0.00	
!86TSA/HAM * 2.00 H2CO Mech 2007				
H2/2.0/ H2O/12.0/ CO/1.75/ CO2/3.6/ AR/0.7/ HE/0.7/				
O+H2 = H+OH	4.589E+04	2.700	6260.00	
!GRI3.0 * 1.19, H2CO Mech 2007				
OH+H2 = H+H2O	1.081E+08	1.510	3430.00	
!GRI3.0 * 0.50 H2CO mech 2007				
OH+OH = O+H2O	3.973E+04	2.400	-2110.00	
!GRI3.0 * 1.11, H2CO mech 2007				
H+O2 = O+OH	2.644E+16	-0.6707	17041.00	
!GRI3.0 * 1.00, H2CO mech 2007				
H+O2(+M) = HO2(+M)	5.116E+12	0.440	0.00	!00TROE
- Based on M=N2 * 1.10, H2CO mech 2007				

LOW/6.328E+19 -1.400 0.00/
 TROE/0.5 1E-30 1E+30/
 O2/0.85/ H2O/11.89/ CO/1.09/ CO2/2.18/ AR/0.40/ HE/0.46/ H2/0.75/
 H2O/0.0/ H2/0.0/ N2/0.0/ CH4/10.0/ CO2/3.8/ CO/1.9/
 H+H+H2O = H2+H2O 5.624E+19 -1.250 0.00 !GRI3.0
 * 0.94, H2CO Mech 2007
 H+OH+M = H2O+M 4.400E+22 -2.000 0.00 !GRI3.0 *
 2.00, H2CO May 07
 H2/2.0/ H2O/6.30/ CO/1.75/ CO2/3.6/ AR/0.38/ HE/0.38/
 O+O+M = O2+M 1.200E+17 -1.000 0.00 !GRI3.0,
 H2CO May 07
 H2/2.4/ H2O/15.4/ CO/1.75/ CO2/3.6/ AR/0.83/ HE/0.83/
 HO2+HO2 = O2+H2O2 1.300E+11 0.000 -1630.00
 !90HIP/TRO H2CO May 07
 DUPLICATE
 HO2+HO2 = O2+H2O2 3.658E+14 0.000 12000.00
 !90HIP/TRO * 0.87 H2CO May 07
 DUPLICATE
 HCO+M = CO+H+M 1.870E+17 -1.000 17000.00
 !02FRI/DAV * 2.00 H2CO May 07
 H2/2.0/ H2O/0.0/ CO/1.75/ CO2/3.6/
 HCO+H2O => CO+H+H2O 2.244E+18 -1.000 17000.00
 !12xM * 2.00 H2CO May 2007
 CO+HO2=CO2+OH 1.51E+14 0 23647
 !1986TSA/HAM1087
 CO+O2 = CO2+O 1.119E+12 0.000 47700.00
 !86TSA/HAM * 0.44 H2CO May 2007
 CO+O(+M)=CO2(+M) 1.362E+10 0.000 2384.00
 !99MUE/KIM * 0.76 H2CO Mech 2007
 LOW/1.173E+24 -2.79 4191./
 H2/2.0/ H2O/12/ CO/1.75/ CO2/3.6/ AR/0.7/ HE/0.7/
 HCO+O = CO+OH 3.000E+13 0.000 0.00 !GRI3.0
 H2CO May 2007
 HCO+O = CO2+H 3.000E+13 0.000 0.00 !GRI3.0
 H2CO May 2007
 H+H+CO2 = H2+CO2 5.500E+20 -2.000 0.00 !GRI3.0,
 H2CO May 2007
 HCO+H = CO+H2 1.200E+14 0.000 0.00
 !02FRI/DAV * 1.00, H2CO May 07
 HCO+OH = CO+H2O 3.020E+13 0.000 0.00
 !86TSA/HAM, H2CO May 07
 CO+OH=CO2+H 8.000E+11 0.140 7352.00
 !This Work * 0.83
 DUP
 CO+OH=CO2+H 8.784E+10 0.030 -16.00 !
 * 1.20
 DUP
 !SERDP PAH MODEL version 0.1, Jun 2007 model

OC6H4CH3 + H (+M) = HOC6H4CH3 (+M)	1.000E+14	0.000	0.00	!
Estimated (C6H5O + H -> C6H5OH) / 2.5				
LOW / 4.000E+93 -21.840 13880.0 / ! 96-DAV-WAN, 97-WAN-FRE				
TROE / 0.043 304.2 60000. 5896.4 /				
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/				
C6H5 + H (+M) = C6H6 (+M)	1.000E+14	0.000	0.00	!SERDP
2007				
LOW / 6.600E+75 -16.300 7000.00 /! (HW, RRKM)				
TROE / 1.0 0.1 584.9 6113. /				
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/				
!C6H6=C6H5+H	2.00E+17	0	118069	
!Kiefer 1985				
C6H5 (+M) = o-C6H4 + H (+M)	4.300E+12	0.616	77313	!
RRKM 00-HAI-FRE				
LOW/ 1.000E+84 -18.866 90064 /				
TROE/ 0.902, 696., 358., 3856. /				
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/				
!C6H5 + H = o-C6H4 + H2	2.000E+11	1.100	24500.00	!
01-MEB-LIN 1 atm				
n-C4H3 + C2H2 = o-C6H4 + H	3.10E+49	-10.59	37700.	!
7600 Torr RRKM				
!l-C6H4 + H = C6H5	1.700E+78	-19.720	31400.00	!
1 atm				
!l-C6H4 + H = o-C6H4+ H	1.400E+54	-11.700	34500.00	!
1 atm				
!l-C6H4 + H = C6H3 + H2	1.330E+06	2.530	9240.00	!
= C4H4+H				
!l-C6H4 + OH = C6H3 + H2O	3.100E+06	2.000	430.00	!
see notes				
C4H2 + C2H2 = o-C6H4	5.00E+78	-19.31	67920.	! 5
atm				
o-C6H4 + OH = CO + C5H5	1.00E+13	0.00	0.	!
Estimated				
o-C6H4 + C2H2 = C8H6	2.00E+13	0.00	20000.	!
Wang				
o-C6H4 + C2H4 = C6H5C2H3	2.00E+13	0.00	10000.	!
Estimated HW Est				
C6H5 + H = o-C6H4 + H2	2.000E+11	1.100	24500.00	!
01-MEB-LIN 1 atm				
C6H3 + O2 => CO + C3H2 + HCCO	5.00E+11	0.0	0.	
C4H2+C2H = C6H3	4.50E+37	-7.68	7100.	
!97WAN/FRE				
C6H2+H = C6H3	1.10E+30	-4.92	10800.0	
!97WAN/FRE				
C6H3+H = C4H2+C2H2	2.80E+23	-2.55	10780.0	
!97WAN/FRE				
!C6H3+H = l-C6H4	3.40E+43	-9.01	12120.0	
!97WAN/FRE				

C6H3+H = C6H2+H2 !97WAN/FRE	3.00E+13	0.00	0.0	
C6H3+OH = C6H2+H2O !97WAN/FRE	4.00E+12	0.00	0.0	
!A. Burcat, M. Dvinyaninov, E. Olchanski, Int. J. Chem. Kinet, 33 (2001), 491-508				
C5H6+CH3=C5H5+CH4 0		6.00E+13		0
C5H6+AC3H5=C5H5+C3H6	6.00E+12	0	0	
C5H5O=C4H5-N+CO !EBG, 1992 470, Burcat cpd	2.51E+11	0	45900	
C5H6+H2CCCH=C5H5+PC3H4 !Burcat cpd, 2001	6.00E+12	0	0	
C5H5+O2=C5H4O+OH !Burcat cpd	4.80E+12	0	12000	
C5H6+O2=C5H5+HO2 !EBG, 1992 462, Burcat	4.00E+13	0	30000	
!C5H5+O=C5H4O+H !bURCAT CPD	5.00E+14	0	0	
C5H5+HO2=C5H5O+OH !EBG, 1992 460, Burcat cpd	1.50E+13	0	0	
C5H5+OH=C5H4OH+H !EBG, 1992 461, Burcat	1.00E+13	0	0	
!C5H5+O=C5H5O !Burcat cpd	1.00E+4	0	0	
!C6H5+O2=C6H5O+O !bURCAT CPD	2.09E+12	0	7470	
C2H3+O2=CH2O+HCO !Burcat	3.98E+13	0	-240	
!A. Lifshitz, C. Tamburu, A. Suslensky, F. Dubnikova, Proc. Combust. Inst. 30 (2005) 1039-1047.				
C5H4-1CH3=C5H5-1CH2	3.00E+12	0	50400	
C5H5-1CH3=>C5H5-1CH2+H	4.50E+15	0	94000	
C5H5-1CH3=>C5H4-1CH3+H	1.50E+15	0	68000	
C5H5-1CH3+H=C5H6+CH3	1.00E+14	0	8000	
C5H5-1CH3+H=C5H5-1CH2+H2	1.00E+14	0	10000	
C5H5-1CH3+H=C5H4-1CH3+H2	1.00E+14	0	10000	
C5H5-1CH3+CH3=C5H5-1CH2+CH4	5.00E+12	0	11500	
C5H5-1CH3+CH3=C5H4-1CH3+CH4	5.00E+12	0	11500	
C5H5-1CH2=n-C6H7	8.00E+13	0	27000	
C5H4-1CH3=n-C6H7	8.00E+13	0	50000	
n-C6H7=C2H2+C4H5-N	3.16E+13	0	43100	
C5H5-1CH2=c-C6H7	1.40E+13	0	17400	
c-C6H7=C6H6+H	7.45E+13	0	28500	
c-C6H7=C4H5-N+C2H2	2.00E+15	0	92000	
C5H5-1CH2+H=>C5H5-1CH3 !Estimated at 298.15K, Lifshitz 2005	4.29E+08	0	-1300	
C5H4-1CH3+H=>C5H5-1CH3 !Estimated at 298.15K, Lifshitz 2005	5.23E+07	0	-4800	
!Dean J. Phys. Chem. Vol 89, 1985				

n-C6H7=PC3H4+H2CCCH !Dean	1.26E+15	0	59417	
!R.S. Tranter, A. Raman, R. Sivaramakrishnan, K. Brezinsky, Int. J. Chem. Kinet. 37 (2005) 306-331.				
C2H6 + OH = C2H5 + H2O oxdn Tranter 2004	14.46E+06	2	864	!Ethane
C2H4OH = CH2O + CH3 oxdn Tranter 2004	1.00E+15	0	21606	!Ethane
C2H4=C2H2 + H2 oxdn 2004	6.00E12	0.44	86770	!Ethane
H+C2H2=C2H3 oxdn 2004	2.66e+08	1.75	2420	!Ethane
C2H4OH = CH3CHO + H oxdn 2004 Tranter	2.51E+14	0	23399	!Ethane
C2H4 + OH = C2H4OH oxdn 2004 Tranter	6.03E12	0	0	!Ethane
C2H4+OH=C2H3+H2O oxdn 2004 Tranter	3.02E+13	0	5955	!Ethane
HO2+C2H2=CH2HCO+O oxdn Tranter 2004	3.0E+12	0	10000	!Ethane
HO2+C2H2=CH2O+HCO oxdn Tranter 2004	3.0E+12	0	10000	!Ethane
C6H5CH3+O2=C6H5CH2+HO2 !Oehslager 2006(adjusted within error limits +20%)	2.615E+07	2.5	44946	
!C. A. Taatjes, D. L. Osborn, T. M. Selby, G. Meloni, A. J. Trevitt, E. Epifanovsky, A. I. Krylov, B. Sirjean, E. Dames, H. Wang, J. Phys. Chem. A. 114 (2010) 3355-3370.				
C6H6+O=C6H5O+H	3.55E+10	0.91	6323	
C6H6+O=C6H5OH DUP	5.84E+35	-5.89	34534	
C6H6+O=C6H5OH DUP	2.53E+13	0	6565	
C6H6+O=C5H6+CO DUP	1.56E+31	-4.73	33568	
C6H6+O=C5H6+CO DUP	4.83E+03	0	14929	
!B. Eiteneer, M. Frenklach, Int. J. Chem. Kinet, 35(2003) 391-414				
C2H2+C2H=C4H2+H	1.77E+13	0.2	85	
C2H2+C2H=n-C4H3	4.50E+37	-7.7	7100	
C2H2+C2H=i-C4H3	2.60E+44	-9.5	14650	
C2H2+C2H2=C4H4	1.51E+05	0	5500	
C2H2+C2H2=C4H2+H2	6.31E+13	0	42700	
C2H2+C2H3=C4H4+H	2.00E+18	-1.7	10600	
C2H4+C2H=C4H4+H	1.20E+13	0	0	
C4H+O=C2H+C2O	5.00E+13	0	0	
C4H+O2=HCCO+C2O	5.00E+13	0	1500	
C4H+H2=H+C4H2	4.90E+05	2.5	560	
C4H2+O=C3H2+CO	2.70E+13	0	1720	

C4H2+OH=H2C4O+H	6.60E+12	0	-410
C4H2+OH=C4H+H2O	3.37E+07	2.0	14000
H2C4O+H=C2H2+HCCO	5.00E+13	0	3000
H2C4O+OH=CH2CO+HCCO	1.00E+07	2.0	2000
H2C4O+O=CH2CO+C2O	2.00E+07	1.9	200
n-C4H3=i-C4H3	4.10E+43	-9.5	53000
n-C4H3+H=i-C4H3+H	2.50E+20	-1.7	10800
n-C4H3+H=C2H2+C2H2	6.30E+25	-3.3	10014
i-C4H3+H=C2H2+C2H2	2.80E+23	-2.5	10780
n-C4H3+H=C4H4	2.00E+47	-10.3	13070
i-C4H3+H=C4H4	3.40E+43	-9.0	12120
n-C4H3+H=C4H2+H2	3.00E+13	0	0
i-C4H3+H=C4H2+H2	6.00E+13	0	0
n-C4H3+OH=C4H2+H2O	2.00E+12	0	0
i-C4H3+OH=C4H2+H2O	4.00E+12	0	0
i-C4H3+O2=HCCO+CH2CO	7.86E+16	-1.8	0
C4H4+H=n-C4H3+H2	6.65E+05	2.5	12240
C4H4+H=i-C4H3+H2	3.33E+05	2.5	9240
C4H4+OH=n-C4H3+H2O	3.10E+07	2.0	3430
C4H4+OH=i-C4H3+H2O	1.55E+07	2.0	430
C4H4+CH3=n-C4H3+CH4	3.98E+11	0	4972
C4H4+CH3=i-C4H3+CH4	3.98E+11	0	4972
C4H4+C2H=n-C4H3+C2H2	3.90E+13	0	0
C4H4+C2H=i-C4H3+C2H2	3.90E+13	0	0
!S. Klippenstein, J. A. Miller, J. Phys. Chem. A., 109 (2005) 4285-4295			
C4H2+H=n-C4H3	8.13E+09	1.305	5018
!Kinf			
C4H2+H=i-C4H3	4.31E+10	1.119	1672
!Kinf			
C4H2+OH=C4H+H2O	9.15E+09	1.03	10944
!Y. Hidaka, Y. Henmi, T. Ohonishi, T. Okuno, T. Koike, Combust. Flame, 130 (2002) 62-82			
C4H2+C2H=C6H2+H	1.20E+14	0	0
C4H+C2H2=C6H2+H	4.00E+13	0	0
C4H4=C2H2+C2H2	3.16E+13	0	77100
!Murakami et al. J. Phys. Chem. A Vol 111 No. 50 2007			
!fit between 10 atm and high pressure limit values between 700 and 1500 K			
C6H5CH2+O2=>C6H5CH2OO	1.75E+09	-0.02	-7700
C6H5CH2OO=>C6H5CH2+O2	6.87E+11	0	17341
C6H5CH2OO=C6H5O+CH2O	1.56E+07	0	33817
C6H5CH2OO=C6H5CHO+OH	1.65E+09	0	29040
!J.C.G. Andrae, T. Brinck, G.T. Kalghatgi, Comb. and Flame 155(2008) 696-712			
C6H5OH+O2=C6H5O+HO2	8.00E+12	0	40000
!Baulch 2005 J. Phys. Chem. Ref. Data			
C6H5C2H5+OH=C6H5CH2CH2+H2O	4.80E+12	0	0
C6H5C2H5+HO2=C6H5CHCH3+H2O2	2.65E+11	0	11286
C6H5C2H5+HO2=C6H5CH2CH2+H2O2	3.19E+12	0	19393
C6H5C2H5+O=C6H5CHCH3+OH	2.23E+13	0	3795

!S.S. vasu, D. F. Davidson and R.K. Hanson, Journal of propulsion and power, 26(4) 2010

C6H5CH2+C6H5CHO=C6H5CH3+C6H5CO	2.18E+07	2.5	46045
C6H5CH3+OH=C6H5CH2+H2O	1.81E+05	2.39	-602
C6H5CH3+H=C6H5CH2+H2	6.47	3.98	3384
C6H5CH3+H=C6H6+CH3	3.90E+08	1.25	2371

!Y. Sakai et al. / Proceedings of the Combustion Institute 32 (2009) 411–418

C6H5CH3+C6H5O=C6H5CH2+C6H5OH	5.431E+12	0	10530
REV/	2.52E+14	-0.6597	7168.6/
C6H5CH3+HCO=C6H5CH2+CH2O	3.771E+13	0	11972
REV/	3.61E+15	-0.5863	11846.5/

!K. Narayanaswamy, G. Blanquart, H. Pitsch, Comb and Flame, Vol 157, Issue 10, Oct 2010, 1879-1898

C6H4CH3+O=OC6H4CH3	1.000e+14	0.000	0.00
REV/	8.59E+19	-1.15	128503/
C6H4CH3+OH=OC6H4CH3+H	3.000e+13	0.000	0.00
REV/	1.96E+20	-1.47	26514.9/
C6H4CH3+HO2=OC6H4CH3+OH	3.000e+13	0.000	0.00
REV/	1.28E+17	-0.86	63046.9/
C6H4CH3+O2=OC6H4CH3+O	8.570e+20	-2.270	7189.29
REV/	2.21E+25	-3.39	16944.7/
C6H4CH3+O2=>C5H4CH2+CO2+H	2.550E+13	-0.440	-1649.14
C6H4CH3+O2=>PC3H4+C2H3+2CO	2.550E+13	-0.440	-1649.14
H2CCCH+H2CCCH=C5H4CH2	8.250E+46	-10.100	16959.85
REV/	3.29E+57	-11.3125	126589.3/
H2CCCH+H2CCCH=C6H6	1.070E+45	-9.570	17014.82
REV/	7.76E+55	-10.3921	160396/
H2CCCH+H2CCCH=C6H5+H	5.770E+37	-7.000	31505.74
REV/	1.27E+46	-7.7974	61605/

!J. P. Senosiain and J. A. Miller, J. Phys. Chem. A 2007, 111, 3740-3747

!10 atm, fit 500-2500 K

!C4H5-N+C2H2=C6H6+H	1.69E+16	-1.03	8967
!C4H5-N+C2H2=C5H4CH2+H	1.74E+19	-1.86	12383
C4H5-N+C2H2=C6H6+H	8.25E+24	-3.76	26562
C4H5-N+C2H2=C5H4CH2+H	9.70E+25	-3.76	10733

!J. A. Miller and S. J. Klippenstein

!10 atm, 1100-2000 K

C5H4CH2=C6H6	2.95E+31	-4.97	175780
REV/	2.636E+45	-8.5096	130754.6/
C5H4CH2=C6H5+H	8.51E+24	-2.505	225187
REV/	1.233E+66	-14.2349	63046.4/

!Fahr et al. J. Phys. Chem. A 1999, 103, 8433-8439

C2H3+CH3=AC3H5+H	3.61E+13	0	0
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!JetSurF version 1.0 - A Jet Surrogate Fuel Model - September 2009

NC3H7+CH3(+M) = C4H10(+M)	1.93E+14	-0.32	0.0 !
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LOW / 2.68E+61 -13.24 6000.0 /

TROE / 1.000 1000.0 1433.9 5328.8 /

H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/

!

! kinf: -0.5 T power = CH3+C2H5, kinf(300K) = TS1 recommendation
! ko: scaled such that Pr(C2H5+C2H5) = Pr(CH3+C2H5) at (T,P), 500 cm-1
! Fc: assumed equal to Fc(CH3+C2H5)

!
C2H5+C2H5(+M) = C4H10(+M) 1.88E+14 -0.50 0.0 !
LOW / 2.61E+61 -13.42 6000.0 /
TROE / 1.000 1000.0 1433.9 5328.8 /
H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/
!n-C4H3+C2H3=C6H6 2.87E+14 0 817 !Dagaut et
al., 2002, Phys. Chem. Chem. Phys.
!R. S. Tranter et al. J. Phys. Chem. A, Vol. 114, No. 32, 2010
C6H5+C6H5=C12H10 1.11E+14 -0.405 -610
PLOG/10 1.11E+14 -0.405 -610/
PLOG/100 3.09E+12 0.036 -1703/
!Grimech 3.0
OH+CH3(+M)<=>CH3OH(+M) 2.790E+18 -1.430 1330.00
LOW / 4.000E+36 -5.920 3140.00/
TROE/ .4120 195.0 5900.00 6394.00/
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH2-S+H2O(+M)<=>CH3OH(+M) 4.820E+17 -1.160 1145.00
LOW / 1.880E+38 -6.360 5040.00/
TROE/ .6027 208.00 3922.00 10180.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH2OH(+M)<=>CH3OH(+M) 1.055E+12 .500 86.00
LOW / 4.360E+31 -4.650 5080.00/
TROE/ .600 100.00 90000.0 10000.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH3O(+M)<=>CH3OH(+M) 2.430E+12 .515 50.00
LOW / 4.660E+41 -7.440 14080.0/
TROE/ .700 100.00 90000.0 10000.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH2O(+M)<=>CH2OH(+M) 5.400E+11 .454 3600.00
LOW / 1.270E+32 -4.820 6530.00/
TROE/ .7187 103.00 1291.00 4160.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+HCO(+M)<=>CH2O(+M) 1.090E+12 .480 -260.00
LOW / 2.470E+24 -2.570 425.00/
TROE/ .7824 271.00 2755.00 6570.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
C2H2+O = HCCO+H 1.350E+07 2.00 1.900E+03
O+C2H2<=>OH+C2H 4.600E+19 -1.410 28950.00
O+C2H2<=>CO+CH2 6.940E+06 2.000 1900.00
!Dooley et al.
!LASKIN ET AL. IJCK 32 589-614 2000
AC3H5+O = CH2CHCHO+H 6.00E+13 0.0 0.0
REV/ 5.47E+16 -0.62 68735.72/

!LASKIN ET AL. IJCK 32 5 89-614 2000

AC3H4+OH = H2CCCH+H2O	5.30E+06	2.0	2000.0
REV/	1.37E+05	2.095	33399/
C5H4CH3CH2=C6H6CH3	1.40E+13	0	17400 !assumed
same as C5H5-1CH2=c-C6H7			
REV/	7.00E+13	0.2611	47396.8/
C6H5CH3+OH=C6H4CH3+H2O	1.758E+13	0	4570
!EBG, 1992 445*(5/6)			
C6H5CH3+HO2=C6H4CH3+H2O2	5.420E+12	0.000	28810.00 !
94-BAULCH			
!MXYLENE+OH=phenyl(CH3)2+H2O	1.41E+13	0	4570
!EBG, 1992 445deg*(4/6)			
!MXYLENE+HO2=phenyl(CH3)2+H2O2	4.34E+12	0.000	28810.00 !
94-BAULCHdeg*(4/5)			
!Zhang and Bozzelli, J. Phys. Chem. A, Vol. 102, No. 20. 1998			
C5H5+O=C5H5O	6.03E+13	0	0
REV/	1.25E+15	0	72500/
C5H5O=C5H4O+H	2.00E+14	0	18680
REV/	4.00E+14	0	2500/
C6H5CH2+O=C6H5CH2O	3.30E+14	0	0
!EBG, 1992 522, overall rate considered			
C6H5CH2+HO2=C6H5CH2OOH	3.70E+37	-16.33	-67470
PLOG/1	3.70E+37	-16.33	-67470/
PLOG/7	8.00E+13	0	0/
C6H5CH2OOH=C6H5CH2O+OH	2.03E+47	-10.27	50710
PLOG/1	2.03E+47	-10.27	50710/
PLOG/7	3.29E+13	0.42	39890/
!HPL rate			
C6H5CH2+HO2=C6H5CH2O+OH	1.19E+09	1.03	-2250
PLOG/1	1.19E+09	1.03	-2250/
!T range 900-1300K			
!PLOG/7	1.24E+10	0	-1433/
!T range >1300K			
PLOG/7	3.86E+10	0	1456/
!HPL rate			
C6H5CH2O=C6H5CHO+H	5.26E+28	-5.081	22250
PLOG/1	5.26E+28	-5.081	22250/
PLOG/10	1.68E+22	-2.901	20760/
PLOG/101	5.07E+08	1.56	16850/
!HPL RATE			
C6H5CH2O=C6H5+CH2O	7.21E+33	-6.210	36850
PLOG/1	7.21E+33	-6.210	36850/
PLOG/10	1.32E+27	-4.009	35070/
PLOG/101	1.09E+14	0.157	31160/
!HPL RATE			
C6H5CH2O=C6H6+HCO	2.37E+32	-6.095	28810
PLOG/1	2.37E+32	-6.095	28810/
PLOG/10	3.82E+31	-5.663	29840/

