THESIS

THE EFFECT OF FUEL REACTIVITY AND EXHAUST GAS RECIRCULATION ON KNOCK PROPENSITY OF NATURAL GAS

Submitted by

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In partial fulfillment of the requirements

For the Degree of Master of Science

Colorado State University

Fort Collins, Colorado

Spring 2020

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ABSTRACT

THE EFFECT OF FUEL REACTIVITY AND EXHAUST GAS RECIRCULATION ON KNOCK PROPENSITY OF NATURAL GAS

The development of high efficiency, spark ignited natural gas engines is currently limited by engine knock at high compression ratio/elevated boost pressures and misfire at lean conditions/high exhaust gas recirculation (EGR) levels. The knock and misfire limits are further confounded by the wide variety in fuel reactivity observed in "pipeline quality" natural gas. In this study, a rapid compression machine was used to characterize the effects of EGR and variation in natural gas fuel reactivity on the homogeneous ignition delay, flame propagation rate, and end-gas autoignition propensity for stoichiometric natural gas/oxidizer/EGR blends. A reduced chemical kinetic mechanism was also developed to accurately model the homogeneous ignition delays measured in the Colorado State University rapid compression machine (CSU RCM). Pipeline quality natural gas with a range of chemical reactivity (68 < Methane Number < 95) was simulated using mixtures of CH_4, C_2H_6, and C_3H_8. Exhaust gas recirculation gases were simulated with mixtures of Ar, CO_2, CO, and NO at substitution rates of 0 to 30 mass percent. Ignition delay period under homogeneous autoignition conditions was measured at compressed pressures of 30.2 to 34.0 bar and compressed temperatures of 667 to 980 K. End-gas autoignition fraction and flame propagation rate were measured by initiating a laser spark in the center of the combustion chamber, after compression, at pressures of 30.7 to 32.7 bar and temperatures of 751 to 795 K. The results indicate that both fuel reactivity and the presence of reactive species (NO and CO) in the exhaust gas recirculation have a strong impact on end-gas autoignition fraction. A chemical kinetic mechanism was developed to predict homogeneous ignition delays for pipeline quality natural gas

in a pressure and temperature range of 1-100 bar and 500-1000 K respectively. This mechanism accurately predicted measured homogeneous ignition delay in the RCM with a total average relative error of 11.0%.

ACKNOWLEDGMENTS

There are many people that I would like to acknowledge for assistance for this work. First, I would like to thank my parents for providing the opportunity to go to Colorado State University for undergraduate and graduate school. Their endless support and words of advice made the completion of this degree possible. I would also like to thank Marie Dutton and her family for giving me a second home in Colorado and being so supportive while I was working on this degree.

Next, I would like to thank my advisor, Dr. Marchese, who was willing to hire me as a freshman in 2012 to be an intern at his lab. His advice and support allowed me to get an understanding of the different paths I could take in energy conversion and emissions research. His support not only gave me a project to work on for my master's degree but allowed me to learn so much about fundamental combustion and chemical kinetics as well. I would also like to thank my committee members, Dr. Olsen and Dr. Reardon for serving on my committee and being available to advise me when I had questions.

As I said, Dr. Marchese, hired me as an undergraduate intern the first semester of my freshman year of undergrad. In the five years of undergrad I worked for many students (Torben Grumstrup, Jessica Tryner, Tim Vaughn, James Tillotson, Marc Baumgardner, Colin Gould, and Siddhesh Bhoite) and each one of them gave me countless words of advice and trained me on how to work in a research lab on a graduate level allowing me to transition from undergrad to graduate school seamlessly.

During my master's degree I worked with another graduate student, Andrew Zdanowicz, running the CSU RCM. His countless hours spent of developing the measurement metrics and

systems made this work possible. I would also like to thank two undergraduate interns, Kara Gustafson and Juan Jimenez for their assistance in running and maintaining the CSU RCM.

I would also like to thank Shannon Wagner who was my supervisor for my Graduate Academic Coach position at CSU. This project, led by Shannon, essentially created mentoring program between the graduate students and the incoming undergraduates. In this program I learned many things such as communication and mentoring skills that most engineers do not have the opportunity to learn in their normal studies. These skills have made me a more well-rounded engineer and I am happy to have had the opportunity to be a GAC.

Finally, I would like to extend a special thanks to Jessica Tryner and Tim Vaughn for not only being among my closest friends in Colorado but for their countless words of advice and support in getting my degree. They were even nice enough to give me a place to stay for the last six months of my degree when my degree ran longer than expected so a big thanks to them for being such good friends.

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1. INTRODUCTION

1.1 Motivation

As concern for human health and human impact on global climate increase, more focus has been placed on limiting emissions from combustion sources such as mobile-heavy truck engines. The current standard for line and heavy haul semi-trucks are compression ignition (CI) diesel engines. These engines benefit from high thermal efficiency, well-established and regulated fuel infrastructure, and relatively low overall emissions. However, with growing concerns of health risks associate with diesel exhaust [1] and rising diesel fuel costs [2] more interest has been placed on developing heavy-duty engines that emit even fewer emissions and still have good thermal efficiency. Spark ignited-natural gas (SI-NG) fueled engines have demonstrated lower gaseous and particulate emissions than diesel engines [3] but struggle with high efficiency due to engine knock limitations [4]. Exhaust gas recirculation (EGR) has been demonstrated as a technology to mitigate knock in engines and could potentially be used to increase thermal efficiency of SI-NG engines [5]. Sponsored by the United States Department of Energy, the Energy Institute at Colorado State University has partnered with Cummins and Woodward Inc. in a three-year program to better understand the limiting factors in mobile natural gas (NG) spark-ignited (SI) engine efficiency and develop a real-time controlled natural gas engine that operates with diesel like efficiencies. The work presented herein is the chemical kinetic analysis of how the reactivity and NG and EGR affect combustion at engine like temperatures and pressures. This information will be used to better understand how NG fuel reactivity and EGR reactivity affect the knock propensity of an engine. Furthermore, the experimental results informed the development of a reduced chemical kinetic model. In future work, the reduced chemical kinetic model will be used to perform three-

dimensional computation fluid dynamics (CFD) simulations to aid development of a SI-NG engine with real time control.

1.2 Natural Gas Fuel Quality in United States

In the United States the majority of natural gas is made up of light alkane fuels. In a survey done by the Southwest Research Institute in 2014 [6] regional fuel composition was measured and averaged. The abbreviated results of that study are included in Table 1, along with a representative sample of the pipeline quality natural gas composition measured at the Colorado State University (CSU) Engines and Energy Conversion Laboratory in fall 2019 and pipeline quality gas measured in the Marcellus shale region in 2013. Natural gas in the United States transmission and distribution systems is composed primarily of methane, followed by lesser concentrations ethane and propane (C_1-C_3) with trace amounts of butane and other containments including nitrogen, hydrogen, carbon dioxide, etc. The data tabulated in Table 1 suggests natural gas composition does not vary substantially by region and contains relatively low levels of hydrocarbons larger than C_2. However, as suggested by the gas composition data acquired at CSU and consistent with observations in the field [7] increased natural gas production from hydraulic fracturing in areas with high levels of natural gas liquids (NGL's; e.g. alkanes of C_3 and greater) has resulted in an overabundance of ethane in the U.S. market [8] resulting in elevated levels of ethane in pipeline quality natural gas in many regions. Conversely, in the northeastern United States, high production in the Marcellus shale, which is very low in NGL's, has produced pipeline quality natural gas that has very low levels of hydrocarbons greater than C_1 [7].

For SI-NG engines, fuel reactivity is quantified by methane number (MN) [9,10], which is analogous to octane number (e.g. RON and MON) for liquid SI fuels [11,12] and represents a measure of fuel knock propensity. By definition, a methane number of 100 corresponds to a

gaseous fuel with the reactivity and knock propensity of 100% methane, whereas a fuel with a methane number of 0 corresponds to a gaseous fuel with the reactivity and knock propensity of 100% hydrogen. However, unlike its gasoline counterpart, natural gas fuel quality is not regulated as an on-road fuel in the United States. As indicated in Table 1, MN of pipeline quality natural gas can vary widely throughout the United States transmission and distribution systems, from the mid-70's for gas originating in production regions with high levels of NGL's to the mid-90's for gas originating in production regions low in NGL's. Whereas gasoline octane number only varies from 85 – 94 nationwide [13] and many gasoline engines are only designed to run on one or two specific octane numbers. Although comparisons should not be made directly between octane number and methane number this illustrates that mobile gasoline engines require a narrow range of fuel quality to run at maximum efficiency. Mobile NG engines face a significant challenge in utilizing a much wider fuel quality ranges across much smaller regions.

Table 1: Regional averages of pipeline quality natural gas composition in the United States in 2014 [6], measured at pipeline quality natural gas at the Colorado State University Engines and Energy Conversion Laboratory in Fall 2019 and measured pipeline quality gas in the Marcellus Shale in 2013 [7].