PLOG/101	1.81E+13	0	22717/	
!HPL RATE				
!MXYLENE Oxidation Model				
MXYLENE=MXYLYL+H	1.95E+16	0	88671	
!Brand et al J.Phys.Chem vol 94 no. 16 1990				
!MXYLYL+H=>MXYLENE	1.50E+14	0	0	
!Brand et al.				
MXYLENE=C6H4CH3+CH3	1.23E+17	0	99068	
!Branching ratio 0.03 to 0.29 from 1100 to 1900K Lange et al J. Phys Chem 1994, 98, 6509-6513				
!Rate constants similar to analogous toluene reactions and adjusted based on number of abstractable H atoms and methyl groups for m-Xylene				
MXYLENE+H=MXYLYL+H2	12.94	3.98	3384	!Hanson
2010, deg*2				
MXYLENE+H=C6H5CH3+CH3	3.90E+08	1.25	2371	!Hanson
2010				
!MXYLENE+H=C6H5CH3+CH3	23.12E+13	0	8088	
!Baulch*2deg*2				
!MXYLENE+H=MXYLYL+H2	3.98E+02	3.44	3120	!Baulch
2005, 1992 515*2deg/2				
MXYLENE+OH=MXYLYL+H2O	3.62E+05	2.39	-602	!Hanson
2010, deg*2				
!MXYLENE+OH=MXYLYL+H2O	2.52E+13	0	2583	
!EBG Model*2deg				
CH3+MXYLENE=CH4+MXYLYL	8.00e-05	5.61504	9000	
!Estimated, *2deg				
!MXYLENE+O2=MXYLYL+HO2	2.28E+07	2.5	44946	!Baulch et
al. 2005*2deg				
!MXYLENE+O=OC6H3(CH3)2+H	1.63E+13	0	3418	
!EBG, 1992 517,				
C6H4CH3+MXYLENE=C6H5CH3+MXYLYL	15.88E+13	0	11935	!Hippler,
1996*2deg				
!MXYLENE+H=phenyl(CH3)2+H2	2.00E+14	0.00	16000	!Kiefer,
JPC, 1987*4/5deg				
!MXYLENE+CH3=phenyl(CH3)2+CH4	3.49E-04	5.00	12300	!Kiefer,
JPC, 1987*4/5deg				
!mxylyl decay				
MXYLYL+MXYLYL=MDICPCH2	2.51E+11	0.4	0	
!EBG, 1992 526,				
MCPHC2H5=MXYLYL+CH3	8.91E+15	0	74720	!Kiefer,
IJCK, 1986,				
!MXYLYL=C2H2+C5H5-1CH2	6.03E+13	0	70000	
!Colket and Seery, 1994				
!MXYLYL+O=C6H4CH3+CH2O	8.00E+13	0	0	
!EBG, 1992 523				
!MXYLYL+HO2=>MCPPHCO+H+OH	3.67E+14	0	0	
!Coll Freq. * 0.7575				

!MXYLYL+HO2=>C6H4CH3+CH2O+OH !Coll Freq. * 0.2525	1.17E+14	0	0	
MXYLYL+OH=MCPCH2OH !EBG, 1992 528	6.00E+13	0	0	
!m-C6H4CH3 decay !C6H5CH3=C6H4CH3+H !Estimated*(5/6)deg	1.67E+17	0	110000	
C6H4CH3+C2H4=C6H5CH3+C2H3 !Lin, JPC, 2004*5/6deg	7.87E-03	4.47	4470	
C6H4CH3+C2H4=MACPHC2H4 !Lin, JPC, 2004	4.04E+03	2.64	1459	
C6H4CH3+PC3H4=C6H5CH3+H2CCCH 2002 PCCP*5/6deg	1.84E+03	2.848	4275.574	!Peeters
C6H4CH3+C2H2=MBCSTYRYL !Lin, JACS, 2003	2.04E+10	0.70	27500	
!C6H4CH3+O2=OC6H4CH3+O !Just, 1994	2.60E+13	0	6120	
!decay of MCC6H4OH HOC6H4CH3+MXYLYL=OC6H4CH3+MXYLENE !EBG, 1992 520f	1.05E+11	0	9500	
!MCPHC2H5 decay MCPHC2H5+H=MACPHC2H4+H2 2005	234.897	1.90	6637	!Baulch,
MCPHC2H5+H=C6H5CH3+C2H5 2005*5/6deg	4.82e+13	0	8088	!Baulch,
MCPHC2H5+C6H5CH2=C6H5CH3+MBCPHC2H4 to Toluene 492, Hippler, 1996*2deg	15.88E+13	0	11935	!Similar
MCPHC2H5+H=MBCPHC2H4+H2 2005	265.012	3.44	1004	!Baulch,
MCPHC2H5+OH=>MCSTYREN+H2O+H !EBG, 1992 543	8.43E+12	0	2583	
MCPHC2H5+O2=>MCSTYREN+HO2+H !EBG, 1992 545	2.00E+14	0	41400	
MCPHC2H5=>MBCPHC2H4+H Markgraf and Troe, JPC, 1988	2.51E+15	0.00	81262	!Muller-
MBCPHC2H4+H=>MCPHC2H5 !calculated using CHEMREV	1.17E+14	-2.117	-5290	
MBCPHC2H4<=>MCSTYREN +H !(Id BPHC2H4):2, Dagaut 2007	5.000E+12	0.0	50670.0	
!decay of MBCPHC2H4, MACPHC2H4 !MBCPHC2H4=MCSTYREN+H !Lin, JPC, 2004	3.79E+06	1.991	32106	
MBCPHC2H4=MACPHC2H4 !Lin, JPC, 2004	5.95E+05	2.074	29582	
MACPHC2H4=MCSTYREN+H !Lin, JPC, 2004	3.74E+08	1.550	44609	
!decay of MCSTYREN				

MXYLENE+C2H4=MCSTYREN+CH4	3.00E+45	-8.65	42422	
!Lin JPC 2004, 100 atm 1000-2500K Rate*2deg				
MACSTYRYL+H=MCSTYREN	1.54E+13	-0.99	-6880	!
[QRRK-HR, 1 atm]				
MCSTYREN+H=MACSTYRYL+H2	5.07E+07	1.93	12951	!
[Knyazev et al. 1996a for C2H4+H]				
!decay of MACSTYRYL				
C6H4CH3+C2H2=MACSTYRYL	2.69E+06	2.05	3720	
!Lin, JACS, 2003				
MACSTYRYL=MBCSTYRYL	4.90E+12	0.45	45740	
!Lin, JACS, 2003				
!decay of MEPHHCO				
MCPHHCO+O2=MCPHCO+HO2	1.02E+13	0	38950	
!EBG, 1992 535				
MCPHHCO+OH=MCPHCO+H2O	1.71E+09	1.18	-447	
!EBG, 1992 536				
MCPHHCO+H=MCPHCO+H2	5.00E+13	0	4928	
!EBG, 1992 537				
MCPHHCO+H=C6H5CHO+CH3	5.78E+13	0	8088	!Baulch
MXYL+MCPHHCO=MXYLENE+MCPHCO	2.18E+07	2.5	46045	!Hanson
2010, deg*2				
!MXYL+MCPHHCO=MXYLENE+MCPHCO	5.54E+03	2.81	5773	
!EBG, 1992 540deg*2				
CH3+MCPHHCO=CH4+MCPHCO	2.77E+03	2.81	5773	
!EBG, 1992 541				
C6H5+MCPHHCO=C6H6+MCPHCO	7.01E+11	0	4400	
!EBG, 1992 542				
MCPHHCO+O=MCPHCO+OH	6.02E+12	0	1809	!Baulch
1994				
C6H4CH3 + HCO=MCPHHCO	1.000E+13	0.000	0.00	!
Est.				
!decay of MCPCH2OH				
MCPCH2OH + OH=>MCPHHCO+H2O+H	5.000E+12	0.000	0.00	!
90a-HIP-REI				
MCPCH2OH+O2=>MCPHHCO+HO2+H	2.00E+14	0	41400	
!EBG, 1992 529				
!MCPCH2OH+OH=>MCPHHCO+H2O+H	8.43E+12	0	2583	
!EBG, 1992 530				
MCPCH2OH+H=>MCPHHCO+H2+H	8.00E+13	0	8235	
!EBG, 1992 531				
MCPCH2OH+MXYL=>MCPHHCO+MXYLENE+H	2.11E+11	0	9500	
!EBG, 1992 533				
MCPCH2OH+C6H4CH3=>MCPHHCO+C6H5CH3+H	1.40E+12	0	4400	
!EBG, 1992 534				
!decay of OC6H3(CH3)2				
OC6H4CH3=CO+C5H4-1CH3	2.51E+11	0	43900	
!EBG, 1992 449				

OC6H4CH3+CH3=HOC6H3(CH3)2 [Lin and Lin 1986]	1.00E+12	0.0	0.0	!
!OC6H3(CH3)2+H=HOC6H3(CH3)2 !EBG, 1992 450*0.5	1.25E+14	0	0	
HOC6H3(CH3)2+OH=OC6H3(CH3)2+H2O !EBG, 1992 548	6.00E+12	0	0	
HOC6H3(CH3)2+H=OC6H3(CH3)2+H2 !EBG, 1992 549	1.15E+14	0	12400	
HOC6H3(CH3)2+H=MXYLENE+OH !EBG, 1992 550	2.21E+13	0	7910	
HOC6H3(CH3)2+H=HOC6H4CH3+CH3 !EBG, 1992 551	1.20E+13	0	5148	
HOC6H3(CH3)2+MXYL=OC6H3(CH3)2+MXYLENE !EBG, 1992 521	1.05E+11	0	9500	
OC6H3(CH3)2=CO+C5H3(CH3)2 !EBG, 1992 449	2.51E+11	0	43900	
!decay of HOC6H4CH3, OC6H4CH3 !OC6H4CH3+H=HOC6H4CH3 !EBG, 1992 450*0.5	1.25E+14	0	0	
C4H5-N+HOC6H4CH3=C4H6-13+OC6H4CH3 !EBG, 1992 456	6.00E+12	0	0	
C2H3+HOC6H4CH3=C2H4+OC6H4CH3 !EBG, 1992 455	6.00E+12	0	0	
C6H4CH3+HOC6H4CH3=C6H5CH3+OC6H4CH3 !EBG, 1992 457	4.91E+12	0	4400	
HOC6H4CH3+OH=OC6H4CH3+H2O !EBG, 1992 451	6.00E+12	0	0	
HOC6H4CH3+H=C6H5CH3+OH !EBG, 1992 452	2.21E+13	0	7910	
HOC6H4CH3+H=OC6H4CH3+H2 !EBG, 1992 453	1.15E+14	0	12400	
HOC6H4CH3+O=OC6H4CH3+OH !EBG, 1992 454	2.81E+13	0	7352	
!C6H4CH3=C6H5CH2 !LL, 1996	1.000E+15	0.000	67000.00	
!Dimethylcyclopentadiene reactions, rate constants taken from analogous methylcyclopentadiene reactions				
!C5H3(CH3)2 1,4-dimethyl-1,3-cyclopentadiene				
C5H3(CH3)2=C5H4CH3CH2 !*2deg	6.00E+12	0	50400	
C5H4(CH3)2=C5H4CH3CH2+H !*2deg	9.00E+15	0	94000	
C5H4(CH3)2=C5H3(CH3)2+H	1.20E+15	0	68000	!*4/5deg
C5H4(CH3)2+H=C5H5-1CH3+CH3 !*2deg	2.00E+14	0	8000	
C5H4(CH3)2+H=C5H4CH3CH2+H2 !*2deg	2.00E+14	0	10000	
C5H4(CH3)2+H=C5H3(CH3)2+H2	0.80E+14	0	10000	!*4/5deg

C5H4(CH3)2+CH3=C5H4CH3CH2+CH4 !*2deg	1.00E+13	0	11500	
C5H4(CH3)2+CH3=C5H3(CH3)2+CH4	4.00E+12	0	11500	!*4/5deg
!C5H4CH3CH2=C6H6CH3	1.40E+13	0	17400	!assumed
same				
!I. V. Tokmakov, M. C. Lin, Int. J. Chem. Kinet. 33 (2001) 633-653.				
CH3+C6H6=>C6H6CH3 !Tokmakov and Lin 2001	2.60E+03	2.84	8502	
C6H6CH3=>CH3+C6H6 !Tokmakov and Lin 2001	1.10E+14	0	22425	
C6H6CH3=>C6H5CH3+H !Tokmakov and Lin 2001	3.76E+13	0	27321	
C6H5CH3+H=>C6H6CH3 !Tokmakov and Lin 2001	1.93E+06	2.17	4163	
!F. Battin-Leclerc, R. Bounaceur, N. Belmekki, P. A. Glaude, Int. J. Chem. Kinet. 38 (2006) 284-302.				
!MXYLENE+O=phenyl(CH3)2+OH	4.00E+13	0.0	14700.0	
!MXYLENE+OH=phenyl(CH3)2+H2O	3.20E+08	1.4	1450.0	
!MXYLENE+HO2=phenyl(CH3)2+H2O2	1.10E+13	0.0	28900.0	
!phenyl(CH3)2+O2=OC6H3(CH3)2+O !<estimated(f)>! *1 par rapport au toluene	2.6E+13	0.0	6.1E3	
!***termination reactions!				
!phenyl(CH3)2+H=MXYLENE !<estimated(g)>! *1 par rapport au toluene	1.0E+14	0.0	0.0	
!phenyl(CH3)2+O=OC6H3(CH3)2 !<estimated(f)>! *1 par rapport au toluene	1.0E+14	0.0	0.0	
!phenyl(CH3)2+OH=HOC6H3(CH3)2 !<estimated(f)>! *1 par rapport au toluene	1.0E+13	0.0	0.0	
MCPCH2OH+H=C6H5CH3+CH2OH Leclerc Model	5.80E+13	0	5148	!Battin-
MCPHHCO+H=C6H5CH3+HCO Leclerc Model	5.80E+13	0	5148	!Battin-
!SERDP PAH MODEL version 0.1, Jun 2007 model				
MCPHHCO+C6H4CH3 = MCPHCO+C6H5CH3 est.(C6H5CH3+C6H5)*4/5 deg	1.68E+12	0.000	4400.00	!
MCPHCO + H2O2 =MCPHHCO + HO2 est.(CH3CO+H2O2 = CH3CHO+HO2)	1.80E+11	0.000	8226.00	!
MCPHCO=C6H4CH3+CO !EBG, 1992 552	3.98E+14	0	29400	
!MCPHHCO+H=C6H4CH3+CH2O SERDP model	2.00E+13	0	2000.0	!
!MCPHCO=C6H4CH3+CO	5.27E+14	0	19013	!SERDP
OC6H3(CH3)2 + H (+M) = HOC6H3(CH3)2 (+M)	1.000E+14	0.000	0.00	!
Estimated (C6H5O + H -> C6H5OH) / 2.5				
LOW / 4.000E+93 -21.840 13880.0 / ! 96-DAV-WAN, 97-WAN-FRE				
TROE / 0.043 304.2 60000. 5896.4 /				
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/				

!3 channels for the reaction of m-xylene+o = products, total rate constant 2.3E+13 0
! 2710
!Thermochemistry of all the dimethyphenol and phenoxy radicals assumed to be the same as
!HOC6H3(CH3)2, OC6H3(CH3)2
!Branching ratios assumed to be the same as corresponding C6H6+O reactions at 50 bar and T
!range of 1200-1700K, original rate*1.5 , Taatjes et al.
MXYLENE+O=HOC6H3(CH3)2 1.54E+13 0 2710!
MXYLENE+O=OC6H3(CH3)2+H 1.80E+13 0 2710!
MXYLENE+O=C5H4(CH3)2+CO 1.04E+12 0 2710!
!G. Da Silva, E. E. Moore, J. W. Bozzelli, J. Phys. Chem. A. 113 (2009) 10264-10278.
MXYLYL=CH2PCH2+H 3.26E+13 0.128 70300
MXYLYL=C7H6f + CH3 4.00E+15 0 76100
!Da Silva et al. J. Phys. Chem. A. Vol 113, No. 21, 2009
C6H5CH2=>C7H6f+H 3.06E+25 -2.89 94320
PLOG/10 3.06E+25 -2.89 94320/
PLOG/100 6.28E+22 -2.056 93400/
!G. Da Silva, J. A. Cole, J. W. Bozzelli, J. Phys. Chem. A. 114 (2010) 2275-2283.
C7H6f+H=>C6H5CH2 1.12E-06 6.25 6040
PLOG/10 2.65E-15 8.75 10810/
PLOG/100 1.12E-06 6.25 6040/
C7H6f+H=>C5H5+C2H2 8.55E-21 10.35 12590
PLOG/10 3.38E+01 4.01 6210/
PLOG/100 8.55E-21 10.35 12590/
C7H6f+H=>ETCPD+H 2.72E-29 12.88 11510
PLOG/10 6.73E-07 6.25 17560/
PLOG/100 2.72E-29 12.88 11510/
ETCPD+H=>C5H5+C2H2 4.44E+20 -1.82 14450
PLOG/10 3.09E+20 -1.91 11330/
PLOG/100 4.44E+20 -1.82 14450/
C5H5+C2H2=>C7H6f+H 1.15E-44 17.07 22460
PLOG/10 2.37E-06 5.60 33540/
PLOG/100 1.15E-44 17.07 22460/
ETCPD+H=>C7H6f+H 8.56E-31 13.10 8670
PLOG/10 2.00E-22 10.69 9170/
PLOG/100 8.56E-31 13.10 8670/
C5H5+C2H2=>ETCPD+H 7.24E+15 -0.61 34040
PLOG/10 4.40E+15 -0.68 30890/
PLOG/100 7.24E+15 -0.61 34040/
!S. Gail, P. Dagaut, Combust. Sci. Technol. 179 (2007) 813-844.
CH2PCH2 +O =CHOPHCH2 +H 3.16E+13 0.0 0
!Brezinsky 1984*2deg
CHOPHCH2+O2= CHOPCHO +OH 6.31E+12 0.0 3000.0
CHOPCHO + H= CHOPCO+H2 5.00E+13 0.0 4928.0
CHOPCHO +O= CHOPCO+OH 9.04E+13 0.0 3080.0
CHOPCO+H=CHOPCHO 3.00E+13 0.0 0!Est
c6h5co+h=c6h5cho
CHOPCO => Y1P4CHO +CO 3.98E+14 0.0 29400.0
Y1P4CHO +H= C6H5CHO 3.98E+15 0.0 83701.0

Y1P4CHO + O2=OY1P4CHO +O	2.09E+12	0.0	7470.0
CHOPCHO+CH3=CHOPCO+CH4	2.77E+03	2.81	5773.0
OY1P4CHO => C5H5CHO + CO	3.980E+14	0.0	29400.0
! (Id PHHCO)			
C5H5CHO =CPDCO	1.00E+12	0.0	0.0
CPDCO =C5H5+CO	2.00E+12	0.0	0.0
C6H5CO+H=C6H5CHO	3.00E+13	0	0
!Buth 1992			
MCPHCO+H=MCPHHCO	3.00E+13	0	0
!Buth 1992			
MXYLENE+O2=MXYL+HO2	5.23E+07	2.5	46045
!Oehslager 2006 * 2 deg (adjusted within error limits +20%)			
!Thermochemistry of CH3C6H4CH2OO frm FBL			
!Murakami et al. J. Phys. Chem. A Vol. 114 No. 40 2009			
MXYL+O2=>CH3C6H4CH2OO	1.17E+09	-0.05	-2414
PLOG /10	1.17E+09	-0.05	-2414/
PLOG/100	3.076E+11	-0.01	751.8/
CH3C6H4CH2OO=>MXYL+O2	1.56E+11	0	6502
PLOG/10	1.56E+11	0	6502/
PLOG/100	7.85E+13	0	10224/
CH3C6H4CH2OO=MCPHHCO+OH	1.106E+11	0	9401
PLOG/10	1.106E+11	0	9401/
PLOG/100	1.795E+12	0	10066/
!fit between 10 atm and high pressure limit values between 700 and 1500 K			
CH3C6H4CH2OO=OC6H4CH3+CH2O	5.55E+09	0	17341
!Baulch 2005 J. Phys. Chem. Ref. Data			
MCPHC2H5+OH=MACPHC2H4+H2O	4.80E+12	0	0
!Baulch 2005 J. Phys. Chem. Ref. Data			
MCPHC2H5+HO2=MACPHC2H4+H2O2	2.65E+11	0	11286!
MCPHC2H5+HO2=MBCPHC2H4+H2O2	3.19E+12	0	19393!
MCPHC2H5+O=MBCPHC2H4+OH	2.23E+13	0	3795!
!Y. Sakai et al. / Proceedings of the Combustion Institute 32 (2009) 411-418			
MXYLENE+C6H5O=MXYL+C6H5OH	1.086E+13	0	10530
!deg*2			
MXYLENE+HCO=MXYL+CH2O	7.542E+13	0	10530
!deg*2			
MXYL+O=CH3C6H4CH2O	3.30E+14	0	0
!EBG, 1992 522, overall rate considered			
MXYL+HO2=CH3C6H4CH2OOH	3.70E+37	-16.33	-67470
PLOG/1	3.70E+37	-16.33	-67470/
PLOG/7	8.00E+13	0	0/
CH3C6H4CH2OOH=CH3C6H4CH2O+OH	2.03E+47	-10.27	50710
PLOG/1	2.03E+47	-10.27	50710/
PLOG/7	3.29E+13	0.42	39890/!HPL rate
MXYL+HO2=CH3C6H4CH2O+OH	1.19E+09	1.03	-2250
PLOG/1	1.19E+09	1.03	-2250/

!T range 900-1300K

!PLOG/7	1.24E+10	0	-1433/
!T range >1300K			
PLOG/7	3.86E+10	0	1456/
!HPL rate			
CH ₃ C ₆ H ₄ CH ₂ O=MCPHHCO+H	5.26E+28	-5.081	22250
PLOG/1	5.26E+28	-5.081	22250/
PLOG/10	1.68E+22	-2.901	20760/
PLOG/101	5.07E+08	1.56	16850/!
CH ₃ C ₆ H ₄ CH ₂ O=C ₆ H ₄ CH ₃ +CH ₂ O	7.21E+33	-6.210	36850
PLOG/1	7.21E+33	-6.210	36850/
PLOG/10	1.32E+27	-4.009	35070/
PLOG/101	1.09E+14	0.157	31160/!
CH ₃ C ₆ H ₄ CH ₂ O=C ₆ H ₅ CH ₃ +HCO	2.37E+32	-6.095	28810
PLOG/1	2.37E+32	-6.095	28810/
PLOG/10	3.82E+31	-5.663	29840/
PLOG/101	1.81E+13	0	22717/!
!!			
!!135-TMB CHEMISTRY!!			
!!			
!Brand et al., JPC, 94, 16, 1990			
C ₉ H ₁₂ =C ₉ H ₁₁ +H	2.24E+16	0	87237
REV/	7.80E+13	0	0/
!Reverse from I. V. Tokmakov, J. Park, s. Gheyas and M. C. Lin, J. Phys. Chem. A 1999, 103, 3636-3645			
C ₉ H ₁₂ =C ₆ H ₃ (CH ₃) ₂ +CH ₃	3.37E+17	0	100437
!Estimated			
REV/	1.38E+13	0	45/
!actual rate constant (1.38+/-0.08)x1e13 exp(-(23+/-36)/T) cm ³ /mols T range = 300-980 K			
!W.Tsang, J. P. Cui and J.A. Walker, 208 (1989), Single pulse shock tube studies on the reactions of hydrogen atoms with unsaturated compounds, 63-73			
!reverse rate from C.T. Brooks, C. P. R. Cummins, S. J. Peacock, Pyrolysis of Toluene using a static system, Trans. Faraday Soc., 67 (1971) 3265-3274			
!reverse rate same as the reverse rate of toluene+h=benzyl+h ₂			
C ₉ H ₁₂ +H=C ₉ H ₁₁ +H ₂	3.70E+14	0	8628
REV/	2.82E+12	0	14500/
!forward and reverse from reverse rate constant taken from M.B. Colket and Seery, Toluene Pyrolysis, Proc. Combust. Inst., same as benzyl+ch ₄ =toluene+ch ₃			
C ₉ H ₁₂ +CH ₃ =C ₉ H ₁₁ +CH ₄	4.74E+12	0	11100
!*3deg			
REV/	1.20E+13	0	27100/
!Baulch et al., J. Phys. Chem. Ref. Data, Vol. 34, No. 3, 2005			
!calculated the reverse using the thermodynamic data provided in Baulch 2005			
C ₉ H ₁₂ +OH=C ₉ H ₁₁ +H ₂ O	1.56E+10	1.0	874 !A*3deg
REV/	1.23E+10	0.7003	29538/
C ₉ H ₁₂ +O ₂ =C ₉ H ₁₁ +HO ₂	3.42E+07	2.50	44946
!A*3 deg			
REV/	1.44E+07	1.974	4085/
!dimethylethylbenzene reactions			

!forward rate constant same as c7h7+ch3=c6h5c2h5 taken from
!U.Brand, H. Hippler, L. Lindemann and J. Troe, J. Phys. Chem. 94(1990) 6305-6316
!Reverse rate constant estimated using rate rules given by A.M. Dean, J. Phys. Chem, 89 (1985)
4600-4608

C9H11+CH3=DIMETB	1.10E+12	0	0
! /10			
REV/	8.00E+14	0	80922/
! /10			
!Baulch et al., J. Phys. Chem. Ref. Data, Vol. 34, No. 3, 2005, same as c6h5c2h5+ !calculated the reverse using the thermodynamic data provided in Baulch 2005			
DIMETB+H=DIMCHCH3+H2	7.26E+07	2.00	5345!A*2.2 deg
REV/	1.98E+06	2.2	22404/
DIMETB+H=DIMCH2CH2+H2	1.59E+08	1.5	7412
!A*2.2 deg			
REV/	6.51E+05	1.564	8720/
DIMETB+O=DIMCHCH3+OH	4.906E+13	0	3795
!A*2.2 DEG			
REV/	3.19E+11	0.18	19027/
DIMETB+HO2=DIMCHCH3+H2O2	1.36E+05	2.50	13522
!A*2.2 deg			
REV/	9.75E+05	2.04	14045/
DIMETB+HO2=DIMCH2CH2+H2O2	7.81E+04	2.50	16849
!A*2.2 deg			
REV/	2.98E+03	1.901	1621/
!Took the total rate constant			
DIMETB+OH=DIMCH2CH2+H2O	4.80E+12	0	0
REV/	8.509E+10	-0.0302	16598/
!I. V. Tokmakov and M. C. Lin, J. Phys. Chem.A 108 (2004) 9697-9714			
C6H3(CH3)2+C2H4=DIMCH2CH2	4.04E+03	2.64	1459
REV/	1.72E+11	0.78	38704/
DIMCH2CH2=DIMSTYR+H	1.83E+06	2.081	33207
REV/	1.63E+06	2.158	1994/
DIMCH2CH2=DIMCHCH3	5.96E+05	2.074	29582
REV/	2.30E+07	1.737	44456/
DIMCHCH3=DIMSTYR+H	3.74E+08	1.55	44609
REV/	1.19E+07	1.925	-108/
!P.Lindstedt, L.Maurice and M. Meyer, Faraday Discuss. 119 (2011) 409-432			
!reverse rate constants same as dimetb			
DIMSTYR+H=DIMCHCH+H2	1.99E+06	2.53	12239
!A*3 deg			
REV/	6.51E+05	1.564	8720/
DIMSTYR+O=>C6H3(CH3)2+CH2HCO	3.50E+13	0	2832
DIMSTYR+O=DIMCHCH+OH	2.27E+06	1.91	3735
!A*3 deg			
REV/	3.19E+11	0.18	19027/
!D. L. Baulch, I. M. Campbell, S. M. Saunders, P. K. K. Louie, J. Chem. Soc. Faraday Trans 85 (1989) 1819-1826			
!directly got from NIST website for rxn C6H5C2H3+OH=>pdts			

DIMSTYR+OH=DIMCHCH+H2O	2.85E+13	0	0
REV/	8.509E+10	-0.0302	16598/
!L.Fusetti et al. Organic Geochemistry 41 (2010) 146-167			
DIMETB+H=MCPHC2H5+CH3	5.80E+13	0	8100
REV/	1.20E+12	0	15900/
DIMSTYR+H=MCSTYREN+CH3	5.80E+13	0	8100
REV/	1.20E+12	0	15900/
!same as that of dimetb			
DIMSTYR+H=MXYLENE+C2H3	5.20E+13	0	4100
REV/	1.20E+11	0	15900/
DIMETB+H=MXYLENE+C2H5	5.20E+13	0	4100
REV/	1.20E+11	0	15900/
!forward W.Tsang, J. P. Cui and J.A. Walker, 208 (1989), Single pulse shock tube studies on the reactions of hydrogen atoms with unsaturated compounds, 63-73			
!reverse L.Fusetti et al. Organic Geochemistry 41 (2010) 146-167			
C9H12+H=MXYLENE+CH3	6.70E+13	0	6468
REV/	8.00E+11	0	15900/
!Tokmakov and Lin, J. Am. Chem. Soc., 125 (2003) 11397-11408			
!same as c6h5+c2h2=styr reactions			
C6H3(CH3)2+C2H2=DIMCHCH	2.69E+06	2.05	3720
REV/	1.35E+14	0.34	45710/
!P.Frank, J. Herzler, Th. Just and C. Wahl, Proc. Combust. Inst. 1994, 833-840			
!same as C6H5+O2=C6H5O+O			
!C6H3(CH3)2+O2=>OC6H3(CH3)2+O	2.60E+12	0	3080
!/10			
!Murakami et al. J. Phys. Chem. A Vol. 114(40) 2009, same as m-xylyl radical reactions			
!LPL rate considered			
!C9H11+O2=>C9H11OO	1.17E+09	-0.05	-2414
!C9H11OO=>C9H11+O2	1.56E+11	0	6502
!C9H11OO=>DIMP HHCO+OH	1.11E+10	0	9401
!/10			
!c9H11OO=OC6H3(CH3)2+CH2O	5.55E+09	0	17341
!REV/	1.00E+13	0	0/
!HPL rate			
C9H11+O2=>C9H11OO	3.076E+11	-0.01	751.8
C9H11OO=>C9H11+O2	7.85E+13	0	10224
C9H11OO=>DIMP HHCO+OH	1.795E+12	0	10066
C9H11OO=OC6H3(CH3)2+CH2O	5.55E+09	0	17341
REV/	1.00E+13	0	0/
!M.A. Grela, A. J. Colussi, J. Phys. Chem 90 (1986) 434-437			
!reverse from R. Buth, K. Hoyer mann and G. Rohde, Proc. Combust. Inst. 1992, pp. 669-694			
DIMP HHCO=DIMP HCO+H	3.98E+15	0	83661
REV/	3.00E+13	0	0/
!R.K. Solly and S. W. Benson, J. Am. Chem. Soc, 93:9 May 5, 1971, 2127-2131			
!reverse rate from G. Nam, W. Xia, J. Park and M.C. Lin, J. Phys. Chem. A, 2000, 104, 1233-1239			
DIMP HCO=C6H3(CH3)2+CO	1.25E+15	0	27646
REV/	1.17E+12	0	2778/
!uic M-xYLENE OXIDAITON MODEL			

!reverse same as hco+ho2->pdts reaction, W. Tsang, R.F. Hampson, J. Phys. Chem. Ref. Data, 15 (1986) 1087-1280

DIMPHHCO+O2=DIMPHCO+HO2	7.14E+13	0	38950
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!EBG, 1992 535, A*7 DEG

REV/	3.01E+13	0	0/
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!REVERSE RATE TSANG (1986) HCO+H2O=CH2O+OH

DIMPHHCO+OH=DIMPHCO+H2O	1.20E+10	1.18	-447
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!EBG, 1992 536, A*7 DEG

REV/	5.14E+11	1.35	26000/
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!REVERSE RATE TSANG (1986) CH3CO+H2=CH3CHO+H

DIMPHHCO+H=DIMPHCO+H2	3.50E+14	0	4928
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!EBG, 1992 537, A*7 DEG

REV/	1.31E+11	1.82	17600/
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!reverse rate tsang(1986) ch3co+oh->pdts

DIMPHHCO+O=DIMPHCO+OH	6.33E+13	0	3080
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!EBG, 1992 539, A*7 DEG

REV/	4.22E+13	0	0/
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DIMPHHCO+H=MCPHHCO+CH3	5.80E+13	0	8100
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REV/	1.20E+12	0	15900/
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!H. Hippler, C. Reihs and J. Troe, Proc. Combust. Inst., 1990, 37-43

!rate constants from corresponding c6h5ch2 reactions

!reverse rate from hco+h->o+ch2,T. Tsuboi, K. Hashimoto, Combust Flame 42 (1981), 61-76 (taken directly from NIST)

C9H11+O=DIMPHHCO+H	4.00E+13	0	0
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!/10

REV/	3.98E+13	0	102540/
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C9H11+OH=>DIMPHCH2OH	2.00E+13	0	0
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DIMPHCH2OH+OH=>DIMPHCH2O+H2O	5.00E+12	0	0
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!L.Fusetti et al. Organic Geochemistry 41 (2010) 146-167

DIMPHCH2OH+H=MCPCH2OH+CH3	5.80E+13	0	8100
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REV/	1.20E+12	0	15900/
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!uic m-xylene oxidation model

!LPL RATE CONSIDERED

!C9H11+HO2=>C9H11OOH	3.70E+37	-16.33	-67470
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!C9H11OOH=>DIMPHCH2O+OH	2.03E+47	-10.27	50710
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!C9H11+HO2=>DIMPHCH2O+OH	1.19E+09	1.03	-2250
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!DIMPHCH2O=>DIMPHHCO+H	5.26E+27	-5.081	22250
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!/10

!DIMPHCH2O=>C6H3(CH3)2+CH2O	7.21E+33	-6.21	36850
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!DIMPHCH2O=>MXYLENE+HCO	2.37E+32	-6.095	28810
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!HPL rate considered

C9H11+HO2=>C9H11OOH	8.00E+13	0	0
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C9H11OOH=>DIMPHCH2O+OH	3.29E+13	0.42	39890
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C9H11+HO2=>DIMPHCH2O+OH	3.86E+10	0	1456
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DIMPHCH2O=>DIMPHHCO+H	5.07E+08	1.56	16850
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DIMPHCH2O=>C6H3(CH3)2+CH2O	1.09E+14	0.157	31160
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DIMPHCH2O=>MXYLENE+HCO	1.81E+13	0	22717
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!W. Muller-Markgraf and J. Troe, J. Phys. Chem. 92 (1988) 4899-4905

C9H11+C9H11=C18H22 !*5	1.58E+12	0.4	0	
REV/	7.94E+14	0	57361/	
!uic mxyl				
C6H3(CH3)2+O2=OC6H3(CH3)2+O !A/100	8.57e+18	-2.270	7189.29	
REV/	2.21E+23	-3.39	16944.7/	
!A/100				
!L.Fusetti et al. Organic Geochemistry 41 (2010) 146-167				
MCPHC2H5+H=C6H5C2H5+CH3	1.70E+14	0	8100	
REV/	1.20E+12	0	15900/	
!same as mcphc2h5				
MCSTYREN+H=C6H5CH3+C2H3	5.20E+13	0	4100	
REV/	1.20E+11	0	15900/	
MCSTYREN+H=C6H5C2H3+CH3	1.70E+14	0	8100	
REV/	1.20E+12	0	15900/	
!Estimated				
MCSTYREN=C6H4CH3+C2H3	8.00E+15	0	114177	
REV/	2.00E+13	0	0/	
MCPHC2H5=C6H4CH3+C2H5	8.00E+15	0	100907	
REV/	2.00E+13	0	0/	
!L.Fusetti et al. Organic Geochemistry 41 (2010) 146-167				
DIMPHHCO+H=MXYLENE+HCO	5.20E+13	0	4100	
REV/	1.20E+11	0	15900/	
C9H11+C9H12=DIMERS238+H	1.70E+12	0	23500	
REV/	5.80E+13	0	29400/	
MXYLYL+C9H12=DIMERS224+H	1.70E+12	0	23500	
REV/	5.80E+13	0	29400/	
C9H11+MXYLENE=DIMERS224+H	2.50E+12	0	23500	
REV/	5.80E+13	0	29400/	
MXYLYL+MXYLENE=DIMERS210+H	2.50E+12	0	23500	
REV/	5.80E+13	0	29400/	
C9H11+C9H12=DIMERS224+CH3	4.20E+12	0	23500	
REV/	1.20E+12	0	29400/	
MXYLYL+C9H12=DIMERS210+CH3	4.20E+12	0	23500	
REV/	1.20E+12	0	29400/	
C9H11+MXYLENE=DIMERS210+CH3	2.50E+12	0	23500	
REV/	1.20E+12	0	29400/	
MXYLYL+MXYLENE=DIMERS196+CH3	2.50E+12	0	23500	
REV/	1.20E+12	0	29400/	
!Forward Fahr and Stein				
!Reactions of vinyl and phenyl radicals with ethyne, ethene and benzene, Symp. Int. Combust. Proc, 22, 1023-1029				
!Reverse NIST database-could not find the rate in the paper				
C9H11+C9H12=C18H22+H	1.99E+11	0	3994	!/2
REV/	1.99E+14	0	29400/	!/2
!FBL m-xylene				
MCPHHCO+O2=CH2C6H4CHO+HO2	2.10E+12	0	41000	

MCPHHCO+H=CH2C6H4CHO+H2	4.00E+13	0	3200	
MCPHHCO+O=CH2C6H4CHO+OH	6.00E+12	0	1800	
MCPHHCO+OH=CH2C6H4CHO+H2O	7.80E+12	0	0	
MCPHHCO+HO2=CH2C6H4CHO+H2O2	3.00E+12	0	11000	
MCPHHCO+CH3=CH2C6H4CHO+CH4	2.00E-06	5.6	1500	
MCPHHCO+C2H5=CH2C6H4CHO+C2H6	1.30E+12	0	7500	
!FORWARD ESTIMATED				
!REV BAULCH 2005 SAME AS C6H5CH2+CH3=C6H5C2H5				
CH2C6H4CHO+CH3=C2H5C6H4CHO	2.00E+13	0	0	
REV/	7.10E+15	0	75109/	
!Estimated				
DIMPHHCO=C6H3(CH3)2+HCO	8.00E+15	0	147206	
REV/	2.00E+13	0	0/	
DIMPHCH2OH=C6H3(CH3)2+CH2OH	8.00E+15	0	148412	
REV/	2.00E+13	0	0/	
!Fusetti et al.				
C9H12+CH3=TETRAMB+H	1.20E+12	0	15900	
REV/	5.80E+14	0	8100/	
!forward W.Tsang, J. P. Cui and J.A. Walker, 208 (1989), Single pulse shock tube studies on the reactions of hydrogen atoms with unsaturated compounds, 63-73				
!reverse L.Fusetti et al. Organic Geochemistry 41 (2010) 146-167				
TETRAMB+H=TMB123+CH3	6.70E+13	0	6468	
REV/	1.20E+12	0	15900/	
TMB123+H=O-XYL+CH3	6.70E+13	0	6468	
REV/	1.20E+12	0	15900/	
TMB124+H=O-XYL+CH3	6.70E+13	0	6468	
REV/	1.20E+12	0	15900/	
!Reactions of vinyl and phenyl radicals with ethyne, ethene and benzene, Symp. Int. Combust. Proc, 22, 1023-1029				
!Reverse NIST database-could not find the rate in the paper				
C9H11+C6H6=DIMERS196+H	1.99E+11	0	3994	!/2
REV/	1.99E+14	0	29400/	!/2
TMB124+C6H5=B124PM+H	1.99E+11	0	3994	!/2
REV/	1.99E+14	0	29400/	!/2
MXYLENE+C6H4CH3=B11MB3+H	1.99E+11	0	3994	!/2
REV/	1.99E+14	0	29400/	!/2
!Fusetti et al.				
DIMERS196+C9H11=RDIMERS196a+C9H12	1.60E+11	0	12800	
REV/	1.60E+09	0	12800/	
DIMERS196+H=RDIMERS196a+H2	4.00E+15	0	8400	
REV/	2.80E+11	0	14500/	
DIMERS196+CH3=RDIMERS196a+CH4	1.60E+12	0	8800	
REV/	6.60E+11	0	27500/	
RDIMERS196a=PTRIARO192+H	4.20E+11	0	23500	
REV/	5.80E+13	0	29400/	
RDIMERS196a=PTRIARO178+CH3	8.40E+11	0	23500	
REV/	1.20E+12	0	29400/	
PTRIARO192+H=RPTRIARO192a+H2	4.00E+15	0	8400	

REV/	2.80E+11	0	14500/
PTRIARO178+H=RPTRIARO178a+H2	4.00E+15	0	8400
REV/	2.80E+11	0	14500/
PTRIARO192+CH3=RPTRIARO192a+CH4	1.60E+12	0	8800
REV/	6.60E+11	0	27500/
PTRIARO178+CH3=RPTRIARO178a+CH4	1.60E+12	0	8800
REV/	6.60E+11	0	27500/
RPTRIARO178a=A3+H	3.50E+13	0	28400
REV/	4.30E+13	0	4500/
RPTRIARO192a=A3CH3+H	3.50E+13	0	28400
REV/	4.30E+13	0	4500/
!forward W.Tsang, J. P. Cui and J.A. Walker, 208 (1989), Single pulse shock tube studies on the reactions of hydrogen atoms with unsaturated compounds, 63-73			
!reverse L.Fusetti et al. Organic Geochemistry 41 (2010) 146-167			
A3CH3+H=A3+CH3	6.70E+13	0	6468
REV/	1.20E+12	0	15900/
A3+H=A3-+H2	2.50E+14	0	15896
A3+OH=A3-+H2O	1.70E+12	1.42	1496
A3-+H=A3	1.00E+14	0	0!
A2C2H*+C2H2=A3-	4.67E+06	1.787	3262
!MIT			
A2-+C4H2=A3-	3.30E+33	-5.7	25334
A2-+C4H4=A3+H	3.30E+33	-5.7	25334
INDENYL+C5H5=A3+2H	5.00E+12	0	8000
!MIT			
A2-+H=A2	1.00E+14	0	0
A2C2H*+H=A2R5	5.00E+13	0	0
INDENE=INDENYL+H	1.10E+15	0	77096
A3-+O2=>CO+HCO+A2R5	2.00E+11	0	7352
!/10			
INDENYL+H2CCCH=A2R5+H2	9.50E+12	0	0
A2-+C2H2=A2R5+H	1.90E+31	-5.26	20863
A2C2H+H=A2R5+H	4.60E+37	-7.03	22949
A2R5-+H=A2R5	1.00E+14	0	0
A2R5+O=A2R5-+OH	2.00E+13	0	14704
A2R5+O=>A2-+HCCO	2.00E+13	0	14704
A2R5+H=A2R5-+H2	2.50E+14	0	15896
A2R5+OH=A2-+CH2CO	1.00E+13	0	9935
A2+O=>INDENYL+CO+H	3.60E+14	0	43899
A2+O=A2-+OH	2.00E+13	0	14704
A2+H=A2-+H2	2.50E+14	0	15896
A2+OH=A2-+H2O	2.10E+13	0	45701
A2+CH3=A2-+CH4	2.00E+12	0	14962
C6H5+H2CCCH=>INDENE	3.860E+11	0	1361
A2-+O=>INDENYL+CO	1.00E+14	0	0
A2-+HO2=>INDENYL+CO+OH	1.00E+13	0	0
A3+C2H=A3C2H+H	5.00E+13	0	0
A3-+C2H2=A3C2H+H	1.200E+26	-3.44	30004

!forward W.Tsang, J. P. Cui and J.A. Walker, 208 (1989), Single pulse shock tube studies on the reactions of hydrogen atoms with unsaturated compounds, 63-73
!reverse L.Fusetti et al. Organic Geochemistry 41 (2010) 146-167
DIMERS196+H=DIMERS182+CH3 6.70E+13 0 6468
REV/ 1.20E+12 0 15900/
!forward W.Tsang, J. P. Cui and J.A. Walker, 208 (1989), Single pulse shock tube studies on the reactions of hydrogen atoms with unsaturated compounds, 63-73
!reverse L.Fusetti et al. Organic Geochemistry 41 (2010) 146-167
DIMERS182+H=C6H5CH2C6H5+CH3 6.70E+13 0 6468
REV/ 1.20E+12 0 15900/
!!http://creckmodeling.chem.polimi.it/
!biphenylmethane
C6H5CH2C6H5=FLUORENE+H2 .1000E+09 .000 32000.0
!BREZINSKY/LITZINGER NIST DATABASE
!C9H11+O2=DIMPHCH2O+O 6.31E+12 0 42900
!SAME AS C6H5
!Estimated
C6H3(CH3)2+H=>MXYLENE 1.0E+14 0.0 0.0
C6H3(CH3)2+O=>OC6H3(CH3)2 1.0E+14 0.0 0.0
C6H3(CH3)2+OH=>HOC6H3(CH3)2 1.0E+13 0.0 0
END

1,3,5-Trimethylbenzene Oxidation Model Thermochemistry File

!135-tmb thermochemistry appended to UIC m-Xylene Oxidation Model 2

!UIC m-Xylene Oxidation Model 2

!S. Gudiyella, T. Malewicki, A. Comandini and K. Brezinsky, "High Pressure Study of m-Xylene Oxidation" (2010)

!Contact:kenbrez@uic.edu

!R. Sivaramakrishnan, R. S. Tranter, K. Brezinsky, Combust. Flame 139 (2004) 340-350.

!R. Sivaramakrishnan, R. S. Tranter, K. Brezinsky, J. Phys. Chem. A 110 (2006) 9388-9399.

!R. Sivaramakrishnan, R. S. Tranter, K. Brezinsky, J. Phys. Chem. A 110 (2006) 9400-9404.

THERMO

300.000 1000.000 5000.000

HE L10/90HE 1 0 0 0G 200.000 6000.000 1000. 1
2.50000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2
-7.45375000E+02 9.28723974E-01 2.50000000E+00 0.00000000E+00 0.00000000E+00 3
0.00000000E+00 0.00000000E+00 -7.45375000E+02 9.28723974E-01 0.00000000E+00 4
!C2H4O 120186C 2H 4O 1 G 0300.00 5000.00 1000.00 1
! 0.59249249E+01 0.11120714E-01 -0.37434083E-05 0.55413918E-09 -0.29549886E-13 2
! -0.93028008E+04 -0.93792849E+01 -0.24173594E+00 0.20761095E-01 0.21481201E-05 3
! -0.16948157E-07 0.81075771E-11 -0.71720117E+04 0.24432190E+02 4
AR 120186AR 1 G 0300.00 5000.00 1000.00 1
0.02500000E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2
-0.07453750E+04 0.04366001E+02 0.02500000E+02 0.00000000E+00 0.00000000E+00 3
0.00000000E+00 0.00000000E+00 -0.07453750E+04 0.04366001E+02 4
C 121086C 1 G 0300.00 5000.00 1000.00 1
0.02602087E+02 -0.01787081E-02 0.09087041E-06 -0.01149933E-09 0.03310844E-14 2
0.08542154E+06 0.04195177E+02 0.02498585E+02 0.08085777E-03 -0.02697697E-05 3
0.03040729E-08 -0.01106652E-11 0.08545878E+06 0.04753459E+02 4
C2 121286C 2 G 0300.00 5000.00 1000.00 1
0.04135979E+02 0.06531618E-03 0.01837099E-05 -0.05295085E-09 0.04712137E-13 2
0.09967272E+06 0.07472923E+01 0.06996045E+02 -0.07400602E-01 0.03234704E-04 3
0.04802535E-07 -0.03295918E-10 0.09897487E+06 -0.01386227E+03 4
!C2H 81193C 2H 1 G 0300.00 4000.00 1000.00 1
! 0.03986367E+02 0.03143123E-01 -0.01267243E-04 0.02924363E-08 -0.02716320E-12 2
! 0.06655884E+06 0.01191063E+02 0.02737704E+02 0.08048446E-01 -0.09244310E-04 3
! 0.06525259E-07 -0.01939580E-10 0.06683813E+06 0.07300220E+02 4
!C2H2 121386C 2H 2 G 0300.00 5000.00 1000.00 1
! 0.04436770E+02 0.05376039E-01 -0.01912817E-04 0.03286379E-08 -0.02156710E-12 2
! 0.02566766E+06 -0.02800338E+02 0.02013562E+02 0.01519045E+00 -0.01616319E-03 3
! 0.09078992E-07 -0.01912746E-10 0.02612444E+06 0.08805378E+02 4
C2H3 MAR94C 2H 3 G 0300.00 5000.00 1671.00 1
3.96047713E+00 7.99426013E-03 -2.85608087E-06 4.58350813E-10 -2.72570140E-14 2
3.35153544E+04 2.25663414E+00 2.73925942E+00 7.03011591E-03 2.36647299E-06 3
-3.59569737E-09 8.91756491E-13 3.42868979E+04 1.01531535E+01 4
C2H4 121286C 2H 4 G 0300.00 5000.00 1000.00 1
0.03528419E+02 0.01148518E+00 -0.04418385E-04 0.07844601E-08 -0.05266848E-12 2
0.04428289E+05 0.02230389E+02 -0.08614880E+01 0.02796163E+00 -0.03388677E-03 3