Region	Methane	Ethane	Propane	Nitrogen	Carbon dioxide	Other	Methane Number
SwRI Western	94.6%	3.2%	0.5%	0.8%	0.8%	0.2%	89
SwRI Central	94.7%	3.5%	0.3%	0.9%	0.6%	0.1%	90
SwRI Eastern	92.7%	4.1%	0.4%	0.9%	1.7%	0.2%	88
Colorado State University, 2019	85.5%	8.9%	1.2%	1.0%	1.6%	1.9%	77
Northeastern Marcellus, 2013	97.7%	1.9%	0.1%	0.0%	0.0%	0.0%	93

The wide variation in fuel reactivity in pipeline quality natural gas represents a challenging design constraint that limits the ability to maximize thermal efficiency and performance in SI-NG engines. Specifically, the compression ratio and/or maximum boost pressure for SI-NG engines must be designed to avoid engine knock for operation with the most reactive fuels (i.e. low MN fuels) which limits the compression ratio and maximum boost pressure. To maximize performance and efficiency, mobile NG engines will need to be able to operate at the threshold of knock for any pipeline quality fuel reactivity. Such engines will likely require high percentage of exhaust gas recirculation (EGR), stoichiometric air/fuel ratios to maintain transient load performance and enable the use of a 3-way catalyst, and sophisticated real time control algorithms to detect the onset of knock and meet low emission requirements [14].

1.3 Natural Gas Engines, Efficiency, and Knock

SI-NG engines offer a multitude of advantages over diesel engines including lower particle emissions and lower cost (engine maintenance, exhaust treatment systems, and fuel) [3,15,16]. However, SI-NG engines continue to have relatively low market penetration in comparison to diesel powered compression ignition (CI) engines for mobile applications due to limited fueling infrastructure, poor transient load response and low thermodynamic efficiency [4]. Development of high efficiency SI-NG engines is currently limited by misfire at lean conditions/high exhaust gas recirculation (EGR) levels and engine knock at high compression ratio/elevated boost pressures. At the lower bound, misfire occurs at lean conditions or conditions with high EGR levels where there is not enough fuel in the engine cylinder to ignite resulting in weak or no combustion. Misfire dramatically reduces the efficiency and power output of the engine and increases unburned hydrocarbon emissions. At the upper bound of engine operation, knock is a scenario where the fuel/air mixture ignites volumetrically causing violent pressure oscillations that eventually damage the engine [17].

Under normal SI-NG engine operation, near the end of the compression stroke, a spark ignites a premixed air/fuel mixture. Around the spark a flame is initiated that propagates outwards consuming the air/fuel mixture. The flame propagates outward until it is quenched by the cold thermal boundary layer against the piston and cylinder walls. This process provides a gradual energy release that is known as the power stroke in the Otto cycle. In order to maximize the efficiency of an Otto cycle. It is desirable to increase the compression ratio of the cycle. However, as compression ratio increases, in-cylinder pressure and temperature also increase. Eventually, abnormal combustion occurs. In an engine operating in this abnormal mode, the same initial steps occur. A spark ignites the premixed air/fuel mixture near the end of the compression stroke. A

flame begins to propagate outward. As the flame propagates outward the air/fuel mixture in front of the flame, called end-gas, is heated and compressed. If the proper (undesirable) conditions occur, the end-gas violently and volumetrically autoignites causing a rapid pressure and temperature increase in the engine cylinder. This combustion phenomenon is known as knock or end-gas autoignition.

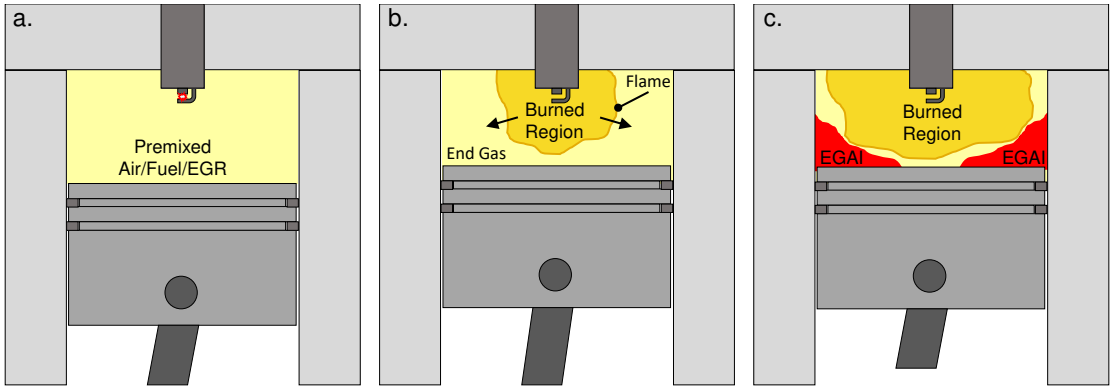

Figure 1: Schematic showing process of knock in SI-NG engine. (a.) Air/fuel mixture is ignited with a spark from the spark plug as piston moves towards top dead center (TDC). (b.) The spark initiates flame that propagates throughout the cylinder consuming air/fuel mixture. (c.) If the proper condition exists, the gas in front of the propagating flame (end-gas) volumetrically autoignites resulting in violent in-cylinder pressure and temperature increase.

Knock affects the engine in many ways. The largest effect is due to physical damage to the piston face, cylinder walls, and cylinder head in the engine. In a properly operating engine, a thin flame front gradually consumes the fuel. As the flame approaches the walls of the cylinder the cold walls quench the flame leaving a cold thermal wall boundary that isolates and protects the inner surfaces of the cylinder and piston. In a knocking engine the flame propagates as normal but the end-gas autoignites volumetrically. The volumetric autoignition allows hot combustion gasses to burn through the cold thermal boundary layer and burn directly against the cylinder wall and piston faces. This high heat along with many reactive radicals from the combustion process chemically attack the cylinder and piston surfaces eventually causing oxidation and pitting. With continued

operation these conditions evolve into cylinder wall scuffing, valve and head erosion, and potentially piston failure [18].

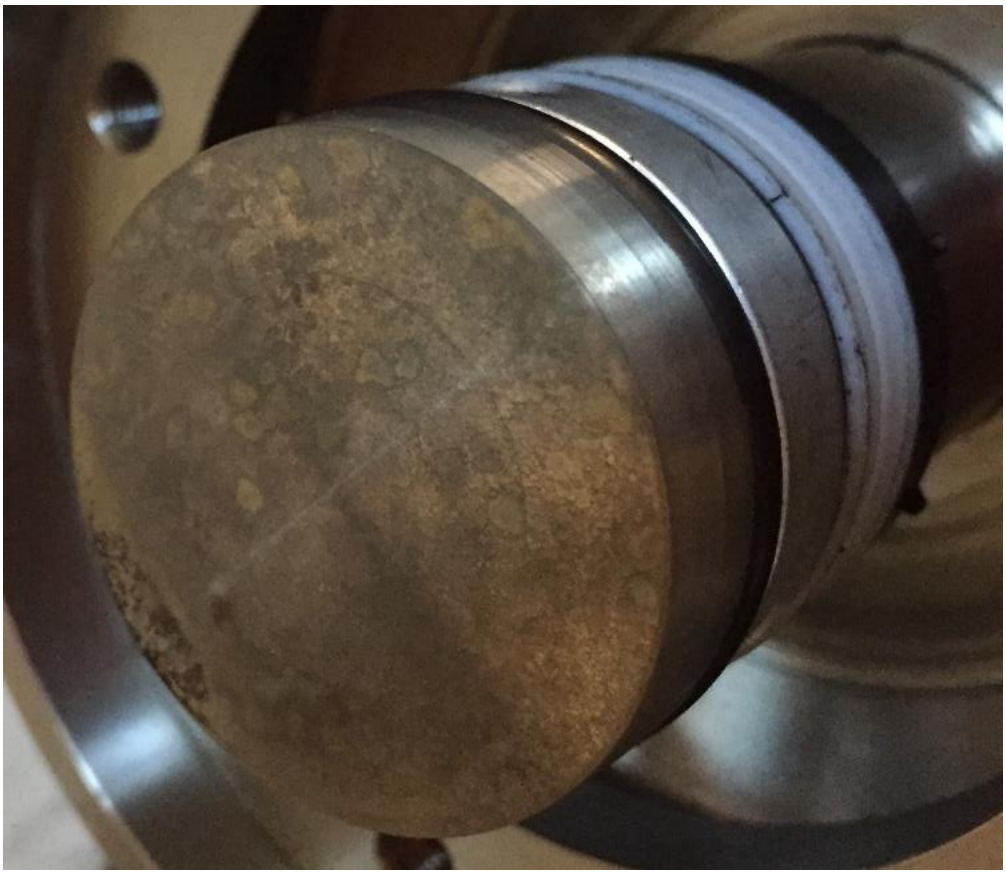

Figure 2: Photograph of piston face of Colorado State University (CSU) rapid compression machine (RCM) showing the chemical oxidization due to knock experiments. These effects were seen after ~50-75 heavy knock experiments in the RCM a SI-NG engine during normal operation would cycle 50-75 times in a couple seconds.

Therefore, the maximum efficiency of an SI-NG is limited by the occurrence of knock and the highest efficiency engines are designed to run right at the threshold of knock. If an engine is operating on a single fuel blend (gasoline car engines) the mechanical design and operating conditions can be found easily during the design of the engine. However, in the case of mobile SI-NG engines, where fuel reactivity can vary greatly, the engine design must be able to actively change its in-cylinder combustion conditions to remain below the threshold of knock. This type of engine would need to be controlled with sophisticated real-time control algorithms that monitor

knock and change engine parameters to remain efficient operating conditions. In order to achieve this, EGR substitution may be utilized to control the in-cylinder combustion conditions. Therefore, a strong understanding of EGR and NG interaction and how this could lead to knock is very important. This study will perform experiments and simulations to better understand how natural gas fuel quality and EGR substitution change the likely hood of knock in an engine.

1.4 Overview of Exhaust Gas Recirculation

Historically, EGR has been used in engines to reduce oxides of nitrogen (NO_x) formation [19,20]. Studies have also shown that EGR can be employed to reduce knock in SI engines [5,21]. However, many laboratory studies [22–24] investigating knock mitigation using EGR employ nitrogen (or another inert gas) with a mixture of just CO_2 or H_2O as surrogate for EGR gas. In reality, EGR gas composition varies greatly depending on the engine and source of the EGR gas. EGR systems vary greatly between different engine designs. The two most common types of EGR systems are low-pressure and high-pressure loop systems as seen in figure 3.

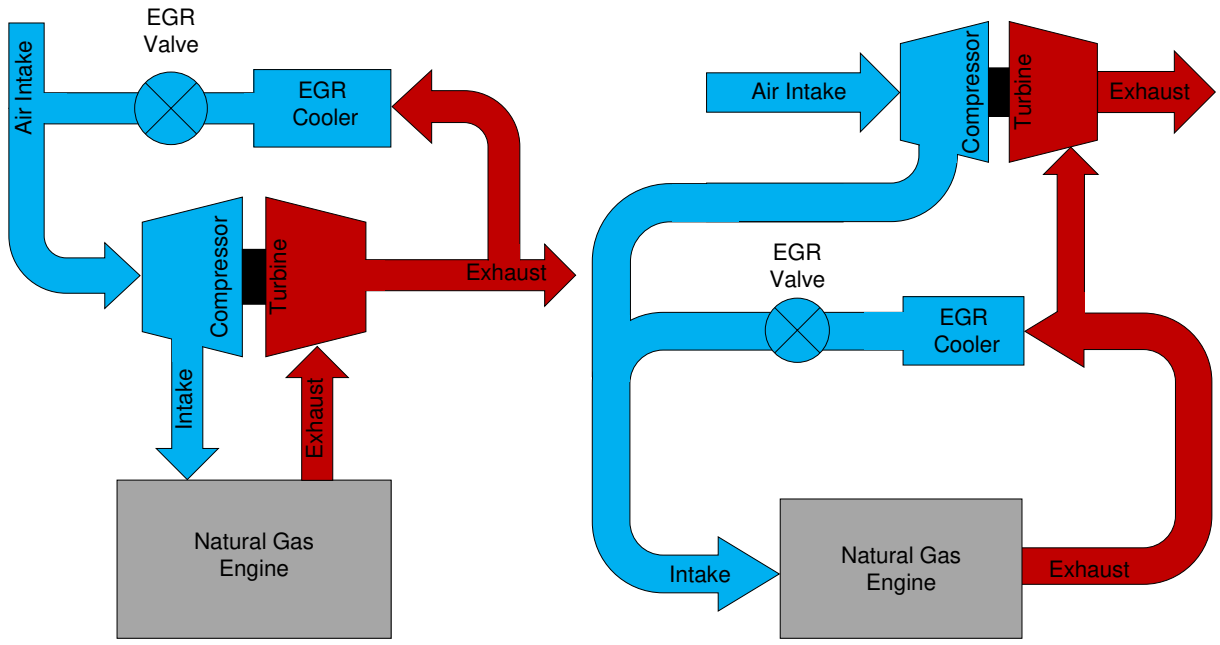

Figure 3: (Left) low-pressure loop EGR configuration. **(Right)** high-pressure loop EGR configuration.

Beyond low- and high-pressure loops EGR can also be cooled to various degrees, dried to remove water vapor, or even catalyzed to remove reactant species [19]. Although there are many different types of EGR systems, EGR consists of the same basic species between engines. EGR gas is comprised of N_2, CO_2, and H_2O in thermodynamically significant quantities. In thermodynamically insignificant but potentially chemically significant quantities, reactive species such as NO, CO, and unburned hydrocarbons are found. However, the quantity of these species change due to engine operating conditions such as fuel type, EGR substitution rate, engine load, boost pressure, etc. There are many benefits to using EGR in an engine. The most common is a reduction of NO_x emissions and the reduced need for post-exhaust treatments [25]. EGR is also effective to increase the thermodynamic efficiency of engines. Canton, explains many thermodynamic reasons for the efficiency increase including; reduced pumping losses due to increased mass flow with EGR substitution, increased ratio of specific heats of the bulk air/fuel/EGR in cylinder mixture, and reduced heat transfer due to the lower maximum in cylinder

temperatures [26]. The final use of EGR is to mitigate engine knock [27]. In early studies (1986) done by Watanabe ERG was found to effectively reduce knock and decrease brake fuel consumption. Watanabe used 99.9% pure N_2 as an EGR surrogate, and an insignificant difference was found between real EGR and nitrogen substitution in engine operation [5]. The influence of reactant species in the EGR surrogate has become of interest in modern studies. In fact, in more recent studies [28,29] there has been evidence that EGR may not be effective in reducing knock and that NO_x concentration could significantly change in cylinder combustion characteristics. Part of the complication in these studies is the complex combustion that occurs inside of an engine. For example, if an engine is being tested at a single power output and speed, as EGR is substituted the quantity of fuel in the intake charge decreases because it is displaced by the substituted EGR. In order to maintain the required power, the intake manifold pressure (IMP) must be increased to maintain the original mass of fuel required by the engine. The corresponding increase in IMP results in different in-cylinder pressures, temperature, turbulence and heat transfer effects. In effect, it is difficult to independently vary the variables that impact combustion kinetics in an engine. One of the goals of this study is to understand how fuel quality and EGR substitution rate influence the likely hood of knock on a chemical kinetic level. This requires a system that can combust air/fuel/EGR mixtures at consistent pressures and temperatures changing as few independent variables as possible. Therefore, a machine designed to study combustion kinetics is used, instead of an engine, for this study.

1.5 Rapid Compression Machines

Rapid Compression Machines (RCM) are commonly utilized in chemical kinetic studies. Most RCM's are purpose-built machines that vary greatly in design and system operation. However, all RCM's operate on the same basic principles. RCM's use one or more pistons to rapidly compress

and heat a mixture to observe changes in combustion kinetics [30]. The RCM used at Colorado State University is known as a horizontally opposed dual-piston RCM. It is hydraulically locked and pneumatically fired (figure 4).

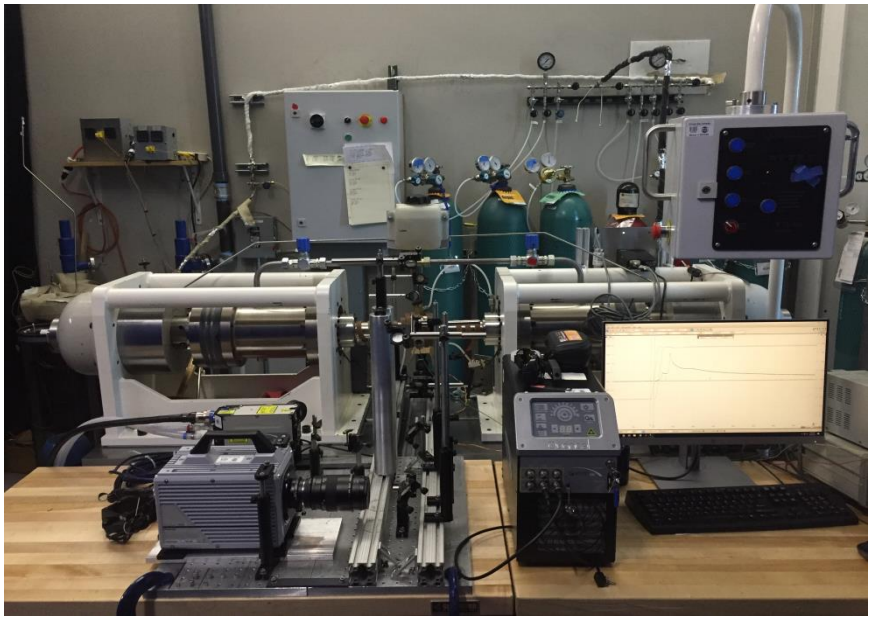

Figure 4: Horizontally opposed dual-piston RCM at CSU

The CSU RCM utilizes two pistons to simulate a single compression stroke of an engine. The CSU RCM has been modified to utilize a laser ignition system and schlieren imaging system. Unlike an SI-NG engine that runs full Otto cycles, the RCM operates as a single shot mode with only a compression stroke. First, the pistons are pulled to bottom dead center (BDC) and the combustion chamber is vacuumed of all reactants using a rotary vane vacuum pump. The air/fuel/inert (reactants) mixture is premixed and loaded into the combustion chamber to the desired pressure and temperature. Upon firing the two pistons come together with a nominal compression ratio of 11.8:1. The mixture is compressed in 15-20ms and the pistons lock at top dead center (TDC) creating a constant volume chamber with a volume of 30.0 cm^3. The reactants, now at elevated temperature and pressure, are then ignited using either a laser spark or ignite from compression ignition depending on the experimental goals. This process completes a single

experiment in the RCM. There are many advantages that RCM's have over engines for chemical kinetic studies. The main advantage is the quiescent volume that remains in the combustion chamber during and after compression. This is made possible using creviced pistons. A complete description of piston geometry and design can be found in section 2.3. The fluid dynamic simplicity not only makes simulation of experiments easier but also allows the collection of remarkably high-resolution video of combustion events inside the RCM. These capabilities make the CSU RCM effective in studying chemical kinetic reactivity of gaseous fuels.