0.02785152E-06-0.09737879E-10 0.05573046E+05 0.02421149E+03 4
 C2H5 JPC93 C 2H 5 0 OG 300.000 5000.000 1375.000 1
 5.60116091E+00 1.06977081E-02-3.63504780E-06 5.61816654E-10-3.24914714E-14 2
 1.14539845E+04-7.02252408E+00 1.47374852E+00 1.63606611E-02-4.32896826E-06 3
 -1.17270665E-09 5.72325883E-13 1.33326992E+04 1.66349852E+01 4
 C2H6 121686C 2H 6 G 0300.00 4000.00 1000.00 1
 0.04825938E+02 0.01384043E+00-0.04557259E-04 0.06724967E-08-0.03598161E-12 2
 -0.01271779E+06-0.05239507E+02 0.01462539E+02 0.01549467E+00 0.05780507E-04 3
 -0.01257832E-06 0.04586267E-10-0.01123918E+06 0.01443229E+03 4
 C3H2 102193H 2C 3 G 0150.00 4000.00 1000.00 1
 0.07670981E+02 0.02748749E-01-0.04370943E-05-0.06455599E-09 0.01663887E-12 2
 0.06259722E+06-0.01236890E+03 0.03166714E+02 0.02482572E+00-0.04591637E-03 3
 0.04268019E-06-0.01482152E-09 0.06350421E+06 0.08869446E+02 4
 AC3H4 101993H 4C 3 G 0300.00 4000.00 1400.00 1
 0.09776256E+02 0.05302138E-01-0.03701118E-05-0.03026386E-08 0.05089581E-12 2
 0.01954972E+06-0.03077061E+03 0.02539831E+02 0.01633437E+00-0.01764950E-04 3
 -0.04647365E-07 0.01729131E-10 0.02251243E+06 0.09935702E+02 4
 PC3H4 101993H 4C 3 G 0300.00 4000.00 1400.00 1
 0.09768102E+02 0.05219151E-01-0.03753140E-05-0.02992191E-08 0.05107878E-12 2
 0.01860277E+06-0.03020678E+03 0.03029730E+02 0.01498961E+00-0.01398500E-04 3
 -0.03969619E-07 0.01388217E-10 0.02148408E+06 0.08004594E+02 4
 C3H6 120186C 3H 6 G 0300.00 5000.00 1000.00 1
 0.06732257E+02 0.01490834E+00-0.04949899E-04 0.07212022E-08-0.03766204E-12 2
 -0.09235703E+04-0.01331335E+03 0.01493307E+02 0.02092518E+00 0.04486794E-04 3
 -0.01668912E-06 0.07158146E-10 0.01074826E+05 0.01614534E+03 4
 C3H8 120186C 3H 8 G 0300.00 5000.00 1000.00 1
 0.07525217E+02 0.01889034E+00-0.06283924E-04 0.09179373E-08-0.04812410E-12 2
 -0.01646455E+06-0.01784390E+03 0.08969208E+01 0.02668986E+00 0.05431425E-04 3
 -0.02126001E-06 0.09243330E-10-0.01395492E+06 0.01935533E+03 4
 C4H10 62090C 4H 10 G 0300.00 4000.00 1500.00 1
 0.01998785E+03 0.01037281E+00-0.09610818E-05-0.04623018E-08 0.08202828E-12 2
 -0.02625571E+06-0.08837907E+03-0.02256618E+02 0.05881732E+00-0.04525783E-03 3
 0.02037115E-06-0.04079458E-10-0.01760233E+06 0.03329595E+03 4
 C4H2 121686C 4H 2 G 0300.00 5000.00 1000.00 1
 0.09031407E+02 0.06047253E-01-0.01948789E-04 0.02754863E-08-0.01385608E-12 2
 0.05294736E+06-0.02385068E+03 0.04005192E+02 0.01981000E+00-0.09865877E-04 3
 -0.06635158E-07 0.06077413E-10 0.05424065E+06 0.01845737E+02 4
 CH 121286C 1H 1 G 0300.00 5000.00 1000.00 1
 0.02196223E+02 0.02340381E-01-0.07058201E-05 0.09007582E-09-0.03855040E-13 2
 0.07086723E+06 0.09178373E+02 0.03200202E+02 0.02072876E-01-0.05134431E-04 3
 0.05733890E-07-0.01955533E-10 0.07045259E+06 0.03331588E+02 4
 AC3H5 82489C 3H 5 G 0300.00 4000.00 1000.00 1
 0.09651539E+02 0.08075596E-01-0.07965424E-05-0.04650696E-08 0.08603280E-12 2
 0.01530096E+06-0.02686774E+03 0.02276486E+02 0.01985564E+00 0.01123842E-04 3
 -0.01014576E-06 0.03441342E-10 0.01789497E+06 0.01372515E+03 4
 C4H4 82489C 4H 4 g 0300.00 4000.00 1000.00 1
 0.01069777E+03 0.06982014E-01-0.06567747E-05-0.03884517E-08 0.07200946E-12 2
 0.03034803E+06-0.03128430E+03 0.03233893E+02 0.01865634E+00 0.01270320E-04 3

-0.09410096e-07 0.02956111e-10 0.03301097e+06 0.09922676e+02 4
 C4H5-N 82489C 4H 5 G 0300.00 4000.00 1000.00 1
 0.01286597E+03 0.07943369E-01-0.08626466E-05-0.04655635E-08 0.08951131E-12 2
 0.03783552E+06-0.04182502E+03 0.02995240E+02 0.02288456E+00 0.01975471E-04 3
 -0.01148245E-06 0.03197824E-10 0.04142218E+06 0.01289454E+03 4
 C4H6-13 120189C 4H 6 G 0300.00 4000.00 1000.00 1
 0.01254437E+03 0.09596525E-01-0.09187012E-05-0.05429640E-08 0.01005364E-11 2
 0.08597330E+05-0.04217451E+03 0.01931624E+02 0.02479030E+00 0.03018071E-04 3
 -0.01154686E-06 0.02586623E-10 0.01255468E+06 0.01701999E+03 4
 C4H6-1 120189C 4H 6 g 0300.00 4000.00 1000.00 1
 0.01200695e+03 0.09576069e-01-0.08995018e-05-0.05369808e-08 0.09934174e-12 2
 0.01729420e+06-0.03802692e+03 0.03726043e+02 0.02053493e+00 0.03021439e-04 3
 -0.08131813e-07 0.01095280e-10 0.02048821e+06 0.08538826e+02 4
 CH2CO 121686C 2H 2O 1 G 0300.00 5000.00 1000.00 1
 0.06038817E+02 0.05804840E-01-0.01920954E-04 0.02794485E-08-0.01458868E-12 2
 -0.08583402E+05-0.07657581E+02 0.02974971E+02 0.01211871E+00-0.02345046E-04 3
 -0.06466685E-07 0.03905649E-10-0.07632637E+05 0.08673553E+02 4
 CH2HCO 110393O 1H 3C 2 G 0300.00 5000.00 1000.00 1
 0.05975670E+02 0.08130591E-01-0.02743624E-04 0.04070304E-08-0.02176017E-12 2
 0.04903218E+04-0.05045251E+02 0.03409062E+02 0.01073857E+00 0.01891492E-04 3
 -0.07158583E-07 0.02867385E-10 0.01521477E+05 0.09558290E+02 4
 CH2O 121286C 1H 2O 1 G 0300.00 5000.00 1000.00 1
 0.02995606E+02 0.06681321E-01-0.02628955E-04 0.04737153E-08-0.03212517E-12 2
 -0.01532037E+06 0.06912572E+02 0.01652731E+02 0.01263144E+00-0.01888168E-03 3
 0.02050031E-06-0.08413237E-10-0.01486540E+06 0.01378482E+03 4
 !CH2OH 120186H 3C 1O 1 G 0250.00 4000.00 1000.00 1
 ! 0.06327520E+02 0.03608271E-01-0.03201547E-05-0.01938750E-08 0.03509705E-12 2
 !-0.04474509E+05-0.08329366E+02 0.02862628E+02 0.01001527E+00-0.05285436E-05 3
 !-0.05138540E-07 0.02246041E-10-0.03349679E+05 0.01039794E+03 4
 CH3 121286C 1H 3 G 0300.00 5000.00 1000.00 1
 0.02844052E+02 0.06137974E-01-0.02230345E-04 0.03785161E-08-0.02452159E-12 2
 0.01643781E+06 0.05452697E+02 0.02430443E+02 0.01112410E+00-0.01680220E-03 3
 0.01621829E-06-0.05864953E-10 0.01642378E+06 0.06789794E+02 4
 PC3H5 82489C 3H 5 G 0300.00 4000.00 1000.00 1
 0.09101018E+02 0.07964168E-01-0.07884945E-05-0.04562036E-08 0.08529212E-12 2
 0.02670680E+06-0.02150559E+03 0.03385811E+02 0.01404534E+00 0.03204127E-04 3
 -0.03824120E-07-0.09053742E-11 0.02909066E+06 0.01126649E+03 4
 SC3H5 82489C 3H 5 G 0300.00 4000.00 1000.00 1
 0.09209764E+02 0.07871413E-01-0.07724523E-05-0.04497357E-08 0.08377272E-12 2
 0.02853967E+06-0.02232370E+03 0.03161863E+02 0.01518100E+00 0.02722659E-04 3
 -0.05177112E-07 0.05435286E-12 0.03095548E+06 0.01197973E+03 4
 CH3CO 120186C 2H 3O 1 G 0300.00 5000.00 1000.00 1
 0.05612279E+02 0.08449886E-01-0.02854147E-04 0.04238376E-08-0.02268404E-12 2
 -0.05187863E+05-0.03274949E+02 0.03125278E+02 0.09778220E-01 0.04521448E-04 3
 -0.09009462E-07 0.03193718E-10-0.04108508E+05 0.01122885E+03 4
 CH3HCO 120186C 2O 1H 4 G 0300.00 5000.00 1000.00 1
 0.05868650E+02 0.01079424E+00-0.03645530E-04 0.05412912E-08-0.02896844E-12 2
 -0.02264569E+06-0.06012946E+02 0.02505695E+02 0.01336991E+00 0.04671953E-04 3

-0.01128140E-06 0.04263566E-10-0.02124589E+06 0.01335089E+03 4
 CH3CHCO MAR94 C 3H 4O 1 OG 300.00 5000. 1392. 1
 9.40386796E 00 9.90994860E-03-3.34130605E-06 5.13787016E-10-2.96102254E-14 2
 -1.42771281E 04-2.42902025E 01 2.69187311E 00 2.49761396E-02-1.61712107E-05 3
 5.46391115E-09-7.62496644E-13-1.18758805E 04 1.19898101E 01 4
 CH3O 121686C 1H 3O 1 G 0300.00 3000.00 1000.00 1
 0.03770800E+02 0.07871497E-01-0.02656384E-04 0.03944431E-08-0.02112616E-12 2
 0.01278325E+04 0.02929575E+02 0.02106204E+02 0.07216595E-01 0.05338472E-04 3
 -0.07377636E-07 0.02075611E-10 0.09786011E+04 0.01315218E+03 4
 CH3OH 121686C 1H 4O 1 G 0300.00 5000.00 1000.00 1
 0.04029061E+02 0.09376593E-01-0.03050254E-04 0.04358793E-08-0.02224723E-12 2
 -0.02615791E+06 0.02378196E+02 0.02660115E+02 0.07341508E-01 0.07170051E-04 3
 -0.08793194E-07 0.02390570E-10-0.02535348E+06 0.01123263E+03 4
 CH4 121286C 1H 4 G 0300.00 5000.00 1000.00 1
 0.01683479E+02 0.01023724E+00-0.03875129E-04 0.06785585E-08-0.04503423E-12 2
 -0.01008079E+06 0.09623395E+02 0.07787415E+01 0.01747668E+00-0.02783409E-03 3
 0.03049708E-06-0.01223931E-09-0.09825229E+05 0.01372219E+03 4
 CO 121286C 1O 1 G 0300.00 5000.00 1000.00 1
 0.03025078E+02 0.01442689E-01-0.05630828E-05 0.01018581E-08-0.06910952E-13 2
 -0.01426835E+06 0.06108218E+02 0.03262452E+02 0.01511941E-01-0.03881755E-04 3
 0.05581944E-07-0.02474951E-10-0.01431054E+06 0.04848897E+02 4
 CO2 121286C 1O 2 G 0300.00 5000.00 1000.00 1
 0.04453623E+02 0.03140169E-01-0.01278411E-04 0.02393997E-08-0.01669033E-12 2
 -0.04896696E+06-0.09553959E+01 0.02275725E+02 0.09922072E-01-0.01040911E-03 3
 0.06866687E-07-0.02117280E-10-0.04837314E+06 0.01018849E+03 4
 C5H3 20387C 5H 3 G 0300.00 5000.00 1000.00 1
 0.10787622E+02 0.09539619E-01-0.03206744E-04 0.04733323E-08-0.02512135E-12 2
 0.06392904E+06-0.03005444E+03 0.04328720E+02 0.02352480E+00-0.05856723E-04 3
 -0.12154494E-07 0.07726478E-10 0.06588531E+06 0.04173258E+02 4
 H 120186H 1 G 0300.00 5000.00 1000.00 1
 0.02500000E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2
 0.02547163E+06-0.04601176E+01 0.02500000E+02 0.00000000E+00 0.00000000E+00 3
 0.00000000E+00 0.00000000E+00 0.02547163E+06-0.04601176E+01 4
 H2 121286H 2 G 0300.00 5000.00 1000.00 1
 0.02991423E+02 0.07000644E-02-0.05633829E-06-0.09231578E-10 0.01582752E-13 2
 -0.08350340E+04-0.01355110E+02 0.03298124E+02 0.08249442E-02-0.08143015E-05 3
 -0.09475434E-09 0.04134872E-11-0.01012521E+05-0.03294094E+02 4
 !C4H3-123 82489C 4H 3 G 0300.00 4000.00 1000.00 1
 ! 0.01131409E+03 0.05014414E-01-0.05350445E-05-0.02825309E-08 0.05403279E-12 2
 ! 0.05181211E+06-0.03062434E+03 0.06545799E+02 0.01242477E+00 0.05603226E-05 3
 !-0.05631141E-07 0.01665218E-10 0.05352503E+06-0.04264082E+02 4
 !C4H4-123 82489C 4H 4 G 0300.00 4000.00 1000.00 1
 ! 0.01062083E+03 0.07199370E-01-0.06806234E-05-0.04021185E-08 0.07378498E-12 2
 ! 0.03358798E+06-0.03193583E+03 0.03849007E+02 0.01713169E+00 0.01644270E-04 3
 !-0.07761590E-07 0.01947860E-10 0.03608372E+06 0.05732121E+02 4
 H2CCCH 82489C 3H 3 G 0300.00 4000.00 1000.00 1
 0.08831047E+02 0.04357195E-01-0.04109067E-05-0.02368723E-08 0.04376520E-12 2
 0.03847420E+06-0.02177919E+03 0.04754200E+02 0.01108028E+00 0.02793323E-05 3

-0.05479212E-07 0.01949629E-10 0.03988883E+06 0.05854549E+01 4
 -0.02989921E+06 0.06862817E+02 0.03386842E+02 0.03474982E-01-0.06354696E-04 3
 0.06968581E-07-0.02506588E-10-0.03020811E+06 0.02590233E+02 4
 H2O2 120186H 2O 2 G 0300.00 5000.00 1000.00 1
 0.04573167E+02 0.04336136E-01-0.01474689E-04 0.02348904E-08-0.01431654E-12 2
 -0.01800696E+06 0.05011370E+01 0.03388754E+02 0.06569226E-01-0.01485013E-05 3
 -0.04625806E-07 0.02471515E-10-0.01766315E+06 0.06785363E+02 4
 !C4H3 82489C 4H 3 G 0300.00 4000.00 1000.00 1
 ! 0.01075274E+03 0.05381153E-01-0.05549638E-05-0.03052266E-08 0.05761740E-12 2
 ! 0.06121419E+06-0.02973025E+03 0.04153882E+02 0.01726287E+00-0.02389374E-05 3
 !-0.01018700E-06 0.04340505E-10 0.06338071E+06 0.06036507E+02 4
 !HCCO 32387H 1C 2O 1 G 0300.00 4000.00 1000.00 1
 ! 0.06758073E+02 0.02000400E-01-0.02027607E-05-0.01041132E-08 0.01965165E-12 2
 ! 0.01901513E+06-0.09071262E+02 0.05047965E+02 0.04453478E-01 0.02268283E-05 3
 !-0.01482095E-07 0.02250742E-11 0.01965892E+06 0.04818439E+01 4
 HCCOH 32387H 2C 2O 1 G 0300.00 4000.00 1000.00 1
 0.07328324E+02 0.03336416E-01-0.03024705E-05-0.01781106E-08 0.03245168E-12 2
 0.07598258E+05-0.01401214E+03 0.03899465E+02 0.09701075E-01-0.03119309E-05 3
 -0.05537732E-07 0.02465732E-10 0.08701190E+05 0.04491875E+02 4
 HCO 121286H 1C 1O 1 G 0300.00 5000.00 1000.00 1
 0.03557271E+02 0.03345573E-01-0.01335006E-04 0.02470573E-08-0.01713851E-12 2
 0.03916324E+05 0.05552299E+02 0.02898330E+02 0.06199147E-01-0.09623084E-04 3
 0.01089825E-06-0.04574885E-10 0.04159922E+05 0.08983614E+02 4
 HO2 20387H 1O 2 G 0300.00 5000.00 1000.00 1
 0.04072191E+02 0.02131296E-01-0.05308145E-05 0.06112269E-09-0.02841165E-13 2
 -0.01579727E+04 0.03476029E+02 0.02979963E+02 0.04996697E-01-0.03790997E-04 3
 0.02354192E-07-0.08089024E-11 0.01762274E+04 0.09222724E+02 4
 N2 121286N 2 G 0300.00 5000.00 1000.00 1
 0.02926640E+02 0.01487977E-01-0.05684761E-05 0.01009704E-08-0.06753351E-13 2
 -0.09227977E+04 0.05980528E+02 0.03298677E+02 0.01408240E-01-0.03963222E-04 3
 0.05641515E-07-0.02444855E-10-0.01020900E+05 0.03950372E+02 4
 O 120186O 1 G 0300.00 5000.00 1000.00 1
 0.02542060E+02-0.02755062E-03-0.03102803E-07 0.04551067E-10-0.04368052E-14 2
 0.02923080E+06 0.04920308E+02 0.02946429E+02-0.01638166E-01 0.02421032E-04 3
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 O2 121386O 2 G 0300.00 5000.00 1000.00 1
 0.03697578E+02 0.06135197E-02-0.01258842E-05 0.01775281E-09-0.01136435E-13 2
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 0.01313877E-07-0.08768554E-11-0.01005249E+05 0.06034738E+02 4
 OH 121286O 1H 1 G 0300.00 5000.00 1000.00 1
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 0.03886888E+05 0.05595712E+02 0.03637266E+02 0.01850910E-02-0.01676165E-04 3
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 CHOCHO THERM C 2H 2O 2 OG 300. 5000. 1396. 1
 9.75438561E 00 4.97645947E-03-1.74410483E-06 2.75586994E-10-1.61969892E-14 2
 -2.95832896E 04-2.48038370E 01 1.88105121E 00 2.36386368E-02-1.83443295E-05 3
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 IC3H7 MAR95C 3H 7 G 300. 5000. 1381. 1

8.38086577E 00 1.55809528E-02-5.32463008E-06 8.26055541E-10-4.78970959E-14 2
 6.28073262E 03-2.03226081E 01 1.29828769E 00 2.67033333E-02-9.18686715E-06 3
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 0.94282923E 01 0.21911845E-01-0.72831863E-05 0.10622090E-08-0.55580591E-13 2
 0.36300923E 04-0.22419800E 02 0.69567555E 00 0.33100396E-01 0.63189173E-05 3
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 PC4H9 BURCT C 4H 9 0 OG 300.00 5000. 1000.00 1
 0.90141239E 01 0.23985498E-01-0.89440655E-05 0.15295127E-08-0.98013882E-13 2
 0.34599041E 04-0.20575729E 02 0.22069454E 01 0.32849152E-01 0.34258574E-05 3
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 C4H8-2 BURCT C 4H 8 0 OG 300.00 5000. 1000.00 1
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 C4H8-1 BURCT C 4H 8 0 OG 300.00 5000. 1000.00 1
 0.20535841E 01 0.34350507E-01-0.15883197E-04 0.33089662E-08-0.25361045E-12 2
 -0.21397231E 04 0.15556360E 02 0.11811380E 01 0.30853380E-01 0.50865247E-05 3
 -0.24654888E-07 0.11110193E-10-0.17904004E 04 0.21075639E 02 4
 C4H7 BURCT C 4H 7 0 OG 300.00 5000. 1000.00 1
 0.55214200E 01 0.26836840E-01-0.12864300E-04 0.30886400E-08-0.30308560E-12 2
 0.11980440E 05-0.44824470E 01-0.10805140E 01 0.46386860E-01-0.34646970E-04 3
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 CH2CHCHO MAR94 C 3H 4O 1 OG 300.00 5000. 1389. 1
 9.95950056E 00 9.86563039E-03-3.42048051E-06 5.35978370E-10-3.13001966E-14 2
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 8.42301579E-09-1.27327985E-12-9.47146816E 03 2.21264233E 01 4
 CH2CHCO MAR94 C 3H 3O 1 OG 300.00 5000. 1391. 1
 9.48105566E 00 7.77714755E-03-2.71155669E-06 4.26495971E-10-2.49722495E-14 2
 3.20858016E 03-2.42916680E 01 7.83370450E-01 2.90353899E-02-2.28846927E-05 3
 9.25645234E-09-1.52213238E-12 6.13409525E 03 2.20858902E 01 4
 HCOH MAR94 C 1H 2O 1 OG 300. 5000. 1398. 1
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 1.86205951E-08-3.45957838E-12 1.12956672E 04 3.48487757E 01 4
 !CH2 LLNL94C 1H 2 0 OG 300.000 5000.000 1350.000 1
 ! 3.44310466E+00 2.32638011E-03-5.33147998E-07 5.74043968E-11-2.42694849E-15 2
 ! 4.59375743E+04 3.23484714E+00 3.49623989E+00 2.20258645E-03-4.23828799E-07 3
 ! 1.36484706E-11 4.31937372E-15 4.59192771E+04 2.94964354E+00 4
 CH2-S ADJNBRC 1H 2 0 OG 300.000 5000.000 1359.000 1
 3.09627180E+00 2.80839185E-03-7.13614526E-07 8.42136298E-11-3.84640828E-15 2
 5.05739697E+04 4.31392269E+00 3.32340701E+00 2.28062579E-03-2.48156016E-07 3
 -1.02065386E-10 2.48826619E-14 5.04954469E+04 3.09401497E+00 4
 C4H6-12 MAR94 C 4H 6 0 OG 300.000 5000.000 1390.000 1

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 1.37697076E 04-3.19920950E 01 1.13142053E 00 3.44939157E-02-2.14418290E-05 3
 6.84195879E-09-8.94244064E-13 1.72036953E 04 1.89295803E 01 4
 !C4H5-1MA 82489C 4H 5 G 0300.00 4000.00 1000.00 1
 ! 0.01156506E+03 0.08030297E-01-0.07649450E-05-0.04476534E-08 0.08313260E-12 2
 ! 0.03256813E+06-0.03014066E+03 0.05068450E+02 0.01571747E+00 0.02968975E-04 3
 !-0.04990587E-07-0.02984224E-11 0.03518855E+06 0.06791893E+02 4
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 ! 1.15707301E 01 1.10521653E-02-3.74679986E-06 5.78988738E-10-3.35056170E-14 2
 ! 3.28916203E 04-3.61427241E 01 3.87375812E 00 2.35292310E-02-7.91954580E-06 3
 !-1.34382648E-09 9.26833346E-13 3.60697147E 04 7.07337245E 00 4
 C4H5-I 82489C 4H 5 G 0300.00 4000.00 1000.00 1
 0.01199776E+03 0.07990580E-01-0.08098173E-05-0.04568733E-08 0.08636910E-12 2
 0.03228493E+06-0.03528495E+03 0.03879443E+02 0.01997664E+00 0.01872777E-04 3
 -0.09306953E-07 0.02386116E-10 0.03526859E+06 0.09842152E+02 4
 CHCHCHO C 3H 3O 1 G 0300.00 5000.00 1380.00 1
 1.02029457E 01 6.98642466E-03-2.40453423E-06 3.75386729E-10-2.18791232E-14 2
 1.44575591E 04-2.82423192E 01 2.03583477E 00 2.55739847E-02-1.81713324E-05 3
 6.28551145E-09-8.46222353E-13 1.73077219E 04 1.57368973E 01 4
 HCCCHO C 3H 2O 1 G 0300.00 5000.00 1383.00 1
 9.53489086E 00 5.27356380E-03-1.86790292E-06 2.96884935E-10-1.75093893E-14 2
 7.94341348E 03-2.51820453E 01 2.96395961E 00 2.11989287E-02-1.69306862E-05 3
 6.91407180E-09-1.15124164E-12 1.01776675E 04 9.92163123E 00 4
 HCCCO C 3H 1O 1 G 0300.00 5000.00 1453.00 1
 4.72901298E 00 8.55263742E-03-3.11261630E-06 4.45053019E-10-2.03272018E-14 2
 2.88623722E 04 6.44697916E 00 6.40938042E 00 1.15715116E-02-1.02639923E-05 3
 4.52524382E-09-8.02150325E-13 2.70126564E 04-5.92675057E 00 4
 C5H2 20587C 5H 2 G 0300.00 5000.00 1000.00 1
 0.01132917e+03 0.07424057e-01-0.02628189e-04 0.04082541e-08-0.02301333e-12 2
 0.07878706e+06-0.03617117e+03 0.03062322e+02 0.02709998e+00-0.01009170e-03 3
 -0.01272745e-06 0.09167219e-10 0.08114969e+06 0.07071078e+02 4
 H2C4O 120189H 2C 4O 1 G 0300.00 4000.00 1000.00 1
 0.01026888e+03 0.04896164e-01-0.04885081e-05-0.02708566e-08 0.05107013e-12 2
 0.02346903e+06-0.02815985e+03 0.04810971e+02 0.01313999e+00 0.09865073e-05 3
 -0.06120720e-07 0.01640003e-10 0.02545803e+06 0.02113424e+02 4
 C2O 121286C 2O 1 G 0300.00 5000.00 1000.00 1
 0.04849809e+02 0.02947585e-01-0.01090729e-04 0.01792562e-08-0.01115758e-12 2
 0.03282055e+06-0.06453226e+01 0.03368851e+02 0.08241803e-01-0.08765145e-04 3
 0.05569262e-07-0.01540009e-10 0.03317081e+06 0.06713314e+02 4
 H2O 20387H 2O 1 G 0300.00 5000.00 1000.00 1
 0.02672146e+02 0.03056293e-01-0.08730260e-05 0.01200996e-08-0.06391618e-13 2
 -0.02989921e+06 0.06862817e+02 0.03386842e+02 0.03474982e-01-0.06354696e-04 3
 0.06968581e-07-0.02506588e-10-0.03020811e+06 0.02590233e+02 4
 C6H2 121686C 6H 2 G 0300.00 5000.00 1000.00 1
 0.01275652e+03 0.08034381e-01-0.02618215e-04 0.03725060e-08-0.01878851e-12 2
 0.08075469e+06-0.04041263e+03 0.05751085e+02 0.02636720e+00-0.01166760e-03 3
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!from ebg.mech