1.6 CSU RCM Experiment Theory and Overview

The CSU RCM has been modified with a laser ignition system, a schlieren imaging system, and creviced and non-creviced pistons. These systems enable both compression ignition (CI) and laser-ignited (LI) experiments to be performed and optically observed inside the RCM. These systems expand the CSU RCM's capability to include measurement of homogeneous autoignition delay, end-gas autoignition (EGAI) fraction (f_{EGAI}), and in cylinder flame propagation measurements. F_{EGAI} has been demonstrated to be proportional to knock propensity in engines [31]. The ability to measure f_{EGAI} and flame propagation rate will be vital to characterize the effect that NG reactivity and EGR composition has on knock propensity. For this study, the CSU RCM will be utilized to perform both CI and LI experiments. CI experiments to measure homogeneous autoignition delay and LI experiments to measure f_{EGAI} and flame propagation rate. In figure 5 below, both experiments are shown conceptually. An in-depth description of physical setup is available in sections 2.2 – 2.5 and an in-depth description of the analysis methods are available in section 3.3 – 3.5.

For the homogeneous ignition delay period experiments shown in figure 5, creviced pistons are employed to minimize roll up vortices and maintain a symmetrical adiabatic core [32]. The

gaseous mixture (fuel/oxidizer/inert) is premixed and filled into the main combustion chamber at a specified temperature and pressure. The reactant mixture is then compressed with a compression ratio of 11.8:1, resulting in compressed pressure and temperatures of 30.2 to 34.0 bar and 667 to 980 K, respectively. The reactant mixture then volumetrically autoignites and the ignition delay period is defined as time interval between when the pistons reach TDC and time of maximum in-cylinder pressure rise rate.

For the laser-ignited RCM experiments shown in figure 5, non-creviced pistons are used to ensure that EGAI does not occur in the piston crevices and to facilitate differentiation between heat release from the propagating flame and heat release during the EGAI event. A detailed description of the non-creviced piston development can be found in section 2.3. In short, during development of the f_{EGAI} metric, it was found that the crevice volume could ignite, and that this ignition was not consistent between operating conditions. Since this combustion varied, it was difficult to effectively separate crevice combustion from the flame propagation and EGAI events inside the RCM [31]. Using non-creviced pistons ensures all combustion is either flame propagation or EGAI. The lack of crevice does cause turbulence effects which are discussed in section 2.3 and 4.2. To perform the LI experiments, the gaseous mixture (fuel/oxidizer/inert) is premixed and filled into the main combustion chamber at a specified temperature and pressure. The reactant mixture is then compressed with a nominal compression ratio of 11.8:1, resulting in compressed pressure and temperatures of 30.7 to 32.7 bar and 751 to 795 K, respectively. The mixture is then ignited 10ms after TDC by a laser spark, which is created at the centerline of the combustion chamber. The laser spark initiates a spherical, outwardly propagating flame, which compresses the end-gas upstream of the propagating flame, resulting in EGAI depending on the reactivity of the mixture. Flame propagation rate is measured optically using a schlieren imaging

system. The EGAI propensity of the mixture is quantified by the f_{EGAI}, which is defined as the fraction of heat released during the EGAI event divided by the total heat release.

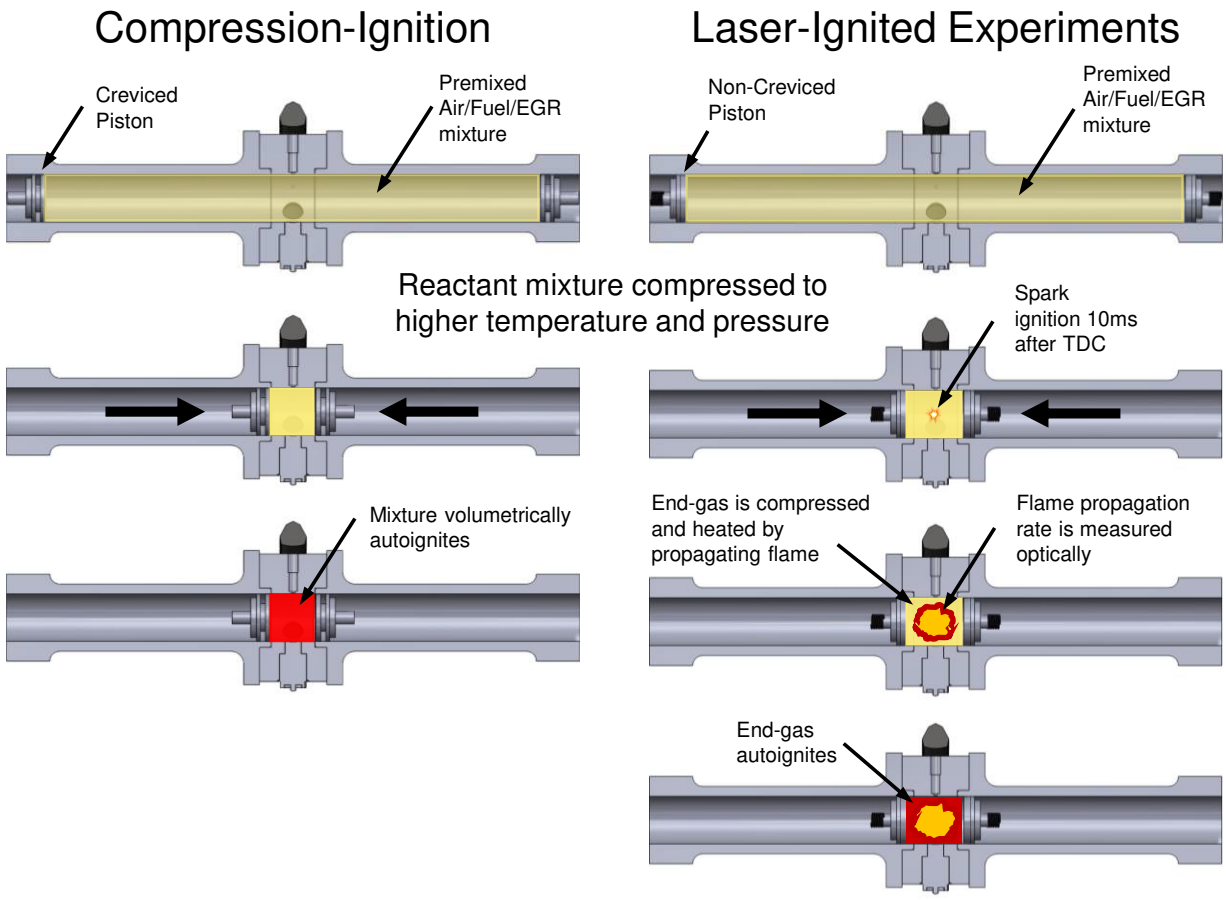

Figure 5: Cross section of rapid compression machine combustion chamber showing the two experimental configurations employed in this study: **(Left)** homogeneous compression ignition experiments used to measure homogeneous ignition delay period and **(Right)** laser-ignited experiments used to measure flame propagation rate and end-gas autoignition fraction.

1.7 Experimental Objectives

In this study, the effect of NG fuel reactivity and EGR substitution on homogeneous ignition delay, flame speed, and end-gas autoignition (EGAI) fraction (f_{EGAI}) of NG blends is investigated using a novel rapid compression machine (RCM) apparatus fitted with a laser ignition system and high-speed Schlieren imaging system. To examine the effect of fuel reactivity a variety of C_1 to C_3 fuel blends were employed, which produced a range of methane numbers from 68 to 95. EGR

gases were simulated with mixtures of Ar, CO_2, CO, and NO at substitution rates of 0 to 30 mass percent. To determine the effect of reactive EGR gases on end-gas autoignition (CO and NO), experiments were also conducted without the reactive species present. The results of this study were used to develop and evaluate a reduced chemical kinetic model for use in computational internal combustion engine models to aid in the development of high efficiency SI-NG engines for mobile applications.

2. EXPERIMENTAL SYSTEMS AND DISCRIPTION

2.1 The Colorado State University Test Facility

The research conducted for this project took place at the Engines and Energy Conversion Laboratory located at the Powerhouse Campus of Colorado State University. A wide variety of research is completed at this facility including algae biofuel development and property testing, biomass cookstove emission studies, laser diagnostics of combustion, and RCM chemical kinetic studies. The RCM test cell, located in the Center for Laser Sensing and Diagnostic Laboratory, contains the CSU RCM, a gas mixing manifold, mixing tanks, and the laser ignition and schlieren imaging system. Each of these systems and will be described in detail in the following sections followed by a full description of experiments and analysis systems used to complete this project

2.2 The Colorado State University Rapid Compression Machine

The RCM was manufactured by Marine Technology, LTD of Galway, Ireland. The RCM is a horizontally opposed, twin-piston system with a nominal compression ratio of 11.8 (figure 6). It operates using a hydraulically locked and pneumatically fired system.