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! 4.43677044E+00 5.37603907E-03-1.91281674E-06 3.28637895E-10-2.15670953E-14 2
! 2.56676641E+04-2.80033827E+00 2.01356220E+00 1.51904458E-02-1.61631888E-05 3
! 9.07899178E-09-1.91274600E-12 2.61244434E+04 8.80537796E+00 4
!C2H4 121286C 2H 4 G 0300.00 5000.00 1000.00 1
! 3.52841878E+00 1.14851845E-02-4.41838529E-06 7.84460053E-10-5.26684849E-14 2
! 4.42828857E+03 2.23038912E+00-8.61487985E-01 2.79616285E-02-3.38867721E-05 3
! 2.78515220E-08-9.73787891E-12 5.57304590E+03 2.42114868E+01 4
!C2H3 BENSON 88 C 2H 3 0 OG 300.000 5000.000 1384.000 01
! 4.98632615E+00 6.74210478E-03-2.31088203E-06 3.59124380E-10-2.08449928E-14 2
! 3.12665642E+04-2.59023245E+00 2.46978485E+00 1.15950612E-02-6.06325764E-06 3
! 1.85458682E-09-2.87093484E-13 3.23161752E+04 1.14112313E+01 4
!CH2O 121286C 1H 2O 1 G 0300.00 5000.00 1000.00 1
! 2.99560618E+00 6.68132119E-03-2.62895469E-06 4.73715289E-10-3.21251747E-14 2
! -1.53203691E+04 6.91257238E+00 1.65273118E+00 1.26314387E-02-1.88816848E-05 3
! 2.05003143E-08-8.41323712E-12-1.48654043E+04 1.37848196E+01 4
!CH2OH 120186H 3C 1O 1 G 0250.00 4000.00 1000.00 1
! 6.32752037E+00 3.60827078E-03-3.20154726E-07-1.93874999E-10 3.50970473E-14 2
! -4.47450928E+03-8.32936573E+00 2.86262846E+00 1.00152725E-02-5.28543581E-07 3
! -5.13853982E-09 2.24604103E-12-3.34967871E+03 1.03979378E+01 4
!CH3 121286C 1H 3 G 0300.00 5000.00 1000.00 1
! 2.84405160E+00 6.13797410E-03-2.23034522E-06 3.78516080E-10-2.45215903E-14 2
! 1.64378086E+04 5.45269728E+00 2.43044281E+00 1.11240987E-02-1.68022034E-05 3
! 1.62182872E-08-5.86495262E-12 1.64237813E+04 6.78979397E+00 4
!CH3O 121686C 1H 3O 1 G 0300.00 3000.00 1000.00 1
! 3.77079964E+00 7.87149742E-03-2.65638391E-06 3.94443145E-10-2.11261638E-14 2
! 1.27832520E+02 2.92957497E+00 2.10620403E+00 7.21659511E-03 5.33847197E-06 3
! -7.37763628E-09 2.07561052E-12 9.78601074E+02 1.31521769E+01 4
!CH4 121286C 1H 4 G 0300.00 5000.00 1000.00 1
! 1.68347883E+00 1.02372356E-02-3.87512864E-06 6.78558487E-10-4.50342312E-14 2
! -1.00807871E+04 9.62339497E+00 7.78741479E-01 1.74766835E-02-2.78340904E-05 3
! 3.04970804E-08-1.22393068E-11-9.82522852E+03 1.37221947E+01 4
!CO 121286C 1O 1 G 0300.00 5000.00 1000.00 1
! 3.02507806E+00 1.44268852E-03-5.63082779E-07 1.01858133E-10-6.91095156E-15 2
! -1.42683496E+04 6.10821772E+00 3.26245165E+00 1.51194085E-03-3.88175522E-06 3
! 5.58194424E-09-2.47495123E-12-1.43105391E+04 4.84889698E+00 4
!CO2 121286C 1O 2 G 0300.00 5000.00 1000.00 1
! 4.45362282E+00 3.14016873E-03-1.27841054E-06 2.39399667E-10-1.66903319E-14 2
! -4.89669609E+04-9.55395877E-01 2.27572465E+00 9.92207229E-03-1.04091132E-05 3
! 6.86668678E-09-2.11728009E-12-4.83731406E+04 1.01884880E+01 4
!H 120186H 1 G 0300.00 5000.00 1000.00 1
! 2.50000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2
! 2.54716270E+04-4.60117638E-01 2.50000000E+00 0.00000000E+00 0.00000000E+00 3
! 0.00000000E+00 0.00000000E+00 2.54716270E+04-4.60117608E-01 4
!H2 121286H 2 G 0300.00 5000.00 1000.00 1
! 2.99142337E+00 7.00064411E-04-5.63382869E-08-9.23157818E-12 1.58275179E-15 2

!-8.35033997E+02-1.35511017E+00 3.29812431E+00 8.24944174E-04-8.14301529E-07 3
 !-9.47543433E-11 4.13487224E-13-1.01252087E+03-3.29409409E+00 4
 !H2O 20387H 2O 1 G 0300.00 5000.00 1000.00 1
 ! 2.67214561E+00 3.05629289E-03-8.73026011E-07 1.20099639E-10-6.39161787E-15 2
 !-2.98992090E+04 6.86281681E+00 3.38684249E+00 3.47498246E-03-6.35469633E-06 3
 ! 6.96858127E-09-2.50658847E-12-3.02081133E+04 2.59023285E+00 4
 !H2O2 120186H 2O 2 G 0300.00 5000.00 1000.00 1
 ! 4.57316685E+00 4.33613639E-03-1.47468882E-06 2.34890357E-10-1.43165356E-14 2
 !-1.80069609E+04 5.01136959E-01 3.38875365E+00 6.56922581E-03-1.48501258E-07 3
 !-4.62580552E-09 2.47151475E-12-1.76631465E+04 6.78536320E+00 4
 !HCCO 32387H 1C 2O 1 G 0300.00 4000.00 1000.00 1
 ! 6.75807285E+00 2.00040033E-03-2.02760731E-07-1.04113183E-10 1.96516472E-14 2
 ! 1.90151328E+04-9.07126236E+00 5.04796505E+00 4.45347792E-03 2.26828277E-07 3
 !-1.48209456E-09 2.25074150E-13 1.96589180E+04 4.81843948E-01 4
 !HCO 121286H 1C 1O 1 G 0300.00 5000.00 1000.00 1
 ! 3.55727124E+00 3.34557286E-03-1.33500600E-06 2.47057264E-10-1.71385089E-14 2
 ! 3.91632446E+03 5.55229950E+00 2.89832974E+00 6.19914662E-03-9.62308423E-06 3
 ! 1.08982494E-08-4.57488518E-12 4.15992188E+03 8.98361397E+00 4
 !HO2 20387H 1O 2 G 0300.00 5000.00 1000.00 1
 ! 4.07219124E+00 2.13129632E-03-5.30814532E-07 6.11226902E-11-2.84116471E-15 2
 ! 9.36629296E+01 3.47602940E+00 2.97996306E+00 4.99669695E-03-3.79099697E-06 3
 ! 2.35419240E-09-8.08902424E-13 4.29135834E+02 9.22272396E+00 4
 !N2 121286N 2 G 0300.00 5000.00 1000.00 1
 ! 2.92664003E+00 1.48797676E-03-5.68476082E-07 1.00970378E-10-6.75335134E-15 2
 !-9.22797669E+02 5.98052788E+00 3.29867697E+00 1.40824041E-03-3.96322230E-06 3
 ! 5.64151526E-09-2.44485487E-12-1.02089990E+03 3.95037222E+00 4
 !O 120186O 1 G 0300.00 5000.00 1000.00 1
 ! 2.54205966E+00-2.75506191E-05-3.10280335E-09 4.55106742E-12-4.36805150E-16 2
 ! 2.92308027E+04 4.92030811E+00 2.94642878E+00-1.63816649E-03 2.42103170E-06 3
 !-1.60284319E-09 3.89069636E-13 2.91476445E+04 2.96399498E+00 4
 !O2 121386O 2 G 0300.00 5000.00 1000.00 1
 ! 3.69757819E+00 6.13519689E-04-1.25884199E-07 1.77528148E-11-1.13643531E-15 2
 !-1.23393018E+03 3.18916559E+00 3.21293640E+00 1.12748635E-03-5.75615047E-07 3
 ! 1.31387723E-09-8.76855392E-13-1.00524902E+03 6.03473759E+00 4
 !OH 121286O 1H 1 G 0300.00 5000.00 1000.00 1
 ! 2.88273048E+00 1.01397431E-03-2.27687707E-07 2.17468370E-11-5.12630534E-16 2
 ! 3.88688794E+03 5.59571219E+00 3.63726592E+00 1.85091049E-04-1.67616463E-06 3
 ! 2.38720266E-09-8.43144185E-13 3.60678174E+03 1.35886049E+00 4
 !C4H4 121686C 4H 4 G 0300.00 5000.00 1000.00 1
 ! 8.89214897E+00 1.09088495E-02-3.59495971E-06 5.19341903E-10-2.68089214E-14 2
 ! 3.32843477E+04-2.17269440E+01 2.14033699E+00 2.46050470E-02-3.63916570E-06 3
 !-1.53040141E-08 8.89646083E-12 3.53740000E+04 1.42824774E+01 4
 !C5H6 20387C 5H 6 G 0300.00 5000.00 1000.00 1
 ! 9.68981457E+00 1.83826201E-02-6.26488418E-06 9.39337719E-10-5.08770814E-14 2
 ! 1.10212422E+04-3.12290802E+01-3.19673920E+00 4.08136100E-02 6.81650533E-07 3
 !-3.13745900E-08 1.57722307E-11 1.52906758E+04 3.86993866E+01 4
 !C6H6 20387C 6H 6 G 0300.00 5000.00 1000.00 1
 1.29107399E+01 1.72329657E-02-5.02421062E-06 5.89349680E-10-1.94752119E-14 2

3.66451172E+03-5.00269928E+01-3.13801193E+00 4.72310297E-02-2.96220787E-06 3
 -3.26281899E-08 1.71869186E-11 8.89003125E+03 3.65757294E+01 4
 !C4H6 PW-APIC 4H 6 G 300.000 5000.000 1
 !+4.55600000E+00+2.57600004E-02-1.21199997E-05+2.18799999E-09+0.00000000E+00 2
 !+1.06500000E+04-1.23400000E-01-2.52900000E+00+5.42100008E-02-5.37399986E-05 3
 !+2.85200003E-08-6.08799998E-12+1.20200000E+04+3.39200000E+01 4
 C6H5 L12/84C 6H 5 0 OG 300.000 5000.000 1000.000 1
 0.11431418E+02 0.17019045E-01-0.58387241E-05 0.88094687E-09-0.48050417E-13 2
 0.33942348E+05-0.38574219E+02-0.23405075E+01 0.42760305E-01-0.25518166E-05 3
 -0.30668716E-07 0.16245519E-10 0.38376734E+05 0.35617355E+02 4
 C6H5O L12/84C 6H 5O 1 OG 300.000 5000.000 1000.000 1
 0.13833984E+02 0.17618403E-01-0.60696257E-05 0.91988173E-09-0.50449181E-13 2
 -0.69212549E+03-0.50392990E+02-0.18219433E+01 0.48122510E-01-0.46792302E-05 3
 -0.34018594E-07 0.18649637E-10 0.42429180E+04 0.33526199E+02 4
 C6H5OH L12/84C 6H 6O 1 OG 300.000 5000.000 1000.000 1
 0.14930705E+02 0.18346462E-01-0.61796381E-05 0.91533114E-09-0.48830826E-13 2
 -0.18379656E+05-0.55983917E+02-0.16495714E+01 0.52105546E-01-0.69632842E-05 3
 -0.36011539E-07 0.20483074E-10-0.13292336E+05 0.32357330E+02 4
 !C4H5 BENSON 88 C 4H 5 0 OG 300.000 5000.000 1400.000 11
 ! 1.09319148E+01 1.12577926E-02-3.82466213E-06 5.90906138E-10-3.41605706E-14 2
 ! 3.55451038E+04-3.26454973E+01 6.94982037E-01 4.01246346E-02-3.60998164E-05 3
 ! 1.71826737E-08-3.27377307E-12 3.86582614E+04 2.06646321E+01 4
 !C5H4O T8/99C 5H 4O 1 OG 200.000 6000.000 1000.000 1
 ! 1.00806824E+01 1.61143465E-02-5.83314509E-06 9.46759320E-10-5.68972206E-14 2
 ! 1.94364771E+03-2.94521623E+01 2.64576497E-01 3.34873827E-02 1.67738470E-06 3
 !-2.96207455E-08 1.54431476E-11 5.11159287E+03 2.35409513E+01 6.64245999E+03 4
 !C5H5 BOZZELLI C 5H 5 0 OG 300.000 5000.000 1400.000 01
 ! 1.34351894E+01 1.26452160E-02-4.42858813E-06 6.98682634E-10-4.09970231E-14 2
 ! 2.06536455E+04-5.32987048E+01-6.29416088E+00 6.57550731E-02-6.00914914E-05 3
 ! 2.73875793E-08-4.92425888E-12 2.67607327E+04 5.00994833E+01 4
 C5H4OH THERM C 5H 5O 1 OG 300.000 5000.000 1406.000 01
 1.49801651E+01 1.29977504E-02-4.44659387E-06 6.90532769E-10-4.00736033E-14 2
 -6.21452008E+02-5.56115890E+01-4.12577307E+00 6.80489898E-02-6.60482345E-05 3
 3.19378134E-08-6.02014894E-12 4.94419361E+03 4.32564735E+01 4
 C6H5CH3 T 9/81C 7H 8 0 OG 300.000 5000.000 1000.000 01
 0.13957725E+02 0.24616607E-01-0.83795358E-05 0.12537165E-08-0.67675520E-13 2
 -0.10295066E+04-0.52245728E+02-0.25368824E+01 0.52898869E-01 0.14038515E-05 3
 -0.40762323E-07 0.20377519E-10 0.44778477E+04 0.37415115E+02 4
 C6H5C2H5 C 8H 10 0 OG 300.000 5000.000 1397.000 21
 2.02816724E+01 2.59464082E-02-8.92667064E-06 1.39161163E-09-8.09786280E-14 2
 -6.88695837E+03-8.65892579E+01-5.93600077E+00 8.94618416E-02-6.81230510E-05 3
 2.66103734E-08-4.21398102E-12 1.94317497E+03 5.33309542E+01 4
 C6H5CH2OH 3/ 8/90 C 7H 8O 1 OG 300.000 5000.000 1396.000 21
 1.81575155E+01 2.26620146E-02-7.79454113E-06 1.21491074E-09-7.06883434E-14 2
 -2.13319736E+04-7.19512787E+01-3.72475901E+00 7.42375044E-02-5.41481788E-05 3
 2.01178934E-08-3.02199053E-12-1.38224993E+04 4.53342817E+01 4
 BIBENZYL C 14H 14 0 OG 300.000 5000.000 1392.000 21
 3.48131330E+01 3.78396057E-02-1.27934440E-05 1.97366490E-09-1.14091685E-13 2

-3.11362732E+02-1.63384186E+02-1.05318902E+01 1.48504587E-01-1.15713218E-04 3
 4.52836955E-08-7.06388895E-12 1.47378885E+04 7.80962493E+01 4
 HOC6H4CH3 AVG CRESOL C 7H 8O 1 OG 300.000 5000.000 1400.000 21
 1.97311724E+01 2.12245074E-02-7.27602659E-06 1.13158989E-09-6.57395287E-14 2
 -2.50451776E+04-8.18783394E+01-4.17663565E+00 8.29479164E-02-6.92618926E-05 3
 2.97047387E-08-5.12027914E-12-1.73715284E+04 4.43681107E+01 4
 OC6H4CH3 AVG CRESOL C 7H 7O 1 OG 300.000 5000.000 1398.000 11
 2.00333477E+01 1.83142467E-02-6.17265091E-06 9.50353551E-10-5.48634044E-14 2
 -7.76864165E+03-8.60606102E+01-3.82920147E+00 7.73376217E-02-6.15929083E-05 3
 2.43728641E-08-3.80779615E-12 2.89377185E+01 4.06647799E+01 4
 C5H5O 5/16/90 THERMC 5H 5O 1 OG 300.000 5000.000 1392.000 01
 1.48322894E+01 1.40483376E-02-4.92302051E-06 7.77041219E-10-4.56103939E-14 2
 1.45523665E+04-5.73228191E+01-2.83112840E+00 5.67277287E-02-4.44757303E-05 3
 1.74924447E-08-2.76004847E-12 2.04992154E+04 3.69634411E+01 4
 C6H5C2H3 TRC TABLES C 8H 8 O 0 OG 300.000 5000.000 1400.000 11
 1.94675525E+01 2.19916239E-02-7.56672249E-06 1.17967158E-09-6.86483959E-14 2
 8.16106600E+03-8.19394370E+01-5.75443698E+00 8.70398896E-02-7.28533682E-05 3
 3.12720079E-08-5.39379278E-12 1.62673706E+04 5.12775455E+01 4
 C6H5CHO 5/16/90 THERMC 7H 6O 1 OG 300.000 5000.000 1386.000 11
 1.74024893E+01 1.89508317E-02-6.58694307E-06 1.03413046E-09-6.04793155E-14 2
 -1.31418522E+04-6.83371315E+01-2.37082285E+00 6.28843128E-02-4.26460754E-05 3
 1.39416083E-08-1.74474949E-12-6.11656186E+03 3.85478773E+01 4
 C6H5CO THERM C 7H 5O 1 OG 300.000 5000.000 1392.000 11
 1.75116258E+01 1.62650511E-02-5.65051892E-06 8.86922680E-10-5.18657990E-14 2
 4.67641545E+03-6.70531966E+01-1.56729686E+00 5.99817511E-02-4.29153585E-05 3
 1.48666854E-08-1.98938453E-12 1.12873830E+04 3.55490009E+01 4
 C6H5CH2 TROE,JPC,1990 C 7H 7 O 0 OG 300.000 5000.000 1392.000 11
 1.77752663E+01 1.88366755E-02-6.58968982E-06 1.03873424E-09-6.09096279E-14 2
 1.65061292E+04-7.37168331E+01-3.82523574E+00 7.22854694E-02-5.81397283E-05 3
 2.40211852E-08-4.03015544E-12 2.37153019E+04 4.12436407E+01 4
 !CH2 120186C 1H 2 G 0250.00 4000.00 1000.00 1
 ! 3.63640785E+00 1.93305663E-03-1.68701632E-07-1.00989939E-10 1.80825576E-14 2
 ! 4.53413398E+04 2.15656066E+00 3.76223707E+00 1.15981908E-03 2.48958543E-07 3
 ! 8.80083562E-10-7.33243544E-13 4.53679063E+04 1.71257758E+00 4
 C6H4O2 O=C6H4=O T10/97C 6H 4O 2 G 0200.00 6000.00 0298.00 1
 1.43886174E+01 1.81624210E-02-6.69934678E-06 1.10097880E-09-6.67372266E-14 2
 -2.12444054E+04-5.02572901E+01 3.79867882E+00 2.51676569E-02 3.79846917E-05 3
 -7.06777516E-08 3.06126573E-11-1.72429606E+04 9.80455363E+00-1.478138819-04 4
 NE L10/90NE 100 0 0 OG 200.000 6000.000 1000. 1
 0.250000000E 01 0.000000000E 00 0.000000000E 00 0.000000000E 00 0.000000000E 00 2
 -0.74537500E 03 0.33553227E 01 0.250000000E 01 0.000000000E 00 0.000000000E 00 3
 0.000000000E 00-0.74537498E 03 0.33553227E 01 0.000000000E 00 0.000000000E+00 4
 C3H3 C 3H 3O 00 OG 300.00 5000.00 1000.00 1
 0.73698450E+01 0.77854710E-02-0.30216960E-05 0.55099410E-09-0.37929260E-13 2
 0.38891950E+05-0.14110520E+02 0.56629250E+01 0.43052760E-02 0.18210260E-04 3
 -0.25694770E-07 0.10163000E-10 0.39782900E+05-0.32569600E+01 4
 !MXYLENE C 8H 10O 0 OG 300.00 5000.00 1000.00 1
 !0.104572604E+02 0.403200160E-01-0.145441770E-04 0.173870560E-08 0.000000000E+00 2

!-0.392485555E+04-0.316838798E+02-0.365621300E+01 0.742185790E-01-0.400008720E-04 3
 !0.741031100E-08 0.000000000E+00 0.307000000E+03 0.427477900E+02 4
 !S. Gail, P. Dagaut, Combust. Sci. Technol. 179 (2007) 813-844.
 MXYLENE (CH₃PCH₃) C 8H 10O 0 OG 300.00 5000.00 1000.00 1
 0.16647870E+02 0.29035770E-01-0.97813380E-05 0.15518060E-08-0.95333120E-13 2
 -0.62956210E+04-0.65045590E+02-0.33455100E+01 0.74388260E-01-0.41786820E-04 3
 0.70195840E-08 0.10659790E-11 0.90807260E+02 0.41601160E+02
 !MXYLYL C 8H 9 G 300.00 5000.00 1000.00 1
 !.808697123E+01 .442230490E-01-.196920930E-04 .391313300E-08-.286780230E-12 2
 !.152828351E+05-.180507988E+02-.244083000E+01 .750206000E-01-.520941000E-04 3
 !.184357000E-07-.267709000E-11 .180599500E+05 .358328500E+02 4
 MXYLYL (CH₂O.PCH₃) C 8H 9O 0 OG 300.00 5000.00 1000.00 1
 0.18378920E+02 0.23689200E-01-0.71096300E-05 0.10401590E-08-0.60499030E-13 2
 0.11252820E+05-0.73134180E+02-0.37325740E+01 0.75464460E-01-0.47955850E-04 3
 0.13161630E-07-0.10021160E-11 0.18250060E+05 0.44449420E+02 4
 C₆H₄CH₃ C 7H 7 G 300.00 5000.00 1000.00 1
 .989521100E+01 .281997140E-01-.985390310E-05 .114532240E-08 .000000000E+00 2
 .307512908E+05-.257557742E+02-.298827000E+01 .621039310E-01-.390118950E-04 3
 .928257830E-08 .000000000E+00 .343676800E+05 .412025200E+02 4
 !C₆H₄CH₃ (C₆H₄CH₃) C 7H 7O 0 OG 300.00 5000.00 1391.00 1
 ! 1.51717348E+01 2.07638164E-02-7.18894216E-06 1.12523916E-09-6.56552624E-14 2
 ! 2.87540716E+04-5.62266630E+01-2.93038658E+00 6.39472228E-02-4.750227752E-05 3
 ! 1.86740296E-08-3.05581252E-12 3.50135512E+04 4.07804853E+01 4
 MCPHHCO (CHOPCH₃) C 8H 8O 1 OG 300.00 5000.00 1000.00 1
 0.34314480E+02 0.53513460E-02-0.92993860E-06 0.91253410E-10-0.40939840E-14 2
 -0.24140030E+05-0.16173510E+03-0.26138220E+01 0.72302110E-01-0.32412460E-04 3
 -0.20096620E-09 0.17424710E-11-0.10469190E+05 0.41807790E+02 4
 MDICPCH₂ C 16H 18O 0 OG 300.00 5000.00 1000.00 1
 0.33497230E+02 0.54076470E-01-0.18088160E-04 0.28564020E-08-0.17497360E-12 2
 -0.70937810E+04-0.14859210E+03-0.73599560E+01 0.14953880E+00-0.88664480E-04 3
 0.16880390E-07 0.17433840E-11 0.56680030E+04 0.68310890E+02 4
 MCPHC₂H₅ (C₂H₅PCH₃) C 9H 12O 0 OG 300.00 5000.00 1000.00 1
 0.19182900E+02 0.34046430E-01-0.11405070E-04 0.18038730E-08-0.11067130E-12 2
 -0.99729390E+04-0.76296090E+02-0.38242200E+01 0.87266150E-01-0.50414030E-04 3
 0.96332090E-08 0.83993700E-12-0.27201520E+04 0.46068790E+02 4
 MCPCH₂OH (CH₂OHPCCH₃) C 8H 10O 1 OG 300.00 5000.00 1000.00 1
 0.16887690E+02 0.32314620E-01-0.11135800E-04 0.17935490E-08-0.11124940E-12 2
 -0.24586000E+05-0.62109060E+02-0.50522800E+01 0.84040540E-01-0.49347200E-04 3
 0.87637670E-08 0.13207010E-11-0.17800800E+05 0.54145290E+02 4
 !MOC₇H₇ (MOC₇H₇) C 7H 7O 1 OG 300.00 5000.00 1000.00 1
 ! 0.63262340E+01 0.37092070E-01-0.13736960E-04 0.23284710E-08-0.14970180E-12 2
 !-0.15663590E+04-0.46862110E+01-0.40396440E+01 0.73990950E-01-0.51594530E-04 3
 ! 0.12037280E-07 0.14321020E-11 0.22570760E+03 0.45316930E+02 4
 !MECPD (MECYCPD) C 6H 8O 0 OG 300.00 5000.00 1394.00 1
 ! 1.78193604E+01 1.86879442E-02-6.51189213E-06 1.02368138E-09-5.99106820E-14 2
 ! 5.71479259E+02-8.87416624E+01-4.01993754E+00 7.70950833E-02-6.84038057E-05 3
 ! 3.14230695E-08-5.79515934E-12 7.49152592E+03 2.60541010E+01 4
 !MECPDY C 6H 7N 00 OG 300.00 5000.00 1000.00 1

! 0.12067100E+02 0.22730360E-01-0.87475070E-05 0.15922850E-08-0.10961430E-12 2
 ! 0.41075070E+05-0.40039970E+02-0.39368920E+01 0.66762740E-01-0.49636890E-04 3
 ! 0.13074990E-07 0.12686790E-11 0.45546340E+05 0.42751860E+02 4
 MCPHCO (COPCH3) C 8H 7O 1 OG 300.00 5000.00 1000.00 1
 0.32990220E+02 0.43029030E-02-0.55945810E-06 0.42393140E-10-0.15349900E-14 2
 -0.61630250E+04-0.15457930E+03-0.15912640E+01 0.60664560E-01-0.15055830E-04 3
 -0.11912520E-07 0.46650820E-11 0.71251610E+04 0.38005990E+02 4
 MCSTYREN (C2H3PCH3) C 9H 10O 0 OG 300.00 5000.00 1000.00 1
 0.25318780E+01 0.57574760E-01-0.23912700E-04 0.43935050E-08-0.29898470E-12 2
 0.11259870E+05 0.16482140E+02-0.43402420E+01 0.88487020E-01-0.59176050E-04 3
 0.13820620E-07 0.14154160E-11 0.11730650E+05 0.47101510E+02
 PHCH2O C 7H 7O 10 OG 300.00 3000.00 1000.00 1
 0.11786960E+02 0.28687710E-01-0.98102230E-05 0.15723720E-08-0.97249460E-13 2
 0.76002110E+04-0.37226230E+02-0.70223900E+01 0.81629680E-01-0.61132220E-04 3
 0.20734560E-07-0.20847660E-11 0.12652870E+05 0.59532670E+02 4
 !MCC6H4OH C 7H 8O 1 OG 300.00 5000.00 1000.00 1
 ! 0.39369160E+01 0.45799220E-01-0.18917840E-04 0.34624380E-08-0.23498170E-12 2
 !-0.18224990E+05 0.74718090E+01-0.38386040E+01 0.77129970E-01-0.53355110E-04 3
 ! 0.12948980E-07 0.10976630E-11-0.17273920E+05 0.43575740E+02 4
 MACPHC2H4 (C2H4PCH3) C 9H 11O 0 OG 300.00 5000.00 1000.00 1
 0.21375000E+02 0.27190600E-01-0.79764670E-05 0.11452270E-08-0.65605530E-13 2
 0.13781850E+05-0.86004420E+02-0.47549540E+01 0.96699280E-01-0.79417750E-04 3
 0.37274610E-07-0.81320850E-11 0.21552180E+05 0.50680390E+02 4
 MBCPHC2H4 (C2H4PCH3) C 9H 11O 0 OG 300.00 5000.00 1000.00 1
 0.19779610E+02 0.29570700E-01-0.89982020E-05 0.13293930E-08-0.77833950E-13 2
 0.67619300E+04-0.78706970E+02-0.23091100E+01 0.78991550E-01-0.43555440E-04 3
 0.76394560E-08 0.84124740E-12 0.13897970E+05 0.39401150E+02 4
 MACSTYRYL C 9H 9O 0 OG 300.00 5000.00 1000.00 1
 0.59224950E+01 0.47364970E-01-0.17948140E-04 0.30915130E-08-0.20099750E-12 2
 0.39277050E+05-0.94177250E-01-0.44372500E+01 0.90770130E-01-0.73354950E-04 3
 0.28968650E-07-0.37540560E-11 0.40644480E+05 0.48029200E+02 4
 MBCSTYRYL C 9H 9O 0 OG 300.00 5000.00 1000.00 1
 0.38672210E+01 0.50532640E-01-0.19469200E-04 0.33915160E-08-0.22218080E-12 2
 0.34658950E+05 0.96695180E+01-0.26840510E+01 0.74822930E-01-0.39813530E-04 3
 0.10572310E-08 0.46766310E-11 0.35450330E+05 0.40359370E+02 4
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 !R. Sivaramakrishnan, R. S. Tranter, K. Brezinsky, J. Phys. Chem. A 110 (2006) 9400-9404.
 C6H5CHCH3 C 8H 9 G 200.000 6000.000 1000.00 1
 0.15287640E+02 0.29990204E-01-0.10786412E-04 0.17441075E-08-0.10457587E-12 2
 0.13540395E+05-0.56228770E+02 0.20579304E+01 0.35354050E-01 0.52500310E-04 3
 -0.88002034E-07 0.34220708E-10 0.18564087E+05 0.19485681E+02 4
 !C6H4 C 6H 4 0 OG 200.000 6000.000 1000.000 1
 ! 0.11268285E+02 0.15349395E-01-0.56344998E-05 0.92384008E-09-0.55940616E-13 2
 ! 0.48518069E+05-0.37146485E+02-0.21078633E+00 0.33398132E-01 0.90937199E-05 3
 !-0.36762523E-07 0.16332537E-10 0.52207261E+05 0.25200286E+02 4
 !LC6H5 CHAIN C 6H 5 G 200.000 6000.000 1000.000 1
 ! 0.13411768E+02 0.14720221E-01-0.50817705E-05 0.79886354E-09-0.46950844E-13 2
 ! 0.58503716E+05-0.41652032E+02 0.77929707E+00 0.54372126E-01-0.47873814E-04 3

! 0.16187164E-07 0.33735744E-12 0.61650312E+05 0.22128592E+02 0.63908517E+05 4
 C12H10 C 12H 10 0 OG 200.000 6000.000 1000.000 1
 0.23054912E+02 0.37211298E-01-0.13575905E-04 0.22166739E-08-0.13383140E-12 2
 0.11423256E+05-0.10106385E+03-0.13137417E+01 0.67444963E-01 0.41935024E-04 3
 -0.10203156E-06 0.42738465E-10 0.19659035E+05 0.33311055E+02 4
 C8H6 C6H5CCH T 9/96C 8H 6 0 OG 200.000 6000.000 1000.00 1
 0.15638086E+02 0.22068432E-01-0.80253111E-05 0.13065013E-08-0.78679279E-13 2
 0.32272867E+05-0.59610868E+02-0.87234720E+00 0.51839614E-01 0.66079738E-05 3
 -0.55950961E-07 0.29284749E-10 0.37461628E+05 0.29096304E+02 0.39467283E+05 4
 C6H5CHCH C 8H 7 G 200.000 6000.000 1000.00 1
 0.15201622E+02 0.24850095E-01-0.89709186E-05 0.14545758E-08-0.87397992E-13 2
 0.39496232E+05-0.55941799E+02 0.35717627E+00 0.44119131E-01 0.22288648E-04 3
 -0.59493882E-07 0.25176903E-10 0.44470559E+05 0.25701259E+02 4
 C6H5CCCH2 C 8H 7 G 200.000 6000.000 1000.00 1
 0.15292349E+02 0.24764175E-01-0.89385839E-05 0.14491892E-08-0.87068705E-13 2
 0.34154585E+05-0.55612559E+02 0.87562719E+00 0.44082140E-01 0.19607851E-04 3
 -0.55930690E-07 0.23845132E-10 0.38955375E+05 0.23527021E+02 4
 C6H4C2H C 8H 5 G 300.000 5000.000 1403.00 1
 1.88370382E+01 1.52445522E-02-5.22469596E-06 8.12518874E-10-4.72045178E-14 2
 5.96821996E+04-7.49107592E+01-1.49929738E+00 7.01891496E-02-6.29429910E-05 3
 2.85073827E-08-5.11137313E-12 6.59494823E+04 3.15838359E+01 4
 C6H5CH2CH2 C 8H 9 G 200.000 6000.000 1000.00 1
 0.15713016E+02 0.29561041E-01-0.10620112E-04 0.17159167E-08-0.10283102E-12 2
 0.21376525E+05-0.57667434E+02 0.19438548E+01 0.38314651E-01 0.45734025E-04 3
 -0.82176543E-07 0.32451043E-10 0.26446509E+05 0.20341568E+02 4
 !CH3C6H4CH2 C 8H 9 G 200.000 6000.000 1000.00 1
 ! 0.15538124E+02 0.29727507E-01-0.10684969E-04 0.17271861E-08-0.10354839E-12 2
 ! 0.13295908E+05-0.56697173E+02 0.15032281E+01 0.42011928E-01 0.36671141E-04 3
 !-0.73698715E-07 0.29716717E-10 0.18295645E+05 0.21976876E+02 4
 !Xylene4 C 8H 10 G 200.000 6000.000 1000.00 1
 ! 0.14714242E+02 0.33186418E-01-0.11937686E-04 0.19302611E-08-0.11573164E-12 2
 !-0.53374060E+04-0.50503587E+02 0.41067722E+01 0.24132089E-01 0.78870118E-04 3
 !-0.11009248E-06 0.40761006E-10-0.64170171E+03 0.13542374E+02 4
 !p-CH3C6H4 C 7H 7 G 200.000 6000.000 1000.00 1
 ! 0.12719765E+02 0.24396683E-01-0.88059622E-05 0.14273815E-08-0.85734838E-13 2
 ! 0.29893851E+05-0.41997747E+02 0.20708625E+01 0.26634291E-01 0.48374631E-04 3
 !-0.77051017E-07 0.29623366E-10 0.34041532E+05 0.19466555E+02 4
 !R1C9H9 C 9H 9 G 200.000 6000.000 1000.00 1
 ! 0.16768085E+02 0.31643066E-01-0.11478226E-04 0.18706995E-08-0.11301675E-12 2
 ! 0.33365581E+05-0.62390466E+02 0.27049358E+01 0.37763739E-01 0.54538651E-04 3
 !-0.92272477E-07 0.35955759E-10 0.38684807E+05 0.17989083E+02 4
 !R4C9H9 C 9H 9 G 200.000 6000.000 1000.00 1
 ! 0.17120394E+02 0.31191509E-01-0.11284715E-04 0.18361120E-08-0.11080573E-12 2
 ! 0.36322192E+05-0.65237314E+02 0.14227277E+01 0.46839532E-01 0.35957214E-04 3
 !-0.76801149E-07 0.31334170E-10 0.41818857E+05 0.22280513E+02 4
 !pc-C9H9 C 9H 9 G 200.000 6000.000 1000.00 1
 ! 0.17853687E+02 0.30287573E-01-0.10878393E-04 0.17578754E-08-0.10537320E-12 2
 ! 0.23528648E+05-0.70743355E+02-0.73945866E+00 0.59495231E-01 0.13057509E-04 3

!-0.59364319E-07 0.26466407E-10 0.29505524E+05 0.30249058E+02 4
 !R2C9H9 C 9H 9 G 200.000 6000.000 1000.00 1
 ! 0.16770528E+02 0.31671831E-01-0.11495510E-04 0.18742252E-08-0.11325824E-12 2
 ! 0.32304781E+05-0.62806283E+02 0.32505929E+01 0.35221379E-01 0.58975459E-04 3
 !-0.95636615E-07 0.36897000E-10 0.37535278E+05 0.15052139E+02 4
 !s-C9H8 C 9H 8 G 200.000 6000.000 1000.00 1
 ! 0.16783183E+02 0.28786366E-01-0.10387265E-04 0.16836020E-08-0.10112900E-12 2
 ! 0.26536867E+05-0.63759322E+02 0.10321802E+01 0.46189544E-01 0.31909218E-04 3
 !-0.72114887E-07 0.29748702E-10 0.31967109E+05 0.23630370E+02 4
 !R3C9H9 C 9H 9 G 200.000 6000.000 1000.00 1
 ! 0.17086183E+02 0.31234676E-01-0.11303477E-04 0.18395251E-08-0.11102749E-12 2
 ! 0.35870324E+05-0.65411567E+02 0.12753067E+01 0.47391407E-01 0.35091586E-04 3
 !-0.76177289E-07 0.31164869E-10 0.41386838E+05 0.22638463E+02 4
 !R13C9H9 C 9H 9 G 200.000 6000.000 1000.00 1
 ! 0.16896527E+02 0.31437513E-01-0.11384195E-04 0.18534120E-08-0.11189553E-12 2
 ! 0.35672282E+05-0.64033565E+02 0.17801818E+01 0.43749859E-01 0.42376835E-04 3
 !-0.82140307E-07 0.32924793E-10 0.41103203E+05 0.20932320E+02 4
 !i-C9H9 C 9H 9 G 200.000 6000.000 1000.00 1
 ! 0.17157630E+02 0.31174366E-01-0.11256170E-04 0.18249879E-08-0.10963670E-12 2
 ! 0.36004392E+05-0.64856663E+02 0.22831734E+01 0.40006534E-01 0.51494066E-04 3
 !-0.90674160E-07 0.35681565E-10 0.41512567E+05 0.19570406E+02 4
 !t-C9H8 C 9H 8 G 200.000 6000.000 1000.00 1
 ! 0.16891476E+02 0.28607750E-01-0.10305310E-04 0.16685780E-08-0.10015953E-12 2
 ! 0.29093074E+05-0.62630640E+02 0.10396307E+01 0.49179949E-01 0.23089163E-04 3
 !-0.63429586E-07 0.26883177E-10 0.34405202E+05 0.24554146E+02 4
 !n-C9H9 C 9H 9 G 200.000 6000.000 1000.00 1
 ! 0.16984624E+02 0.31264546E-01-0.11273301E-04 0.18260509E-08-0.10962712E-12 2
 ! 0.38406533E+05-0.64131001E+02 0.21663444E+01 0.38449695E-01 0.56080928E-04 3
 !-0.95164737E-07 0.37160062E-10 0.43974587E+05 0.20380623E+02 4
 !R22C9H9 C 9H 9 G 200.000 6000.000 1000.00 1
 ! 0.16665042E+02 0.31820900E-01-0.11538163E-04 0.18759830E-08-0.11292044E-12 2
 ! 0.22266677E+05-0.66405185E+02 0.65118202E+00 0.40264151E-01 0.59215245E-04 3
 !-0.10090515E-06 0.39485409E-10 0.28250059E+05 0.24755482E+02 4
 !C9H8 INDENE T 9/96C 9H 8 0 0G 200.000 6000.000 1000.00 1
 ! 0.17318671E+02 0.28982768E-01-0.10605059E-04 0.17334553E-08-0.10467919E-12 2
 ! 0.11151429E+05-0.71555323E+02-0.68190289E+00 0.41658733E-01 0.70741234E-04 3
 !-0.13430875E-06 0.59915845E-10 0.17705036E+05 0.29781396E+02 0.19741190E+05 4
 !p-C9H9 C 9H 9 G 200.000 6000.000 1000.00 1
 ! 0.17315694E+02 0.30959254E-01-0.11161635E-04 0.18078597E-08-0.10853324E-12 2
 ! 0.38046803E+05-0.66075791E+02 0.14017306E+01 0.44426304E-01 0.43920997E-04 3
 !-0.85102699E-07 0.34166308E-10 0.43739036E+05 0.23247085E+02 4
 !c-C9H9 C 9H 9 G 200.000 6000.000 1000.00 1
 ! 0.16927926E+02 0.31493602E-01-0.11398983E-04 0.18511768E-08-0.11133750E-12 2
 ! 0.27867587E+05-0.68530018E+02-0.81686465E+00 0.47168530E-01 0.48044980E-04 3
 !-0.93082369E-07 0.37448108E-10 0.34181757E+05 0.30904400E+02 4
 !f-C9H9 C 9H 9 G 200.000 6000.000 1000.00 1
 ! 0.17276784E+02 0.31046687E-01-0.11208121E-04 0.18172778E-08-0.10918757E-12 2
 ! 0.35316782E+05-0.67026979E+02 0.18049647E+01 0.45752272E-01 0.37506041E-04 3

!-0.77840523E-07 0.31600686E-10 0.40770230E+05 0.19411030E+02 4
 !s-C9H9 C 9H 9 G 200.000 6000.000 1000.00 1
 ! 0.16551057E+02 0.31836474E-01-0.11523531E-04 0.18714042E-08-0.11255261E-12 2
 ! 0.16983352E+05-0.65713371E+02 0.42263518E-01 0.42046485E-01 0.56899198E-04 3
 !-0.99568912E-07 0.39203817E-10 0.23076369E+05 0.27888305E+02 4
 !C10H7-1 TB 1/99 BLYP00C 10H 7 0 OG 300.000 5000.000 1401.000 1!Howard
 ! 2.32134837E+01 2.19245132E-02-7.57801031E-06 1.18526564E-09-6.91369406E-14 2
 ! 3.75456274E+04-1.03911378E+02-7.74269427E+00 1.04220941E-01-9.25076899E-05 3
 !4.12403544E-08-7.28199643E-12 4.72057155E+04 5.86484815E+01 4
 !C10H8 Naphthalene T 7/98C 10H 8 0 OG 200.000 6000.000 1000.00 1
 ! 1.86129884E+01 3.04494175E-02-1.11224825E-05 1.81615474E-09-1.09601281E-13 2
 ! 8.91578988E+03-8.00230396E+01-1.04919475E+00 4.62970781E-02 7.07591636E-05 3
 !-1.38408111E-07 6.20475407E-11 1.59848987E+04 3.02121626E+01 1.81107678E+04 4
 C6H5CHCH3 C 8H 9 G 200.000 6000.000 1000.00 1
 0.15287640E+02 0.29990204E-01-0.10786412E-04 0.17441075E-08-0.10457587E-12 2
 0.13540395E+05-0.56228770E+02 0.20579304E+01 0.35354050E-01 0.52500310E-04 3
 -0.88002034E-07 0.34220708E-10 0.18564087E+05 0.19485681E+02 4
 !F. Battin-Leclerc, R. Bounaceur, N. Belmekki, P. A. Glaude, Int. J. Chem. Kinet. 38 (2006) 284-302.
 phenyl(CH3)2 121686C 8H 9 G 0300.00 5000.00 1000.00 1
 0.19200632E+02 0.21541221E-01-0.60772045E-05 0.84370538E-09-0.46977508E-13 2
 0.24025320E+05-0.77264038E+02-0.60923421E+00 0.62652625E-01-0.29779714E-04 3
 0.10032059E-08 0.21823782E-11 0.30694578E+05 0.29707020E+02 4
 !PC8H9 121686C 4H 2 G 0300.00 5000.00 1000.00 1! KINGAS
 ! 0.19200632E+02 0.21541221E-01-0.60772045E-05 0.84370538E-09-0.46977508E-13 2
 ! 0.24025320E+05-0.77264038E+02-0.60923421E+00 0.62652625E-01-0.29779714E-04 3
 ! 0.10032059E-08 0.21823782E-11 0.30694578E+05 0.29707020E+02 4
 !OC6H3(CH3)2 121686C 8H 9 G 0300.00 5000.00 1000.00 1
 ! 0.19200632E+02 0.21541221E-01-0.60772045E-05 0.84370538E-09-0.46977508E-13 2
 ! 0.24025320E+05-0.77264038E+02-0.60923421E+00 0.62652625E-01-0.29779714E-04 3
 ! 0.10032059E-08 0.21823782E-11 0.30694578E+05 0.29707020E+02 4
 OC6H3(CH3)2 120186C 8H 9O 1 G 0300.00 5000.00 1000.00 1
 0.53072834E+01 0.48387561E-01-0.18405339E-04 0.31713454E-08-0.20584210E-12 2
 -0.40204531E+04 0.20877609E+01-0.38544981E+01 0.86276419E-01-0.60131446E-04 3
 0.14155940E-07 0.17449911E-11-0.30307119E+04 0.44200062E+02 4
 HOC6H3(CH3)2 120186C 8H 10O 1 G 0300.00 5000.00 1000.00 1
 0.29777200E+01 0.57097003E-01-0.23658878E-04 0.43309059E-08-0.29348648E-12 2
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 0.14350504E-07 0.16610515E-11-0.21290064E+05 0.42264072E+02 4
 !trimetbenz C 9H 12O 0 G 0300.00 5000.00 1000.00 1! KINGAS
 ! 0.57078276E+01 0.57825219E-01-0.23154053E-04 0.41373713E-08-0.27558928E-12 2
 !-0.50093848E+04-0.44507904E+01-0.44493732E+01 0.94222344E-01-0.61137929E-04 3
 ! 0.14483445E-07 0.10342963E-11-0.32379512E+04 0.44531319E+02 4
 !CH3C6H4CH2O OC 8H 9O 1 G 0300.00 5000.00 1000.00 1! KINGAS
 ! 0.18246092E+02 0.27164159E-01-0.84199683E-05 0.12545508E-08-0.73559119E-13 2
 ! 0.99993750E+03-0.70436073E+02-0.63662777E+01 0.87856986E-01-0.59508522E-04 3
 ! 0.17500103E-07-0.13271282E-11 0.84847363E+04 0.59329815E+02 4
 !CH3C6H4CH2OOH OC 8H 10O 2 G 0300.00 5000.00 1000.00 1! KINGAS

! 0.19242598E+02 0.32511316E-01-0.11088881E-04 0.17690666E-08-0.10879589E-12 2
 !-0.17093045E+05-0.70666519E+02-0.36816618E+01 0.88307552E-01-0.53304513E-04 3
 ! 0.90592671E-08 0.19138287E-11-0.10222102E+05 0.50064514E+02 4
 !CH2C6H4CHO OC 8H 7O 1 G 0300.00 5000.00 1000.00 1 !KINGAS
 ! 0.34244980E+02 0.35322688E-02-0.38477933E-06 0.19851797E-10-0.19177666E-15 2
 !-0.49546621E+04-0.16077888E+03-0.30528524E+01 0.73702835E-01-0.39264185E-04 3
 ! 0.65173680E-08-0.49082781E-12 0.86914395E+04 0.44091377E+02 4
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 ! 0.19242598E+02 0.32511316E-01-0.11088881E-04 0.17690666E-08-0.10879589E-12 2
 !-0.17093045E+05-0.70666519E+02-0.36816618E+01 0.88307552E-01-0.53304513E-04 3
 ! 0.90592671E-08 0.19138287E-11-0.10222102E+05 0.50064514E+02 4
 !CH3C6H4CH2O OC 8H 9O 1 G 0300.00 5000.00 1000.00 1 !KINGAS
 ! 0.18246092E+02 0.27164159E-01-0.84199683E-05 0.12545508E-08-0.73559119E-13 2
 ! 0.99993750E+03-0.70436073E+02-0.63662777E+01 0.87856986E-01-0.59508522E-04 3
 ! 0.17500103E-07-0.13271282E-11 0.84847363E+04 0.59329815E+02 4
 CH3C6H4CH2OOH 120186C 8H 10O 2 G 0300.00 5000.00 1000.00 1
 0.19242598E+02 0.32511316E-01-0.11088881E-04 0.17690666E-08-0.10879589E-12 2
 -0.17093045E+05-0.70666519E+02-0.36816618E+01 0.88307552E-01-0.53304513E-04 3
 0.90592671E-08 0.19138287E-11-0.10222102E+05 0.50064514E+02 4
 !CH3C6H4CH2OOH 120186C 8H 10O 2 G 0300.00 5000.00 1000.00 1
 ! 0.19242598E+02 0.32511316E-01-0.11088881E-04 0.17690666E-08-0.10879589E-12 2
 !-0.17093045E+05-0.70666519E+02-0.36816618E+01 0.88307552E-01-0.53304513E-04 3
 ! 0.90592671E-08 0.19138287E-11-0.10222102E+05 0.50064514E+02 4
 CH3C6H4CH2OO 120186C 8H 9O 2 G 0300.00 5000.00 1000.00 1
 0.20481600E+02 0.27565336E-01-0.85213878E-05 0.12697395E-08-0.74590595E-13 2
 0.20709570E+03-0.79043121E+02-0.50324097E+01 0.92347950E-01-0.64420106E-04 3
 0.19109828E-07-0.12973675E-11 0.77472412E+04 0.54727161E+02 4
 CH3C6H4CH2O OC 8H 9O 1 G 0300.00 5000.00 1000.00 1
 0.18246092E+02 0.27164159E-01-0.84199683E-05 0.12545508E-08-0.73559119E-13 2
 0.99993750E+03-0.70436073E+02-0.63662777E+01 0.87856986E-01-0.59508522E-04 3
 0.17500103E-07-0.13271282E-11 0.84847363E+04 0.59329815E+02 4
 C6H5CH2OO OC 7H 7O 2 G 0300.00 5000.00 1000.00 1
 0.13219616E+02 0.30663764E-01-0.10623842E-04 0.17133914E-08-0.10614950E-12 2
 0.75553516E+04-0.40278488E+02-0.55591817E+01 0.86046316E-01-0.65238055E-04 3
 0.21014056E-07-0.14211486E-11 0.12285444E+05 0.55260597E+02 4
 !1 Dec 2006, HPST NGB-NOx Model
 C2H4OH mar96C 2H 5O 1 OG 300.000 5000.00 1405.000 1
 8.75544496e 00 9.49453147e-03-3.08803575e-06 4.63537621e-10-2.62730044e-14 2
 -8.09602047e 03-2.03271929e 01 7.76157606e-01 2.91002514e-02-2.13980569e-05 3
 8.16833894e-09-1.25591600e-12-5.46808396e 03 2.21060185e 01 4
 !Burcat Database 2006
 CH3CHO C 2H 4O 10 OG 300.00 5000.00 1000.00 1
 0.56469620E+01 0.91476260E-02-0.36161100E-05 0.66456890E-09-0.45910180E-13 2
 -0.22534160E+05-0.38819790E+01 0.57694260E+01-0.61437480E-02 0.43337420E-04 3
 -0.49301540E-07 0.18135580E-10-0.21806880E+05-0.80332070E+00 4
 !Burcat Database 2010
 !SERDP PAH version 0.1, 2007
 n-C6H7 C 6H 7 G 300.000 3000.000 1000.000 1