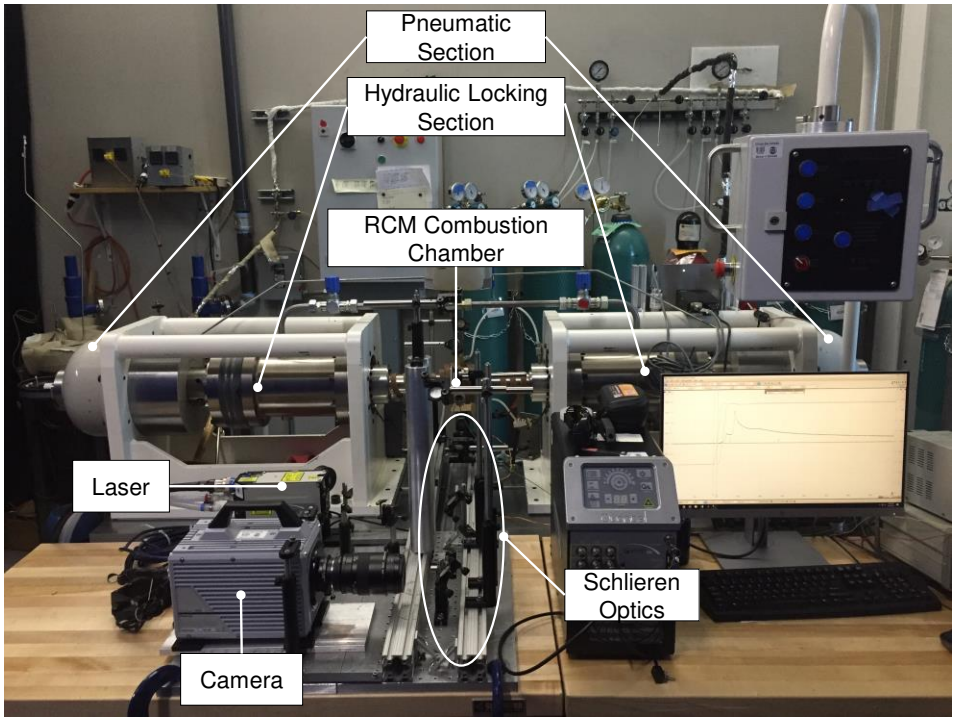

Figure 6: CSU RCM showing pneumatic drive sections, hydraulic locking sections, combustion chamber, laser system, and schlieren system.

The combustion chamber is externally heated using an OMEGA SRT201 heat wrap controlled by a Lightobject JLD612 PID controller. Initial chamber pressure is measured by a dual capacitance manometer that is gas independent to allow accurate pressure measurement of gas mixtures (MKS PDR2000 and MKS 722B13TCE2FA). These systems allow consistent and accurate initial pressure and temperature measurement which are vital to accurate calculation of the in-chamber temperature during compression. Piston position is measured using Positek Limited p100 series linear transducers. Pneumatic bellows on the backside of the piston assemblies are charged to 13.8 bar with air to provide the compressive force. Upon firing, the test gas mixture in the combustion chamber is compressed in 15 to 20ms. After compression, the pistons are held at TDC to maintain a constant volume of 30.0 cm^3 for the remainder of the experiment. A thermally compensated, high speed pressure transducer (Kistler 601CAA) is used to measure the pressure inside the combustion chamber during compression and combustion. The

signal from the pressure transducer passes through a Kistler Type 5018 charge amplifier. The pressure data and piston positions are recorded using a 12-bit Picoscope 4424 data acquisition system with a sample rate of 2 MHz. Due to the rapid temperature changes during compression and combustion it is difficult to accurately measure in chamber temperature. Therefore, temperature inside the combustion chamber is estimated using ideal gas law and adiabatic compression assumption from the measured pressure. Using equation 1 below.

$$T = T_0 * \frac{P}{P_0} * \frac{1}{R_{ad}} \quad (1)$$

Where: T is the estimated temperature inside the chamber, T_0 is the initial chamber temperature, P is the measured pressure inside the chamber, P_0 is the initial chamber pressure, and R_{ad} is the adiabatic compression ratio (see equation 2)

The assumption of adiabatic compression is an approximation with a limited accuracy. However, by using creviced pistons this approximation has become the accepted standard for RCM experiments [30]. Therefore, when possible, the creviced pistons are used for all CSU experiments. However, as discussed in the next section non-creviced pistons were required and to complete the f_{EGAI} experiments.

2.3 CSU RCM Non-Creviced Piston Development and Characterization

The CSU RCM currently has two options for piston selection, creviced and non-creviced. The original pistons that were delivered with the RCM are a creviced design. Creviced pistons are used to absorb the cold wall thermal boundary as the pistons compress. This prevents the formation of roll-up vortices which create temperature gradients inside the chamber destabilizing the adiabatic core [32] (figure 7).

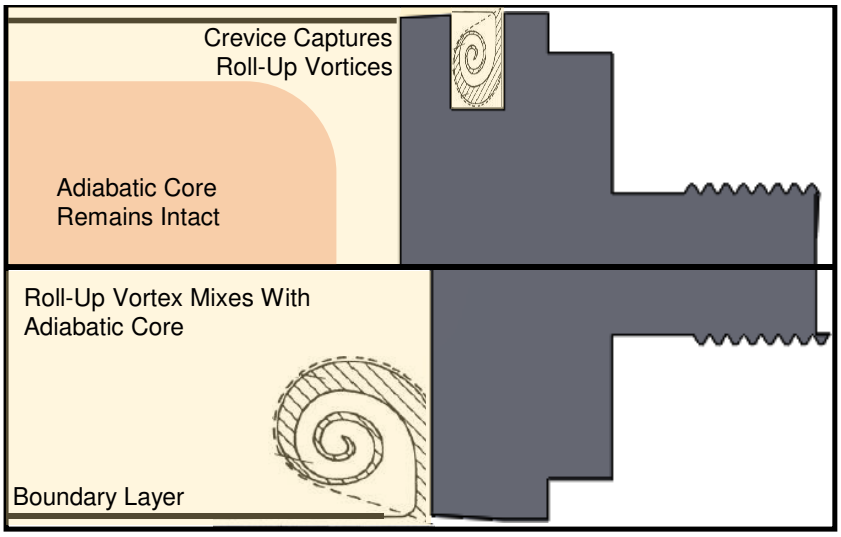

Figure 7: Schematic of creviced vs. non-creviced piston. Piston movement is from right to left. **(Top)** cold thermal wall boundary layer is captured in crevice volume during compression maintaining the adiabatic core. **(Bottom)** cold thermal layer is mixed with adiabatic core by roll-up vortices caused by the non-creviced piston. This makes the adiabatic temperature calculations less accurate and increases turbulent effects inside RCM combustion chamber.

During development of the f_{EGAI} metric combustion in the crevice became a concern [31]. The f_{EGAI} metric is essentially the heat release attributed to EGAI divided by the total heat release of the entire combustion event. Therefore, the ability to accurately distinguish between the heat release due to the flame propagation and EGAI is important. For extremely reactive mixtures it is possible for the mixture in the crevice volume of the piston to autoignite. This crevice has a narrow opening around the perimeter of the piston that could quench and extinguish the propagating flame but still autoignite creating a percentage of the chamber that could only autoignite which would cause error in f_{EGAI} calculation. Furthermore, since the crevice is designed to absorb the cold-wall thermal boundary the temperature in the crevice is significantly different than the temperature in the main chamber. This temperature difference, along with varied fuel reactivity, could result in no combustion, partial combustion, or complete combustion of the crevice volume causing significant error in f_{EGAI} calculation.

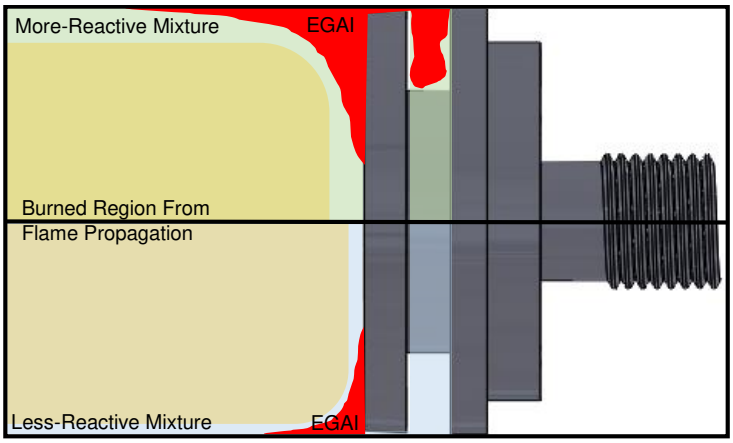

Figure 8: Schematic demonstrating potential error caused by inconsistent combustion in crevice volume of creviced-piston. **(Top)** a highly reactive mixture may be able to autoignite inside the crevice volume artificially increasing f_{EGAI}. **(Bottom)** low reactivity mixture may not autoignite in the crevice volume artificially reducing f_{EGAI}.

Combustion in the crevice volume could be mitigated in a couple ways. The ideal option would be the development of a crevice containment system that allows the crevice to be open during compression then sealed off when the pistons reach TDC. Unfortunately, this would require a re-design of the entire RCM combustion chamber, pistons, and piston ring seals to be implemented and was ultimately beyond the scope of this project. Therefore, the next best option was to remove the crevice from the piston and develop non-creviced pistons to eliminate the crevice volume and improve consistency of f_{EGAI} calculation (figure 9). This method sacrifices turbulent consistency and temperature accuracy for LI experiments in the RCM. However, general trends could still be observed even with the large error and LI experiments could still be completed successfully.

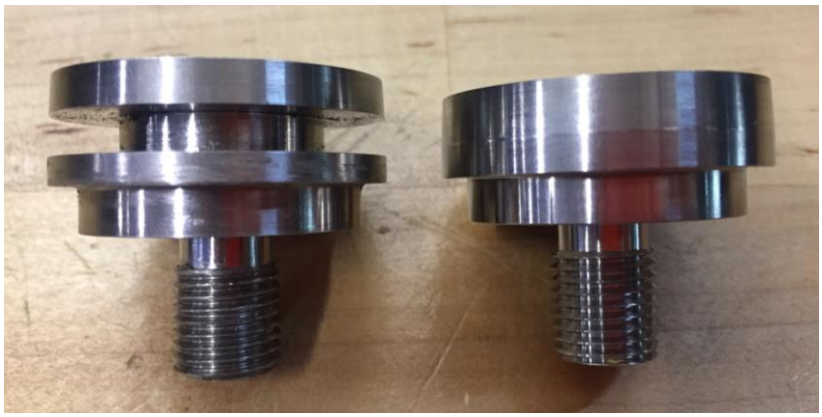

Figure 9: Pistons used in CSU RCM creviced piston **(Left)**, non-creviced piston **(Right)**. Note the non-creviced piston is shorter to maintain nominal compression ratio.

The non-creviced pistons were designed to maintain the nominal compression ratio. This was accomplished by maintaining the same "wetted" volume between the creviced and non-creviced piston designs. In this case the "wetted" volume is the volume contained in the piston crown that contacts the reactant mixture inside the combustion chamber. Modifications were also made to the tolerances of the piston ring seal assembly to reduce potential for blow-by and leakage of the pistons during compression. After the new non-creviced pistons were manufactured a set of benchmark tests were run to characterize the performance of the non-creviced pistons. This was accomplished by running sequential compression runs with N_2 at an initial pressure and temperature of 1.00 bar and 328 K respectively. Figure 10 below shows the results of the benchmark testing where three replicates were run for each piston type. Interestingly, even though the nominal compression ratio is the same between the two piston types the maximum compressed pressure of the non-creviced pistons were markedly higher than the creviced pistons (6.1%). This illustrates the importance of maintaining consistent piston ring seal and minimizing chamber leakage between experiments. Since the ring seals were sealing better with the new non-creviced piston design there was less leakage resulting in a higher compressed pressure. Furthermore, the surface area between the two piston types is not consistent changing the rate of heat transfer as

well. Ultimately, the difference in performance between the two piston designs are only important if comparison experiments between the two pistons are desired. In this project they are not compared beyond this initial benchmark. However, these results demonstrate the importance of adiabatic compression ratio to maintain experimental consistency. Although the nominal (physical) compression ratio is the same between the two pistons designs the effective adiabatic ratio is significantly different. The adiabatic compression ratio calculated using the pressure ratio between the initial and compressed pressures of an experiment.

$$R_{ad} = \left(\frac{P_{max}}{P_0}\right)^{\frac{1}{\gamma}} \tag{2}$$

Where: R_{ad} is the adiabatic compression ratio. P_{max} is the maximum measured compressed pressure, P_0 is the initial chamber pressure, and γ is the ratio of specific heats for the mixture in the chamber.

Monitoring the adiabatic compression ratio between experiments allows more consistent experimental results and a good indicator or leakage through the piston ring seals or general chamber seals (i.e. window seals).

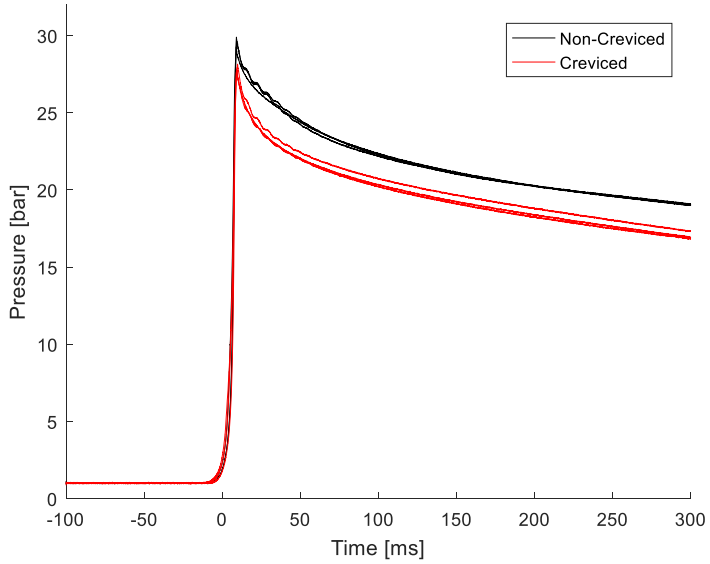

Figure 10: Results of nitrogen benchmark testing for non-creviced and creviced piston designs. Initial pressure and temperature were 1.00 bar and 328 K respectively. Non-creviced pistons reached a maximum compressed pressure 6.1% higher than creviced pistons. The adiabatic compression ratio for the creviced pistons and non-creviced pistons were 11.25:1 and 10.78:1 respectively.

The other side-effect of removing the crevice from the piston is the introduction of turbulence into the RCM experiments. As discussed earlier in this section, the crevice absorbs the roll-up vortices from the cylinder wall. In the non-creviced piston these vortices are no longer captured and turbulent effects can be seen in experimental results. This effect becomes more pronounced with varied piston offset. Piston offset is a side effect of the dual piston design of the CSU RCM. Since the pistons are not mechanically coupled when fired one piston can reach TDC before the other side. The time difference between each piston hitting top dead center is termed as piston offset. The turbulent effects are difficult to quantify inside the combustion chamber of the RCM. However, in experimental data the effect is seen in statistical variation of the results. In order to manage error, strict selection criteria must be placed on experimental data which will be discussed in sections 3.3 – 3.5.

2.4 Gas Mixing Systems and Methods

Precise and accurate mixing of reactants is vital to the repeatability and accuracy of all RCM experiments. In past projects the reactant mixture was mixed directly in the RCM combustion chamber using partial pressure. However, this method suffers from the physical separation of the pressure transducer from the RCM combustion chamber by nearly three meters of quarter inch tubing. This can be seen in figure 11 as the distance from HV 8 to HV11. This length coupled with the valve locations have a significant impact on experimental error. In fact, in a benchmark test case of stoichiometric propane and air, changing the order in which the reactants were added to the chamber resulted in a mixture that would ignite if propane was added first or would not ignite if propane was added last. For this reason, the gas mixing methods have been re-developed for the experiments of this project. The gas mixing system consists of four main parts, parent gas bottles, gas mixing manifold, gas blend bottle, and the liquid mixing tanks. These parts are used together to create batch mixtures that are used to accurately fill the RCM combustion chamber.

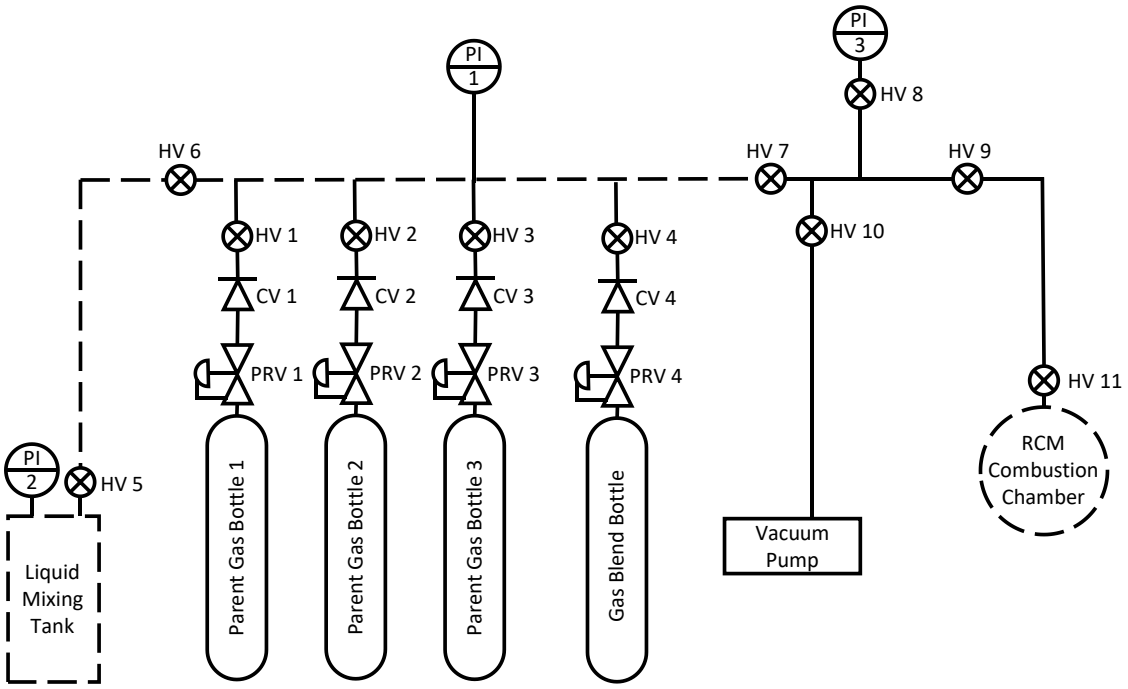

Figure 11: Piping and instrumentation diagram of gas mixing system for CSU RCM. Where: PI = pressure indicator, HV = hand valve, PRV = pressure regulated valve, CV = check valve, dotted lines indicate temperature-controlled sections of the system.