0.22577469E+02-0.30737517E-02 0.14225234E-04-0.69880848E-08 0.10232874E-11 2
 0.41228980E+05-0.91568619E+02 0.13248032E+00 0.57103366E-01-0.43712644E-04 3
 0.15538603E-07-0.12976356E-11 0.47730512E+05 0.25339081E+02 4
 c-C6H7 C 6H 7 G 300.000 3000.000 1000.000 1
 0.19996841E+02 0.11189543E-02 0.11649756E-04-0.62779471E-08 0.94939508E-12 2
 0.16730059E+05-0.83746933E+02-0.30328493E+01 0.50804518E-01-0.69150292E-05 3
 -0.29715974E-07 0.16296353E-10 0.23895383E+05 0.38909180E+02 4
 C6H3 H6W/94C 6H 3 G 300.000 3000.000 1000.000 1
 0.58188343E+01 0.27933408E-01-0.17825427E-04 0.53702536E-08-0.61707627E-12 2
 0.85188250E+05-0.92147827E+00 0.11790619E+01 0.55547360E-01-0.73076168E-04 3
 0.52076736E-07-0.15046964E-10 0.85647312E+05 0.19179199E+02 4
 o-C6H4 D11/99C 6H 4 G 300.000 3000.000 1000.000 1
 0.88432961E+01 0.20301474E-01-0.88674269E-05 0.17264292E-08-0.11786047E-12 2
 0.49317113E+05-0.24014301E+02-0.38454189E+01 0.58391564E-01-0.48644750E-04 3
 0.16770320E-07-0.78580680E-12 0.52592500E+05 0.40587132E+02 4
 l-C6H4 H6W/94C 6H 4 G 300.000 3000.000 1000.000 1
 0.12715182E+02 0.13839662E-01-0.43765440E-05 0.31541636E-09 0.46619026E-13 2
 0.57031148E+05-0.39464600E+02 0.29590225E+00 0.58053318E-01-0.67766756E-04 3
 0.43376762E-07-0.11418864E-10 0.60001371E+05 0.22318970E+02 4
 !Estimated
 C5H4(CH3)2 C 7H 10 G 200.000 5000.000 1000.00 1
 0.11632437E+02 0.36524986E-01-0.14741400E-04 0.27181784E-08-0.18803879E-12 2
 0.15969013E+04-0.38953480E+02 0.28308857E+01 0.34627371E-01 0.43760755E-04 3
 -0.73387078E-07 0.28114231E-10 0.52124026E+04 0.12784872E+02 4
 !Estimated
 C5H4CH3CH2 C 7H 9 G 200.000 5000.000 1000.00 1
 0.12519850E+02 0.32658116E-01-0.13168869E-04 0.24273969E-08-0.16791112E-12 2
 0.12109056E+05-0.42056746E+02 0.57086666E+00 0.48734487E-01 0.10295915E-04 3
 -0.44935354E-07 0.19602667E-10 0.16084831E+05 0.23520081E+02 4
 C5H3(CH3)2 C 7H 9 G 200.000 5000.000 1000.00 1
 0.12480689E+02 0.32665289E-01-0.13162226E-04 0.24248571E-08-0.16766692E-12 2
 0.11564589E+05-0.40172000E+02 0.19652163E+01 0.43160408E-01 0.18445249E-04 3
 -0.50213562E-07 0.20883630E-10 0.15246021E+05 0.18450767E+02 4
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 C6H6CH3 0C 7H 9 G 200.000 5000.000 1000.00 1
 0.11364119E+02 0.33451206E-01-0.13398619E-04 0.24583354E-08-0.16948947E-12 2
 0.20145814E+05-0.36761028E+02-0.13784319E+00 0.44869625E-01 0.21357899E-04 3
 -0.55302107E-07 0.22917979E-10 0.24175678E+05 0.27376650E+02 4
 !V. Detilleux, J. Vandooren, J. Phys. Chem. A. 113 (2009) 10913-10922.
 C7H6f C 7H 6 G 300.000 5000.000 1000.000 1
 8.63047626E+00 3.28146569E-02-1.67463533E-05 4.12422205E-09-3.97875311E-13 2
 3.78424508E+04-2.14598163E+01-4.83808621E+00 7.96144479E-02-7.75198421E-05 3
 3.84238455E-08-7.26609427E-12 4.09670495E+04 4.54480924E+01 4
 !S. Gail, P. Dagaut, Combust. Sci. Technol. 179 (2007) 813-844.
 CH2PCH2 C 8H 80 00 0G 300.00 5000.00 1000.00 1
 0.15476290E+02 0.28401490E-01-0.10924750E-04 0.19882460E-08-0.13684680E-12 2
 0.19727180E+05-0.60584360E+02-0.52720640E+01 0.87208690E-01-0.69407880E-04 3
 0.22830400E-07-0.55471570E-12 0.25439360E+05 0.46331680E+02 4

CHOPHCH2 (CH2.PCHO) C 8H 7O 1 OG 300.00 5000.00 1412.00 1
0.34346760E+02 0.34427470E-02-0.41094190E-06 0.32036820E-10-0.13594020E-14 2
-0.59815660E+04-0.16137820E+03-0.32634220E+01 0.75194690E-01-0.42944220E-04 3
0.10297690E-07-0.18682390E-11 0.77373650E+04 0.44983270E+02 4
!ETPHHCO (C2H5PCHO) C 9H 10O 1 OG 300.00 5000.00 1394.00 1
! 2.48768072E+01 2.86157476E-02-9.98543930E-06 1.57119199E-09-9.20123997E-14 2
!-2.34637635E+04-1.06701809E+02-1.38438397E+01 1.39861798E-01-1.36441537E-04 3
! 6.74549879E-08-1.30927664E-11-1.19013389E+04 9.42061081E+01 4
!ETPCO (C2H5PCO) C 9H 9O 1 OG 300.00 5000.00 1390.00 1
!3.66927500E+02 7.19301100E-02-1.16809300E-05 1.08915500E-09-4.01239970E-14 2
!-1.03188100E+05-1.72760000E+03-1.24763200E+01 7.20352900E-01-2.27880300E-04 3
!-9.76765300E-08 4.58716400E-11 3.95783400E+04 3.74687700E+02 4
!Y1P4ET C 8H 9O 0 OG 300.00 5000.00 1000.00 1
! 0.17092570E+02 0.25160310E-01-0.76713050E-05 0.11329450E-08-0.66206600E-13 2
! 0.24964010E+05-0.66017090E+02-0.33699920E+01 0.72990540E-01-0.40671690E-04 3
! 0.41082490E-08 0.25791680E-11 0.31238690E+05 0.42350110E+02 4
!OY1P4ET C 8H 9O 1 OG 300.00 5000.00 1000.00 1
! 0.10277390E+02 0.39502630E-01-0.14047970E-04 0.23161530E-08-0.14616930E-12 2
!-0.58172150E+04-0.23495450E+02-0.36556660E+01 0.85033070E-01-0.58641880E-04 3
! 0.13630500E-07 0.15076010E-11-0.29440840E+04 0.45332310E+02 4
CHOPCHO (CHOPCHO) C 8H 6O 2 OG 300.00 5000.00 1000.00 1
0.40088810E+02 0.44874150E-02-0.56398100E-05 0.14695110E-08-0.24215690E-12 2
-0.37707640E+05-0.19367790E+03-0.13773190E+01 0.70842940E-01-0.27313200E-04 3
-0.26711310E-08 0.70707500E-12-0.21349500E+05 0.38384010E+02 4
Y1P4CHO C 7H 5O 1 OG 300.00 5000.00 1000.00 1
0.28227590E+02 0.29564700E-02-0.37829220E-06 0.31517300E-10-0.14050850E-14 2
0.12272520E+05-0.12906200E+03-0.21486650E+01 0.58373270E-01-0.25400040E-04 3
-0.23565660E-08 0.23662650E-11 0.23404450E+05 0.38067950E+02 4
CHOPCO (CHOPCO) C 8H 5O 2 OG 300.00 5000.00 1000.00 1
0.40368540E+02 0.19636600E-04-0.26725790E-05 0.52614130E-09-0.10980140E-12 2
-0.20293260E+05-0.19453320E+03-0.21450400E+00 0.58212050E-01-0.75333540E-05 3
-0.16830580E-07 0.45042690E-11-0.37697960E+04 0.34674600E+02 4
OY1P4CHO C 7H 5O 2 OG 300.00 5000.00 1000.00 1
0.26552100E+02 0.83426330E-02-0.19088890E-05 0.22710780E-09-0.11366680E-13 2
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0.70111160E-08 0.12923850E-11-0.10671540E+05 0.41921660E+02 4
C5H5CHO C 6H 5N 0O 1G 300.00 5000.00 1000.00 1
0.13683560E+02 0.19570760E-01-0.77577490E-05 0.14329340E-08-0.99461230E-13 2
0.26920580E+05-0.46588200E+02-0.18152280E+01 0.60316250E-01-0.40687750E-04 3
0.47398430E-08 0.42769330E-11 0.31321290E+05 0.33996780E+02 4
CPDCO C 6H 5N 0O 1G 300.00 5000.00 1000.00 1
0.12909980E+02 0.19528300E-01-0.76528380E-05 0.14059090E-08-0.97294450E-13 2
0.17499310E+05-0.40053340E+02-0.32914680E+01 0.66252740E-01-0.55444870E-04 3
0.19607610E-07-0.10299610E-11 0.21905320E+05 0.43199810E+02 4
!Burcat database
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1.12002638E+01 2.50104924E-02-8.94914815E-06 1.44109704E-09-8.61256818E-14 2
7.66096956E+03-3.68265351E+01 2.93206487E+00 1.12663266E-02 9.41193663E-05 3

-1.36178031E-07 5.64768524E-11 1.15372662E+04 1.42303662E+01 1.35013031E+04 4
 C5H5-1CH2 C 6H 7 G 200.000 6000.000 1000.000 1
 1.27079227E+01 2.13529273E-02-7.71585835E-06 1.25058460E-09-7.50743824E-14 2
 3.41136541E+04-4.24117660E+01 1.64289716E+00 2.65257755E-02 5.29482958E-05 3
 -9.65595872E-08 4.29631206E-11 3.82157747E+04 2.03616391E+01 4.01818508E+04 4
 C5H4-1CH3 C 6H 7 G 200.000 6000.000 1000.000 1
 1.28996538E+01 2.12183240E-02-7.67565006E-06 1.24495899E-09-7.47731827E-14 2
 2.12053775E+04-4.47534535E+01 5.64034275E-01 3.84201803E-02 1.94958520E-05 3
 -5.95545053E-08 2.86869522E-11 2.53304225E+04 2.27464371E+01 2.72743433E+04 4
 C5H5 C 5H 5 G 200.000 6000.000 1000.000 1
 0.10844072E+02 0.15392831E-01-0.55630422E-05 0.90189440E-09-0.54156619E-13 2
 0.26950886E+05-0.35254983E+02-0.95902849E+00 0.31396777E-01 0.26724050E-04 3
 -0.68942183E-07 0.33301983E-10 0.30779441E+05 0.29072780E+02 0.32004580E+05 4
 C5H6 T1/90C 5H 6 G 200.000 6000.000 1000.000 1
 0.99757848E+01 0.18905543E-01-0.68411461E-05 0.11099340E-08-0.66680236E-13 2
 0.11081693E+05-0.32209454E+02 0.86108957E+00 0.14804031E-01 0.72108895E-04 3
 -0.11338055E-06 0.48689972E-10 0.14801755E+05 0.21353453E+02 0.16152485E+05 4
 !C5H5-3CH2 C 6H 7 G 200.000 6000.000 1
 ! 1.31180563E+01 2.10247437E-02-7.60660029E-06 1.23388906E-09-7.41144871E-14 2
 ! 2.35701438E+04-4.51867987E+01-4.65377649E-02 3.96188470E-02 2.21522238E-05 3
 !-6.60053606E-08 3.19768019E-11 2.79177074E+04 2.66778342E+01 4
 C4H C 4H 1 G 300.000 3000.000 1000.000 1
 6.73918671E+00 6.64086480E-03-2.67303014E-06 4.70935449E-10-2.74941451E-14 2
 9.68657883E+04-1.08586007E+01 8.72345580E-01 3.13510263E-02-4.47574650E-05 3
 3.39766851E-08-1.02921293E-11 9.80821833E+04 1.73977335E+01 4
 !delH298 taken frm Bozzelli J. Phys. Chem. A, Vol 114, No. 6, 2010 and S298 using nist group
 !additivity of a different isomer of ethynyl cpd
 ETCPD C 7H 6 G 200.000 5000.000 1000.00 1
 0.11876590E+02 0.24170930E-01-0.96683010E-05 0.17735466E-08-0.12231349E-12 2
 0.38015828E+05-0.38781201E+02-0.72792433E+00 0.52746504E-01-0.19767937E-04 3
 -0.13335846E-07 0.91156557E-11 0.41628856E+05 0.27488916E+02 4
 !S. Klippenstein, J. A. Miller, J. Phys. Chem. A., 109 (2005) 4285-4295
 n-C4H3 00000C 4H 3 G 0300.00 3000.00 1000.00 1
 7.25330164E+00 1.19580846E-02-5.26715675E-06 1.09981875E-09-8.84016751E-14 2
 6.28977574E+04-1.05283126E+01-3.55175031E-02 4.30508503E-02-5.75729147E-05 3
 4.15883142E-08-1.20750857E-11 6.43506593E+04 2.43816855E+01 4
 i-C4H3 00000C 4H 3 G 0300.00 4000.00 1000.00 1
 7.29283596E+00 1.21664949E-02-5.50925306E-06 1.19291350E-09-1.00493092E-13 2
 5.71961011E+04-1.05737251E+01 3.02566263E+00 3.04693624E-02-3.68345185E-05 3
 2.60035352E-08-7.62154351E-12 5.80551505E+04 9.87268458E+00 4
 !Proceedings of the Combustion Inst 32(2009) 287-294
 !J. Chem. Theory. Comput. Vol. 5 No. 12 2009
 !Used vibrational frequencies, H and S from the paper-used FITDAT to get NASA polynomials
 C6H5CH2OOH C 7H 8O 2 G 200.000 5000.000 1000.00 1
 0.14923993E+02 0.32904975E-01-0.13190531E-04 0.24226188E-08-0.16718743E-12 2
 -0.98040932E+04-0.50844770E+02 0.13244434E+01 0.48791993E-01 0.20745714E-04 3
 -0.58712725E-07 0.24744444E-10-0.51586243E+04 0.24392990E+02 4
 C6H5CH2O C 7H 7O 1 G 200.000 5000.000 1000.00 1

0.13058251E+02 0.29414636E-01-0.11924927E-04 0.22068091E-08-0.15309821E-12 2
 0.86220068E+04-0.43457004E+02 0.43257879E+00 0.44385449E-01 0.18916671E-04 3
 -0.53886134E-07 0.22753107E-10 0.12923735E+05 0.26337538E+02 4
 CHD4F1Y25 C 7H 7O 1 G 200.000 5000.000 1000.00 1
 0.13058251E+02 0.29414636E-01-0.11924927E-04 0.22068091E-08-0.15309821E-12 2
 0.86220068E+04-0.43457004E+02 0.43257879E+00 0.44385449E-01 0.18916671E-04 3
 -0.53886134E-07 0.22753107E-10 0.12923735E+05 0.26337538E+02 4
 O1O47D5Y C 7H 7O 1 G 200.000 5000.000 1000.00 1
 0.13521263E+02 0.28714363E-01-0.11578674E-04 0.21353025E-08-0.14779295E-12 2
 0.13454758E+05-0.47638270E+02-0.13805545E+01 0.55737185E-01-0.32362387E-05 3
 -0.36010767E-07 0.17534836E-10 0.18064343E+05 0.32400494E+02 4
 POXYMETHYL C 7H 7O 1 G 200.000 5000.000 1000.00 1
 0.13431389E+02 0.28665143E-01-0.11523244E-04 0.21207731E-08-0.14658554E-12 2
 0.86817573E+04-0.45119511E+02-0.30780363E+00 0.52548817E-01-0.73910815E-06 3
 -0.36141748E-07 0.17187319E-10 0.12983251E+05 0.28932427E+02 4
 !K. Narayanswamy, G. Blanquart, H. Pitsch, Comb. and Flame, Vol. 157, Issue 10, Oct 2010, 1879-1898
 C5H4CH2 FULVENE G3B3 H 6C 6O 0N 0G 300.000 3000.000 1000.000 1
 2.78194214E+00 4.06322016E-02-2.35029327E-05 6.51056017E-09-6.96809087E-13 2
 2.43155607E+04 7.84215958E+00-5.34007612E+00 7.17283827E-02-6.45824457E-05 3
 2.78691157E-08-3.95001455E-12 2.58936616E+04 4.70844323E+01 1.58884208E+04 4
 !Grimech 3.0
 CH2OH GUNL93C 1H 3O 1 G 200.000 3500.000 1000.000 1
 3.69266569E+00 8.64576797E-03-3.75101120E-06 7.87234636E-10-6.48554201E-14 2
 -3.24250627E+03 5.81043215E+00 3.86388918E+00 5.59672304E-03 5.93271791E-06 3
 -1.04532012E-08 4.36967278E-12-3.19391367E+03 5.47302243E+00 4
 CH2O L 8/88H 2C 1O 1 G 200.000 3500.000 1000.000 1
 1.76069008E+00 9.20000082E-03-4.42258813E-06 1.00641212E-09-8.83855640E-14 2
 -1.39958323E+04 1.36563230E+01 4.79372315E+00-9.90833369E-03 3.73220008E-05 3
 -3.79285261E-08 1.31772652E-11-1.43089567E+04 6.02812900E-01 4
 C2H2 L 1/91C 2H 2 G 200.000 3500.000 1000.000 1
 4.14756964E+00 5.96166664E-03-2.37294852E-06 4.67412171E-10-3.61235213E-14 2
 2.59359992E+04-1.23028121E+00 8.08681094E-01 2.33615629E-02-3.55171815E-05 3
 2.80152437E-08-8.50072974E-12 2.64289807E+04 1.39397051E+01 4
 HCCO SRIC91H 1C 2O 1 G 300.00 4000.00 1000.000 1
 0.56282058E+01 0.40853401E-02-0.15934547E-05 0.28626052E-09-0.19407832E-13 2
 0.19327215E+05-0.39302595E+01 0.22517214E+01 0.17655021E-01-0.23729101E-04 3
 0.17275759E-07-0.50664811E-11 0.20059449E+05 0.12490417E+02 4
 C2H L 1/91C 2H 1 G 200.000 3500.000 1000.000 1
 3.16780652E+00 4.75221902E-03-1.83787077E-06 3.04190252E-10-1.77232770E-14 2
 6.71210650E+04 6.63589475E+00 2.88965733E+00 1.34099611E-02-2.84769501E-05 3
 2.94791045E-08-1.09331511E-11 6.68393932E+04 6.22296438E+00 4
 CH2 L S/93C 1H 2 G 200.000 3500.000 1000.000 1
 2.87410113E+00 3.65639292E-03-1.40894597E-06 2.60179549E-10-1.87727567E-14 2
 4.62636040E+04 6.17119324E+00 3.76267867E+00 9.68872143E-04 2.79489841E-06 3
 -3.85091153E-09 1.68741719E-12 4.60040401E+04 1.56253185E+00 4
 ! Wang & Brezinsky 1998
 C5H4O G3B3 H 4C 5O 1N 0G 300.000 3000.000 1000.000 1

4.25344911E+00 3.13639818E-02-1.82864085E-05 5.08408365E-09-5.44845492E-13 2
 3.87579835E+03 1.54537057E+00-3.64380971E+00 6.14329196E-02-5.92149236E-05 3
 2.83233356E-08-5.02726134E-12 5.46809680E+03 3.98672083E+01 1.52084482E+04 4
 !135-tmb thermochemistry
 !Thermochemistry evaluated using thergas
 C9H12 C 9H 12 G 298.000 5000.000 1000.00 1
 0.21966928E+02 0.29572912E-01-0.93862263E-05 0.14293999E-08-0.85467705E-13 2
 -0.12589250E+05-0.95378777E+02-0.35709381E+01 0.82623795E-01-0.42265205E-04 3
 0.54366023E-08 0.12604019E-11-0.38881404E+04 0.42746967E+02 4
 !new thermochemistry calc using grp additivity
 !C9H12 C 9H 12 G 298.000 2000.000 1000.00 1
 ! 0.13164372E+03-0.35670138E+00 0.47585689E-03-0.25713835E-06 0.49546629E-10 2
 !-0.36623827E+05-0.63420814E+03 0.35154965E+01 0.39962480E-01 0.54634656E-04 3
 !-0.92172562E-07 0.37267439E-10-0.52057307E+04 0.12898723E+02 4
 !old thermochemistry
 C9H11 C 9H 11 G 300.000 2000.000 1000.00 1
 0.64723117E+01 0.63593671E-01-0.35294671E-04 0.95915460E-08-0.10301899E-11 2
 0.14149653E+05-0.70148611E+01-0.34836930E+01 0.95095512E-01-0.70064167E-04 3
 0.24449032E-07-0.26640170E-11 0.16556963E+05 0.43097651E+02 4
 !C9H11 C 9H 11 G 200.000 5000.000 1000.00 1
 ! 0.15846555E+02 0.41220136E-01-0.16655719E-04 0.30752532E-08-0.21301106E-12 2
 ! 0.11245298E+05-0.56636429E+02 0.18125060E+01 0.58475173E-01 0.15783460E-04 3
 !-0.57432023E-07 0.24634097E-10 0.15996165E+05 0.20790032E+02 4
 C6H3(CH3)2 C 8H 9 G 200.000 5000.000 1000.00 1
 0.12906776E+02 0.35493099E-01-0.14391896E-04 0.26631392E-08-0.18472945E-12 2
 0.49689363E+05-0.40074591E+02 0.27209334E+01 0.38010509E-01 0.39170929E-04 3
 -0.71271370E-07 0.27855388E-10 0.53637830E+05 0.18622701E+02 4
 DIMPHHCO C 9H 10O 1 G 200.000 5000.000 1000.00 1
 0.16376982E+02 0.41240732E-01-0.16812980E-04 0.31233310E-08-0.21727881E-12 2
 -0.20647236E+05-0.57191050E+02 0.43615940E+01 0.44772913E-01 0.44682803E-04 3
 -0.82403228E-07 0.32296703E-10-0.16017690E+05 0.11908592E+02 4
 DIMPHCH2OH C 9H 12O 1 G 200.000 5000.000 1000.00 1
 0.17182015E+02 0.45699331E-01-0.18440484E-04 0.34011371E-08-0.23538089E-12 2
 -0.28796705E+05-0.61673091E+02 0.41707572E+01 0.49740336E-01 0.47504044E-04 3
 -0.88565906E-07 0.34757386E-10-0.23794252E+05 0.13099711E+02 4
 DIMPHCO C 9H 9O 1 G 200.000 5000.000 1000.00 1
 0.16685340E+02 0.37974015E-01-0.15488552E-04 0.28786934E-08-0.20034871E-12 2
 0.94964580E+02-0.57707015E+02 0.44576705E+01 0.46657226E-01 0.31827832E-04 3
 -0.68893030E-07 0.27799449E-10 0.45518718E+04 0.11341288E+02 4
 DIMETB C 10H 14 G 200.000 5000.000 1000.00 1
 0.16586463E+02 0.52308829E-01-0.21142605E-04 0.39028328E-08-0.27022103E-12 2
 -0.13460342E+05-0.61059980E+02 0.45155719E+01 0.46868854E-01 0.67602670E-04 3
 -0.10898423E-06 0.41382429E-10-0.83599868E+04 0.10605979E+02 4
 DIMSTYR C 10H 12 G 200.000 5000.000 1000.00 1
 0.16956778E+02 0.46059311E-01-0.18621207E-04 0.34387679E-08-0.23819025E-12 2
 0.10536678E+04-0.62991467E+02 0.32590286E+01 0.53969981E-01 0.39833281E-04 3
 -0.82411219E-07 0.32944388E-10 0.61372341E+04 0.14812338E+02 4
 C8H9O C 8H 9O 1 G 200.000 5000.000 1000.00 1