The mixtures were blended using partial pressure and technique was adapted from ASTM Standard D4051-10. Due to the high level of accuracy required to mix the NG fuel blends, the CH_4, C_2H_6, and C_3H_8 were mixed separately in a size 300, CGA 350 gas cylinder (gas blend bottle). Partial pressure was measured using and OMEGA DPGM409-3.5BA pressure transducer. The exact procedure used to blend the fuel mixture is described in detail in the Appendix A. The accuracy in the fuel blends were verified using a gas chromatograph. The results of these measurements demonstrated a mixing accuracy of 0.25% in the fuel blend. By mixing the fuel blend separately in the gas blend bottle, this cylinder can then be used as a parent fuel bottle, then loaded into the liquid mixing tank as a homogeneous fuel blend. This increases the partial pressure of the fuel reactants to the sum of the three fuel components and therefore increases the measurement accuracy of the fuel component in the final batch mixture in the liquid mixing tank.

The total air/fuel/EGR reactant mixture was blended in a similar way. To mix the total reactive mixture the liquid mixing tank was utilized. The liquid mixing tank was developed by Marc Baumgardner. It was designed to allow the vaporization of hydrocarbon fuels that are normally liquid at room temperature and pressure to be utilized in gaseous form in the RCM. The liquid mixing tank has a volume of 20 liters and was designed to have a working pressure of 2 bar. The liquid mixing tank is externally heated using PID controlled wrap heaters and insulated to provide a consistent working temperature. A magnetic stir bar is used to promote mixing of the reactants. The liquid mixing tank is designed to be used with the full reactant mixture (fuel/inert/oxidizer) and are designed to remain intact in case of accidental ignition. In the unlikely case that the pressure during an accidental ignition event rises too high, a burst disk ruptures at 6.89 bar to insure the in-tank pressure remains below the rupture pressure of the tank walls. More detail on the liquid mixing tank can be found in reference [33]. For the experiments completed in this project, the liquid mixing tanks were utilized to batch mix the total reactant mixture before running experiments. The liquid mixing tanks we filled by partial pressure and measured using an OMEGA DPGM409-3.5BA pressure transducer. The exact step by step process can be found in appendix A. This method reduced error when mixing by partial pressure since the working pressure is higher and the pressure transducer location is more direct when compared to mixing the reactants directly in the RCM combustion chamber (figure 11 PI-2). Furthermore, since the liquid mixing tank is temperature controlled the temperature of the liquid mixing tank can be set to match the initial temperature of the RCM combustion chamber to ensure more accurate initial temperatures for the RCM experiments. Finally, the liquid mixing tanks contain enough mass to fill the RCM combustion chamber 25-30 times ensuring that each experimental replicate was run with the same

initial reactant mixtures. This method effectively delivers accurate and repeatable reactant mixtures to the RCM.

2.5 Laser Ignition System and Schlieren Imaging System

In order to run flame propagation and f_{EGAI} experiment an ignition system is necessary to initiate flame propagation. A laser system was chosen for its ability to create a spark without the requirement of metal electrodes that a conventional spark plug would use. The lack of electrodes provides many advantages. First, the laser spark ignites the mixture as a plasma that forms at the focal point of the laser energy. Therefore, the position of the spark is easy to control and change by simply moving the focusing lens that is external to the RCM chamber. Second, the lack of electrodes allows an unimpeded spherical flame propagation which allows for easier and more accurate experiments. Finally, the energy of the laser can be easily changed to suit the required ignition energy of the mixture.

To image the flame propagation and f_{EGAI} a schlieren optical system is used. Schlieren utilizes collimated (parallel) light rays that are diffracted by density gradients. In other words, it is a density gradient imagining system. In these experiments, the density gradients are caused by the large temperature differential from the flame front propagating throughout the chamber. Therefore, this method is quite effective in imaging the flame propagation rates inside the RCM combustion chamber. The schlieren the RCM was originally developed by Ciprian Dumitrache [34] and has been modified as needed for the current experiments. A description of the actual instruments used in both the laser ignition and schlieren system is made below.

Shown schematically in figure 12, the laser ignition system starts with a 1064 nm Nd: YAG laser (Quantel Q-smart 100). The laser energy is steered through a beam splitter that directs a small portion of the beam to a photodiode to measure laser timing. Another beam splitter directs another

small portion of the remaining beam to an energy meter (Ophir PE25BF-DIF-C) to measure relative spark energy. The remaining portion of the energy is then steered to the combustion chamber where a lens focuses the energy down to a point creating a spark in the center of the RCM combustion chamber. The schlieren system uses a 405 ± 15nm LED and a series of optics to pass collimated light into the chamber through a 16.1 mm sapphire window. The collimated light is refracted in the chamber by density gradients, exits the chamber through a second 16.1 mm sapphire window, where it is focused to a point and split by a knife edge. The light is re-collimated and reflected, by a dielectric mirror, into the high-speed Photron SA5 camera operating at 50,000 frames per second with a resolution of 155 pixels/mm^2. The dielectric mirror only reflects a notch of the visible wavelengths (350-400 nm). This reduces the intensity of the broad band radiance from the combustion process giving higher quality schlieren images. A representative sequence of Schlieren images of an outwardly propagating flame are shown in figure 12.

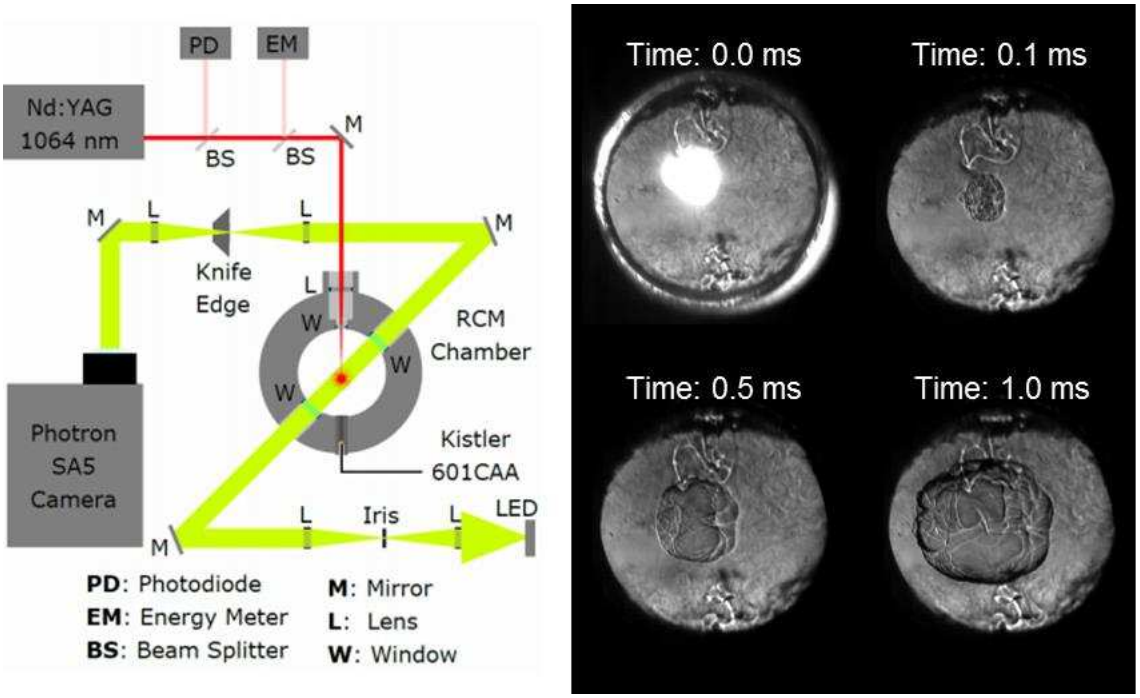

Figure 12: (Left) Schematic diagram of laser ignition and schlieren system (credit Andrew Zdanowicz [31]) and **(Right)** representative sequence of schlieren images showing outwardly propagating flame.

In order to accurately trigger the laser and schlieren. A Berkeley Nucleonics 555 pulse generator is used. The pulse generator is triggered by the signal coming from the charge amplifier of the in-cylinder pressure measurement. When triggered, the pulse generator appropriately delays the laser system and high-speed camera allowing effective synchronization of the RCM, laser ignition, and Schlieren systems.

3. EXPERIMENTAL TEST CONDITONS AND ANALYSIS METHODS

3.1 Experiment Overview

Two sets of experiments were conducted in this study. The first set of experiments utilize compression ignition, which were used to measure the homogeneous ignition delay period of NG blends of various reactivity with and without EGR gas addition. This data will also be used to characterize performance of the reduced chemical kinetic mechanism. The second set of experiments were laser ignited experiments, which enabled the measurement of flame propagation rate and end-gas autoignition fraction, $f_{EGAI.}$ Overall, three different fuel blends were tested at three different EGR substitution rates. The intermediate fuel blend was tested with two type of EGR gas, non-reactive EGR (NR-EGR) and reactive EGR (R-EGR). The following sections will describe the conditions used for the experiments followed by the methods used to analyze the data.

3.2 Gas Composition

In this study, three fuel blends with varying mole fractions of CH_4, C_2H_6 and C_3H_8 were formulated to simulate dry, intermediate, and wet reactivity pipeline quality fuel composition as shown below in Table 2. These formulations ranged in MN from 68 to 95 and were mixed in the gas blend bottle.

Table 2: Fuel blends of varying chemical reactivity used in this study.