0.16164210E+02 0.34729563E-01-0.14222761E-04 0.26509003E-08-0.18486627E-12 2
 -0.11842189E+05-0.58074205E+02 0.29079977E+01 0.47764771E-01 0.26208891E-04 3
 -0.64293176E-07 0.26548563E-10-0.71914646E+04 0.15876767E+02 4
 !DIMPCH2OH C 8H 10O 1 G 200.000 5000.000 1000.00 1
 ! 0.15605679E+02 0.38433704E-01-0.15512222E-04 0.28624871E-08-0.19821528E-12 2
 !-0.26903528E+05-0.56215614E+02 0.26244347E+01 0.52450674E-01 0.20324334E-04 3
 !-0.58936558E-07 0.24728548E-10-0.22411879E+05 0.15888388E+02 4
 DIMPCH2O C 9H 11O 1 G 200.000 5000.000 1000.00 1
 0.18098202E+02 0.41798025E-01-0.16855067E-04 0.31084535E-08-0.21516097E-12 2
 -0.21275891E+05-0.66130766E+02 0.35624522E+01 0.59182392E-01 0.18206330E-04 3
 -0.61024443E-07 0.26007721E-10-0.16330809E+05 0.14185481E+02 4
 C18H22 C 18H 22 G 200.000 5000.000 1000.00 1
 0.30460833E+02 0.86207207E-01-0.34986692E-04 0.64777681E-08-0.44950279E-12 2
 -0.14715038E+05-0.12974085E+03 0.60341574E+01 0.90919854E-01 0.97435421E-04 3
 -0.17479770E-06 0.68117877E-10-0.51799998E+04 0.11352251E+02 4
 !o-xyl,FBL
 O-XYL C 8H 10O 0G 300.00 5000.00 1000.00 1 !KINGAS
 0.17985743E+02 0.26968898E-01-0.88121678E-05 0.13625736E-08-0.81932447E-13 2
 -0.64873730E+04-0.72853989E+02-0.17060317E+01 0.70138752E-01-0.37771289E-04 3
 0.56106786E-08 0.11293696E-11-0.31772705E+02 0.32762829E+02 4
 !m-xyl, FBL
 C2H5C6H4CHO C 9H 10O 1 G 200.000 5000.000 1000.00 1
 0.16685340E+02 0.37974015E-01-0.15488552E-04 0.28786934E-08-0.20034871E-12 2
 0.94964580E+02-0.57707015E+02 0.44576705E+01 0.46657226E-01 0.31827832E-04 3
 -0.68893030E-07 0.27799449E-10 0.45518718E+04 0.11341288E+02 4
 !N. A. Slavinskaya, P. Frank, Combust. Flame, 156 (2009) 1705 - 1722
 A3 OC 14H 10O 0G 0200.00 6000.00 1000.00 1
 0.26602474E+02 0.39769744E-01-0.14572026E-04 0.23843296E-08-0.14409548E-12 2
 0.12132838E+05-0.12266672E+03-0.33646717E+01 0.85073271E-01 0.37531110E-04 3
 -0.12664499E-06 0.61445705E-10 0.22019878E+05 0.40596218E+02 0.24908263E+05 4
 A3CH3 C 15H 12 G 300.000 5000.000 2025.00 1
 2.86721901E+01 4.57935671E-02-1.67466881E-05 2.72794395E-09-1.63863026E-13 2
 6.77859249E+03-1.31269124E+02 2.45407326E-01 1.03437006E-01-5.52427842E-05 3
 1.17708807E-08-4.92994185E-13 1.69368456E+04 2.37077261E+01 4
 A3- OC 14H 9O 0G 0200.00 3000.00 1000.00 1
 1.30899250E+01 6.54850270E-02-3.46655370E-05 8.77017890E-09-8.62784060E-13 2
 4.64475940E+04-4.75652960E+01-7.67067940E+00 1.23515340E-01-8.47954330E-05 3
 1.59995970E-08 4.76798380E-12 5.19694990E+04 5.90610150E+01 4
 A2C2H C 12H 8 G 200.000 6000.000 1000.00 1
 2.34108373E+01 3.12979308E-02-1.13777419E-05 1.85217551E-09-1.11546889E-13 2
 3.49196941E+04-1.00594596E+02-2.59169367E+00 8.63306190E-02-1.76590976E-05 3
 -5.26006488E-08 3.15924760E-11 4.27720678E+04 3.73574503E+01 4
 P2- OC 12H 9O 0G 0300.00 5000.00 1000.00 1
 0.23851303E+02 0.31960227E-01-0.11076719E-04 0.16847825E-08-0.92641173E-13 2
 0.40171297E+05-0.10270549E+03-0.31376228E+01 0.82217276E-01-0.40171444E-05 3
 -0.60809782E-07 0.32074482E-10 0.48868754E+05 0.42730362E+02 4
 A2 OC 10H 8O 0G 0200.00 6000.00 1000.00 1
 1.86129884E+01 3.04494175E-02-1.11224825E-05 1.81615474E-09-1.09601281E-13 2

8.91578988E+03-8.00230396E+01-1.04919475E+00 4.62970781E-02 7.07591636E-05 3
 -1.38408111E-07 6.20475407E-11 1.59848987E+04 3.02121626E+01 4
 A2- C 10H 7 G 200.000 6000.000 1000.00 1
 1.83535073E+01 2.77474314E-02-1.00885968E-05 1.64229575E-09-9.89002001E-14 2
 3.89261241E+04-7.48978150E+01-1.89559772E+00 5.83077290E-02 2.79388931E-05 3
 -9.14375172E-08 4.46422302E-11 4.55409775E+04 3.52453263E+01 4
 A2R5 G3B3 H 8C 12O 0N 0G 300.000 3000.000 1000.000 1
 3.65432884E+00 7.52647236E-02-4.54864951E-05 1.29795341E-08-1.41730827E-12 2
 2.65223472E+04 7.23303392E-01-1.05497902E+01 1.25536790E-01-1.03646045E-04 3
 3.52989130E-08-1.64508384E-12 2.94426605E+04 7.02667419E+01 4
 A2R5- HR 4/99 BLYP00C 12H 7 0 0G 300.000 3000.000 1000.000 1
 1.19534280E+01 5.23860720E-02-2.76952570E-05 6.98583910E-09-6.84938560E-13 2
 5.31995200E+04-4.03924920E+01-7.33802680E+00 1.11965800E-01-9.32829450E-05 3
 3.58663420E-08-4.26602220E-12 5.80597670E+04 5.73507140E+01 4
 A2C2H* C 12H 7 G 300.000 3000.000 1000.00 1
 1.33715110E+01 4.99657190E-02-2.62269020E-05 6.59494350E-09-6.45885050E-13 2
 6.84904150E+04-4.64872350E+01-6.25389030E+00 1.14753010E-01-1.05430910E-04 3
 4.79127480E-08-7.92157250E-12 7.32491920E+04 5.19412620E+01 4
 INDENE C 9H 8 G 200.000 6000.000 1000.00 1
 0.17318671E+02 0.28982768E-01-0.10605059E-04 0.17334553E-08-0.10467919E-12 2
 0.11151429E+05-0.71555323E+02-0.68190289E+00 0.41658733E-01 0.70741234E-04 3
 -0.13430875E-06 0.59915845E-10 0.17705036E+05 0.29781396E+02 4
 INDENYL C 9H 7 G 200.000 6000.000 1000.00 1
 0.18554959E+02 0.25035076E-01-0.91457509E-05 0.14934838E-08-0.90133030E-13 2
 0.25721156E+05-0.76300347E+02-0.26698729E+01 0.62177216E-01 0.15067018E-04 3
 -0.79645699E-07 0.40918972E-10 0.32386969E+05 0.37861193E+02 4
 A3C2H C 16H 10 G 300.000 3000.000 1000.00 1
 5.21651460E+01-1.31973180E-02 3.43530560E-05-1.62838920E-08 2.36773620E-12 2
 3.42350550E+04-2.54066510E+02-1.16026740E+01 1.68243940E-01-1.64320300E-04 3
 8.63943800E-08-1.93105670E-11 5.21728360E+04 7.55153660E+01 4
 !Ranzi model, <http://creckmodeling.chem.polimi.it/tot1101NOx.CKT>
 C6H5CH2C6H5 C 13H 12 G 300.00 5000.00 1000.00 1
 .185418955E+02 .513343070E-01-.178726910E-04 .207043850E-08 .000000000E+00 2
 .668552054E+04-.690121392E+02-.940899900E+01 .125451300E+00-.822539730E-04 3
 .202856220E-07 .000000000E+00 .144845500E+05 .760677200E+02 4
 !Thermochemistry taken from SERDP PAH model 2007
 FLUORENE HR11/99 BLYP C 13H 10 0 0G 300.000 5000.000 1400.000 01
 3.04476803E+01 3.11178654E-02-1.07640759E-05 1.68444388E-09-9.82875496E-14 2
 5.92347405E+03-1.45855799E+02-1.14291780E+01 1.40625771E-01-1.21919889E-04 3
 5.33286885E-08-9.28204948E-12 1.91832070E+04 7.47141338E+01 4
 !calculated using NIST ga estimates
 DIMERS224 C 17H 20 G 298.000 2000.000 1000.00 1
 0.13790184E+03-0.31552463E+00 0.46837253E-03-0.26544915E-06 0.52810830E-10 2
 -0.34649215E+05-0.65776943E+03 0.18137909E+01 0.10817902E+00 0.13789870E-04 3
 -0.83042585E-07 0.37371326E-10-0.13991783E+04 0.28938868E+02 4
 DIMERS238 C 18H 22 G 298.000 2000.000 1000.00 1
 0.84378661E+02-0.13053609E+00 0.25736122E-03-0.16066698E-06 0.33864724E-10 2
 -0.25911847E+05-0.38892937E+03 0.83545408E+00 0.13260812E+00-0.30812174E-04 3

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-0.39579994E-07 0.21350131E-10-0.56517751E+04 0.31875466E+02      4
DIMERS210      C 16H 18      G 298.000 2000.000 1000.00      1
0.11571585E+03-0.25247727E+00 0.38577232E-03-0.22116168E-06 0.44324030E-10  2
-0.25014091E+05-0.54779029E+03-0.90177959E+00 0.11355744E+00-0.12626037E-04  3
-0.55998580E-07 0.28142204E-10 0.33312239E+04 0.39931289E+02      4
DIMERS196      C 15H 16      G 298.000 2000.000 1000.00      1
0.93529853E+02-0.18942990E+00 0.30317211E-03-0.17687422E-06 0.35837229E-10  2
-0.15328644E+05-0.43919503E+03-0.36173501E+01 0.11893586E+00-0.39041945E-04  3
-0.28954576E-07 0.18913081E-10 0.81119491E+04 0.49539830E+02      4
DIMERS182      C 14H 14      G 298.000 2000.000 1000.00      1
0.71343860E+02-0.12638254E+00 0.22057190E-03-0.13258676E-06 0.27350429E-10  2
-0.56431975E+04-0.32991035E+03-0.63329206E+01 0.12431427E+00-0.65457853E-04  3
-0.19105715E-08 0.96839590E-11 0.12892674E+05 0.59837794E+02      4
TMB123         C 9H 12      G 298.000 2000.000 1000.00      1
-0.19774624E+02 0.13937042E+00-0.11136614E-03 0.41000907E-07-0.53191850E-11  2
0.27212619E+03 0.12452197E+03-0.38723182E+01 0.99577511E-01-0.87401249E-04  3
0.48840630E-07-0.13233194E-10-0.40991508E+04 0.41848451E+02      4
TMB124         C 9H 12      G 298.000 2000.000 1000.00      1
0.55934547E+02-0.10866548E+00 0.18224537E-03-0.10806872E-06 0.22113722E-10  2
-0.18201012E+05-0.25360279E+03-0.17841084E+00 0.69769995E-01-0.16383297E-04  3
-0.21665966E-07 0.12017122E-10-0.46776022E+04 0.28613889E+02      4
TETRAMB        C 10H 14      G 298.000 2000.000 1000.00      1
0.24113684E+01 0.76323057E-01-0.28765930E-04-0.32865542E-08 0.31676156E-11  2
-0.94133207E+04 0.15237282E+02-0.11567477E+01 0.94199093E-01-0.60985341E-04  3
0.21796625E-07-0.40040722E-11-0.88798760E+04 0.31550486E+02      4
B124PM         C 15H 16      G 298.000 2000.000 1000.00      1
0.93529853E+02-0.18942990E+00 0.30317211E-03-0.17687422E-06 0.35837229E-10  2
-0.15328644E+05-0.43919503E+03-0.36173501E+01 0.11893586E+00-0.39041945E-04  3
-0.28954576E-07 0.18913081E-10 0.81119491E+04 0.49539830E+02      4
B11MB3         C 15H 16      G 298.000 2000.000 1000.00      1
0.16923902E+03-0.43746580E+00 0.59678362E-03-0.32594385E-06 0.63270136E-10  2
-0.33499845E+05-0.81882444E+03 0.76557277E-01 0.89128341E-01 0.31976007E-04  3
-0.99461172E-07 0.44163398E-10 0.78354354E+04 0.34800611E+02      4
!Battin-Leclerc m-xylene model
CH2C6H4CHO     OC 8H 7O 1   G 0300.00 5000.00 1000.00      1 !KINGAS
0.34244980E+02 0.35322688E-02-0.38477933E-06 0.19851797E-10-0.19177666E-15  2
-0.49546621E+04-0.16077888E+03-0.30528524E+01 0.73702835E-01-0.39264185E-04  3
0.65173680E-08-0.49082781E-12 0.86914395E+04 0.44091377E+02      4
!h and s, freq calc using ub3lyp/6-31g(d), used fitdat in chemkin
DIMCHCH3       C 10H 13      G 200.000 5000.000 1000.00      1
0.17399679E+02 0.48555478E-01-0.19625213E-04 0.36232247E-08-0.25090902E-12  2
0.74182887E+04-0.61671796E+02 0.43216935E+01 0.52314158E-01 0.47566659E-04  3
-0.89724619E-07 0.35224367E-10 0.12461549E+05 0.13560240E+02      4
DIMCH2CH2      C 10H 13      G 200.000 5000.000 1000.00      1
0.17819746E+02 0.48088368E-01-0.19421555E-04 0.35837826E-08-0.24808920E-12  2
0.15634292E+05-0.64294742E+02 0.42485920E+01 0.55037038E-01 0.41159358E-04  3
-0.84139439E-07 0.33516703E-10 0.20715320E+05 0.13012219E+02      4
C9H11OOH       C 9H 12O 2    G 200.000 5000.000 1000.00      1

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0.19598545E+02 0.46359675E-01-0.18732464E-04 0.34582956E-08-0.23950111E-12 2
 -0.14057673E+05-0.71930435E+02 0.55712252E+01 0.52767403E-01 0.46208273E-04 3
 -0.89537081E-07 0.35434731E-10-0.87671320E+04 0.81686622E+01 4
 C9H11OO C 9H 11O 2 G 200.000 5000.000 1000.00 1
 0.19050195E+02 0.44370257E-01-0.18040825E-04 0.33449974E-08-0.23236796E-12 2
 -0.18269393E+04-0.68539137E+02 0.45960300E+01 0.53166411E-01 0.42295700E-04 3
 -0.85899857E-07 0.34333972E-10 0.35149188E+04 0.13448978E+02 4
 DIMCHCH C 10H 11 G 200.000 5000.000 1000.00 1
 0.17523993E+02 0.42742023E-01-0.17334906E-04 0.32089931E-08-0.22269055E-12 2
 0.32833989E+05-0.62079799E+02 0.28735045E+01 0.59241424E-01 0.21069824E-04 3
 -0.64496714E-07 0.27229375E-10 0.37869214E+05 0.19125980E+02 4
 PTRIARO178 C 14H 12 G 200.000 5000.000 1000.00 1
 0.22283250E+02 0.53663832E-01-0.22007060E-04 0.41054578E-08-0.28647362E-12 2
 0.12954527E+05-0.98771614E+02-0.32546286E+01 0.89925723E-01 0.22434541E-04 3
 -0.91411901E-07 0.40065272E-10 0.21356584E+05 0.40906296E+02 4
 PTRIARO192 C 15H 14 G 200.000 5000.000 1000.00 1
 0.24085485E+02 0.60715897E-01-0.24857414E-04 0.46315757E-08-0.32289802E-12 2
 0.90025717E+04-0.10500607E+03-0.11804531E+01 0.89826712E-01 0.39405770E-04 3
 -0.11016348E-06 0.46364102E-10 0.17653406E+05 0.34875711E+02 4
 RDIMERS196a C 15H 15 G 200.000 5000.000 1000.00 1
 0.25714507E+02 0.61521796E-01-0.25034296E-04 0.46451029E-08-0.32288835E-12 2
 0.19838733E+05-0.11048777E+03 0.28550768E+00 0.95688566E-01 0.25039391E-04 3
 -0.96286584E-07 0.41797340E-10 0.28301994E+05 0.29079763E+02 4
 RPTRIARO192a C 15H 13 G 200.000 5000.000 1000.00 1
 0.24737808E+02 0.57138121E-01-0.23415589E-04 0.43664603E-08-0.30461414E-12 2
 0.20111275E+05-0.10639047E+03-0.15594656E+01 0.94912811E-01 0.21043980E-04 3
 -0.92687655E-07 0.40812515E-10 0.28741450E+05 0.37332270E+02 4
 RPTRIARO178a C 14H 11 G 200.000 5000.000 1000.00 1
 0.22932560E+02 0.50084469E-01-0.20563603E-04 0.38399442E-08-0.26815869E-12 2
 0.24181162E+05-0.99267415E+02-0.36651437E+01 0.95263251E-01 0.34862757E-05 3
 -0.73405343E-07 0.34346172E-10 0.32561305E+05 0.44354141E+02 4
 END

VITA

Education

University of Illinois at Chicago (UIC), Chicago, United States Doctor of Philosophy in Chemical Engineering GPA: 4.0/4.0	Aug 2006-May 2012
Osmania University College of Technology, Hyderabad, India Bachelor of Technology in Chemical Engineering GPA: 3.76/4.0	Sep 2002-May 2006

Research Experience

UIC Mechanical and Industrial Engineering Department <i>Graduate Research Assistant, High Pressure Shock Tube (HPST) Laboratory</i>	May 2007-Present
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- Investigate the combustion chemistry of jet fuels and biodiesels at high pressure (20 – 60 atm) and high temperature conditions (900 – 1700 K)
- Conduct experiments on m-xylene, n-propylbenzene and 1,3,5-trimethylbenzene in the High Pressure Single Pulse Shock Tube (HPST) and use gas chromatography and mass spectrometry (GC and GC/MS) for qualitative and quantitative analysis
- Develop chemical kinetic (CK) models to simulate the experimental data of m-xylene, n-propylbenzene and 1,3,5-trimethylbenzene
- Troubleshoot and solve high pressure equipment related issues. Maintain adequate inventory to conduct the experiments in a timely and orderly fashion
- Participate in lab discussions and present research periodically in lab meetings
- Publish the experimental and modeling results in peer-reviewed journals (listed in page 2)
- Participate in conferences at the national and international level (listed in pages 2 and 3)
- Assist in peer-reviewing papers submitted to scientific journals such as Combustion and Flame, Journal of Propulsion and Power, Combustion Science and Technology, Energy and Fuels and Journal of Physical Chemistry
- Guide the undergraduate students in their research projects

Teaching Experience

UIC Department of Chemical Engineering <i>Teaching Assistant, Unit Operations Laboratory</i>	Aug 2006-May 2007
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- Coordinated with the Professor and the lab maintenance staff and planned the experiments
- Guided the undergraduate students in conducting experiments and interpreting their experimental results
- Informed the students about the laboratory safety procedures and handling of different chemicals

Skills

Chemical Kinetic Modeling Software

- Used *Chemkin*, *Cantera*, *Gaussian 03*, *Gaussview* and *Thergas* in the process of developing CK models

Graphing and Chemical Structure Software

- Used *Origin 8*, *Chem3D*, *Molekel* and *ChemSketch* while preparing manuscripts for publications

Process Control Software

- Learned the basics of *Aspen Plus* while auditing the Process Simulation course (CHE 494)

Programming Languages and Environments

- Used *C*, *C++*, *MATLAB* to develop codes for molecular modeling and flow field simulations
- Proficient in using *Windows 7 and 2000 environments* and *Microsoft Office Home and Professional Editions*

Languages

- Fluent in *English*, *Telugu* and *Hindi*

Accomplishments

- Worked on projects sponsored by major funding agencies such as *Air Force Office of Scientific Research (AFOSR)*, *Department of Defense's (DOD) Strategic Environmental Development and Research Program (SERDP)*, *National Science Foundation (NSF)*
- First paper was published in special issue of *Combustion and Flame* journal (Vol. 158, year 2011, p.593), which discussed the notable experimental and theoretical advances in combustion kinetics

Affiliations

Member of the

- Combustion Institute, American Chemical Society,
- Golden Key International Honor Society, Society of Women Engineers

Activities

- Mentoring an undergraduate student, as a participant in the UIC Women in Science and Engineering (WISE) Mentoring Program
- Swimming, salsa, craft projects, movie making and writing creative non-fiction

Completed Projects

University of Illinois at Chicago

Aug 2007-May 2012

- **Combustion of Aromatic Surrogate Fuel Components of Jet Fuels**

Sponsor: Air Force Office of Scientific Research, AFOSR

Studying the combustion of aromatic surrogate fuel components of jet fuels such as n-propylbenzene and 1,3,5-trimethylbenzene and developing an experimental and chemical kinetic modeling validation database.

- **Soot Precursors Formation from the Combustion of m-Xylene:**

Sponsor: Strategic Environmental Development and Research Program, SERDP

Conducted experimental studies on the oxidation and pyrolysis of m-xylene in the HPST and detected the formation of polycyclic aromatic hydrocarbons (PAHs) from our experiments. Investigating the chemical kinetic pathways responsible for the formation of these PAHs.

- **Combustion of m-Xylene at Afterburner Conditions:**

May 2007-Mar 2010

Sponsor: Air Force Office of Scientific Research, AFOSR

Studied the oxidation of m-xylene at low pressure (6 atm) and fuel rich conditions in the HPST and identified the importance of including the pressure dependent reactions in simulating the fuel decay at these conditions.

- **Combustion of Surrogate Fuel Components of Biodiesel:**

Sponsor: National Science Foundation, NSF

Assisted in experimentally and theoretically investigating the chemical pathways responsible for the production of greater NO_x by biodiesels by using saturated and unsaturated C₇ hydrocarbons

Publications

- S. Gudiyella and K. Brezinsky, "High Pressure Study of n-Propylbenzene Pyrolysis", submitted to Proceedings of the Combustion Institute, (2012)
- S. Gudiyella and K. Brezinsky, "High Pressure Study of n-Propylbenzene Oxidation", *Combustion and Flame*, 159 (2012) 940-958
- S. Gudiyella, T. Malewicki, A. Comandini and K. Brezinsky, "High Pressure Study of m-Xylene Oxidation", *Combustion and Flame*, 158 (2011) 687-704

Paper Presentations

- S. Gudiyaella (presenter) and K. Brezinsky, “*High Pressure Study of 1,3,5-Trimethylbenzene Oxidation*”, Eastern States Fall Technical Meeting, Storrs, United States, Oct 2011
- S. Gudiyaella (presenter) and K. Brezinsky, “*High Pressure Study of n-Propylbenzene Oxidation*”, 7th U. S. National Combustion Meeting, Atlanta, United States, Mar 2011
- S. Gudiyaella (presenter), “*Oxidation of Aromatic Surrogate Fuel Components of Jet Fuels*”, Preliminary Examination, UIC, Chicago, United States, Oct 2009
- S. Gudiyaella (presenter), “*High Pressure Study of m-Xylene Oxidation*”, Combustion Kinetics Laboratory, University of Southern California, Los Angeles, United States, Sep 2009
- S. Gudiyaella (presenter), “*m-Xylene Oxidation Experiments and Modeling*”, Lab presentation during Dr. Frederique Battin-Leclerc’s visit to HPST lab, Feb 2009
- S. Gudiyaella, T. Malewicki and K. Brezinsky (presenter), “*Detailed Studies on the Oxidation of Surrogate Fuel Components, Surrogate Mixtures and Real Fuels*”, Multi-Agency Co-ordination Committee for Combustion Research (MACCCR), Fuels Research Review, Chicago, United States, Sep 2011
- A. Comandini, S. Gudiyaella and K. Brezinsky (presenter), “*Aromatic Radicals-Acetylene Particulate Matter Chemistry*”, Washington, United States, Dec 2010 and Dec 2009
- S. Gudiyaella, T. Malewicki and K. Brezinsky (presenter), “*Detailed Studies on the Surrogate Fuel Components of JP-8*”, Multi-Agency Co-ordination Committee for Combustion Research (MACCCR), Fuels Research Review Princeton, United States, Sep 2010
- A. Fridlyand, S. Gudiyaella and K. Brezinsky (presenter), “*Low Pressure Shock Tube Fuel Studies*”, Augmentor Design Systems Conference, Jacksonville, United States, Mar 2010
- S. Gudiyaella, T. Malewicki and K. Brezinsky (presenter), “*Oxidation of Potential Surrogate Fuel Components of JP-8*”, Multi-Agency Co-ordination Committee for Combustion Research (MACCCR), Fuels Research Review, Los Angeles and Gaithersburg, United States, Sep 2009 and Sep 2008
- S. Gudiyaella, T. Malewicki and K. Brezinsky (presenter), “*Comprehensive JP-8 Mechanism for Vitiated Flows*”, UIC, Chicago, United States, Oct 2008

Poster Presentations

- S. Gudiyaella (presenter) and K. Brezinsky, “*High Pressure Study of n-Propylbenzene Oxidation*”, International Conference on Chemical Kinetics, Boston, United States, Jul 2011
- S. Gudiyaella (presenter) and K. Brezinsky, “*High Pressure Study of n-Propylbenzene Pyrolysis*”, International Conference on Chemical Kinetics, Boston, United States, Jul 2011
- S. Gudiyaella (presenter) and K. Brezinsky, “*Oxidation of Aromatic Surrogate Fuel Components of Jet Fuels*”, UIC Student Research Forum, Chicago, United States, Apr 2011
- S. Gudiyaella, T. Malewicki, A. Comandini and K. Brezinsky (presenter), “*High Pressure Study of m-Xylene Oxidation*”, Work in Progress Poster, 33rd International Symposium on Combustion, Beijing, China, Aug 2010
- S. Gudiyaella, T. Malewicki and K. Brezinsky (presenter), “*High Pressure Study of n-Propylbenzene Oxidation*”, Work in Progress Poster, 33rd International Symposium on Combustion, Beijing, China, Aug 2010
- A. Comandini (presenter), S. Gudiyaella, T. Malewicki and K. Brezinsky, “*The Formation of Polycyclic Aromatic Hydrocarbons in Pyrolytic Reactions of the Phenyl Radical in the Presence of Acetylene*”, Partners in Environment Technology Technical Symposium and Workshop, Poster Presentation, Washington, United States, Dec 2010 and Dec 2009
- T. Malewicki, S. Gudiyaella (presenter) and K. Brezinsky, “*Oxidation of Potential Surrogate Fuel Components of JP-8*”, Poster Presentation, UIC Chemistry Department, Chicago, United States, Sep 2008
- T. Malewicki (presenter), S. Gudiyaella (presenter) and K. Brezinsky, “*Oxidation of Potential Surrogate Fuel Components of JP-8*”, Work in Progress Poster, 32nd International Symposium on Combustion, Montreal, Canada, Aug 2008