	% Mole Fraction		
Species	**Dry**	**Intermediate**	**Wet**
CH_4	99%	95%	82%
C_2H_6	0.5%	4%	15%
C_3H_8	0.5%	1%	3%
MN	95	86	68

Each of the fuel blends were then mixed with two unique synthetic EGR mixtures. The compositions of the synthetic EGR mixtures used in this study was informed from exhaust composition measurements of a Cummins medium duty SI-NG mobile engine. In actual SI-NG engines, EGR gas composition varies with engine operating conditions and EGR substitution rate. For the experiments described herein, the EGR gas composition was kept constant for all EGR substitution rates to maintain simplicity. In addition, to maintain compatibility with the RCM, two modifications to the measured engine EGR compositions were made. Firstly, H_2O was eliminated and replaced by additional CO_2. This substitution was required to ensure good mixing and delivery of the synthetic EGR with the rest of the reactants in the liquid mixing tank and RCM combustion chamber and to eliminate the potential for condensation. The carbon dioxide substitution percentage was selected to maintain ratio of specific heats (γ) of the original measured EGR blend including H_2O. Secondly, the synthetic EGR blends contained 100% Ar as the inert species in place of N_2. In an actual engine that runs on air, all the inert species in the reactive charge is nitrogen. Therefore, the exhaust gas that leaves the engine and is used as EGR is also mostly nitrogen. In RCM experiments it is typical to vary the inert species (e.g. substituting a fraction of the N_2 with Ar, or CO_2) as a means of varying the specific heat ratio to produce a desired range of compressed pressure and temperature for a given compression ratio. To achieve the elevated

compressed conditions desired in the present study, the inert species for the 0% EGR conditions consisted of 100% Ar. Therefore, the inert species in the synthetic EGR gas was also changed to 100% Ar. This ensures that the relative change of γ for the RCM experiments as EGR is substituted is similar to the relative change of γ for an engine running on air as EGR is substituted.

To examine the effect of reactive species such as NO, CO and unburned hydrocarbons present in EGR gas, two synthetic EGR blends were tested: a reactive EGR blend (R-EGR) and a non-reactive EGR blend (NR-EGR). The compositions of each are listed below in Table 3. The R-EGR and NR-EGR were tested at substitution percentages of 0 to 30% by mass using equation 3 below.

$$\%\, EGR\ Rate = \frac{m_{EGR}}{(m_{EGR}+m_{Air}+m_{Fuel})} * 100 \quad (3)$$

Where *m* is mass and the subscripts indicate reactant type.

The R-EGR mixture was purchased from Airgas. Since the NO and CO concentrations were low in the R-EGR mixture the accuracy of a professional grade mixing system was desired. The NR-EGR mixture was mixed in the liquid mixing tank as part of the standard reactant blending.

Table 3: Gas composition of synthetic EGR mixtures, which include a reactive EGR blend and nonreactive EGR blend.

	% Mole Fraction	
Species	**Reactive EGR**	**Non-Reactive EGR**
Argon	79.3%	80.0%
Carbon Dioxide	20.0%	20.0%
Carbon Monoxide	0.35%	-
Nitrogen Monoxide	0.35%	-

3.3 Homogeneous Ignition Delay Test Conditions and Analysis

For the homogeneous ignition delay experiments, each fuel blend was tested at a fixed initial pressure (1.0 bar) and three different initial temperatures (308, 318, and 328 K) resulting in three different compressed temperatures at similar compressed pressure. Each fuel blend was tested with 0, 10, 20, and 30% R-EGR substitution rates and the intermediate fuel was also tested with 0, 10, 20, and 30% NR-EGR substitution rates. A table that outlines the compressed pressure and temperature for each experimental condition is available in Appendix B.

Homogeneous ignition delay was measured using a MATLAB script. The MATLAB script requires the initial pressure and temperature of each experiment. The initial pressure, measured using the MKS Instruments dual-capacitance monometer, is used to "peg" the pressure output from the high-speed piezoelectric pressure transducer. The construction of piezoelectric pressure transducers provides good relative pressure measurements but poor absolute pressure measurements. Therefore, pegging is necessary to obtain the correct absolute pressure measurements in the RCM combustion chamber. To peg the pressure measurements the initial 50ms of high-speed pressure data is averaged. The difference between the average and pressure measured using the dual capacitance monometer is applied to the entire pressure trace. After the pressure is pegged, it is filtered using an 8th order Butterworth filter. The derivative of the filtered pressure trace is calculated. In chamber temperature with respect to time is calculated using equation 1. In order to select data, the average temperature between the pistons reaching TDC and ignition was calculated. Experimental data were selected for analysis when the compressed temperature (averaged between TDC and ignition of each replicate) was within +/- 10 K of the weighted average compressed temperature of five replicates.

3.4 Flame Propagation Measurement

The goal of the flame propagation tests was to test at a consistent compressed pressure and temperature to allow comparisons between flame types and EGR substitution rates. Fortunately, the ratio of specific heats for the EGR mixtures is very similar to the ratio of specific heats of the air/fuel mixture. This simplified testing by allowing all the testing to be completed at the same initial conditions but still maintain a similar compressed pressure and temperature across fuel type and EGR substitution rate. Initial conditions were maintained at 1.0 bar initial pressure and 298 K initial temperature. Each fuel blend was tested with 0, 10, 20, and 30% R-EGR substitution rates and the intermediate fuel was also tested with 0, 10, 20, and 30% NR-EGR substitution rates. A table outlining the test conditions for each experimental condition is available in Appendix C.

Unfortunately, due to the non-creviced pistons, it was found that the flame speed was highly sensitive to a phenomenon known as piston offset. Since the CSU RCM is a dual piston RCM and the pistons are not mechanically linked, one piston can reach TDC before the other piston reached TDC. The delta in time between each piston reaching TDC is termed as piston offset. In order to maintain repeatable conditions strict data selection criteria were used. Each test condition was replicated a total of ten times. Only the experiments where the piston offset was less than 4ms were used to measure flame propagations rate.

The methods used for flame propagation rate calculation were developed by Andrew Zdanowicz [31]. The schlieren images were collected in sequence and the projected flame area for each image was measured to calculate an equivalent spherical flame radius as a function of time. A second-order polynomial was fit to the equivalent flame radius versus time data. Flame stretch effects were eliminated through the non-linear extrapolation of Kelley and Law [35,36] to yield the zero-stretch flame speed with respect to the burned gases according to equation 4:

$$s_b^0 t + c = r_f + 2L_b \, ln(r_f) - 4\frac{{L_b}^2}{r_f} - \frac{8}{3}\frac{{L_b}^3}{{r_f}^2} \quad (4)$$

where s_b^0 the zero-stretch burned propagation rate in cm/s, t the time in s, c a measurement constant, rf the equivalent spherical flame radius in cm, and Lb the Markstein length in cm.

The extrapolated zero-stretch burned propagation rate was then converted to an unburned propagation rate by using equation 5:

$$s_u = s_b \left(\frac{\rho_b}{\rho_u}\right) \quad (5)$$

where s is the flame propagation rate in cm/s, ρ is the density in kg/m3, and the u and b subscripts represent the unburned and burned regions across the flame, respectively [36].

Unburned density was calculated using the initial pressure and known compression ratio. Burned density was approximated using the ideal gas law, along with the burned temperatures and molecular weight of the combustion products as predicted by chemical equilibrium calculations.

3.5 End-Gas Autoignition Fraction

For the EGAI experiments, initial conditions were maintained at 1.0 bar initial pressure and 298 K initial temperature. Each fuel blend was tested with 0, 10, 20, and 30% R-EGR substitution rates and the intermediate fuel was also tested with 0, 10, 20, and 30% NR-EGR substitution rates. A table is available in Appendix C that outlines the test conditions for all the experimental conditions. Each test case was replicated ten times. The process used to analyze f_{EGAI} was developed by Andrew Zdanowicz [31]. Since EGAI is strongly governed by the temperature history in the end-gas upstream of the propagating flame, the f_{EGAI} data were categorized by time-integrated temperature in the combustion chamber prior to spark ignition. Specifically, the time-integrated temperature (Θ) was evaluated by integrating, with respect to time, the calculated bulk mean temperature of the gases in the combustion chamber during the 10 ms interval prior to spark ignition:

$$\Theta = \int_{-10\ ms}^{0} T_m dt \tag{6}$$

Where T_m is the calculated bulk-mean temperature in K and t the time in s. Each of the data points presented below consist of ten replicates with time-integrated temperature of $8.2 < \Theta < 8.9$ K-s.

End-gas autoignition fraction, f_{EGAI}, is defined as the fraction of the total heat release that is attributed to EGAI with respect to the net total amount of heat release during the entire combustion event. This parameter is calculated from the apparent heat release rate (AHHR), which is derived from the high-speed pressure data. Since combustion does not occur until after TDC, during which the volume in the combustion chamber remains constant, the AHRR is calculated as follows:

$$AHRR = \frac{dQ}{dt} = \frac{1}{\gamma - 1} V \frac{dP}{dt} \tag{7}$$

Where V is the gas volume after compression in m^3, γ the ratio of specific heats of the mixture, P the pressure in Pa and t the time in s.

Note that dQ/dt represents the net rate of external heat addition to the gases in the combustion chamber that would result in the measured pressure rise dP/dt due to conversion of chemical energy to thermal energy in a homogeneous chemically reacting system.

The EGAI fraction, f_{EGAI}, is calculated by integrating the AHRR profile as follows:

$$f_{EGAI} = \left[\int \frac{dQ}{dt}\, dt\right]_{EGAI} / \left[\int \frac{dQ}{dt}\, dt\right]_{total} \tag{8}$$

where $\frac{dQ}{dt}$ is the apparent heat release rate in W. The numerator represents the integrated apparent heat release during EGAI in J, and the denominator represents the integrated total apparent heat release in J.

A more detailed description of the flame propagation rate and EGAI fraction calculations can be found in Andrew Zdanowicz's thesis [31].

4.1 Homogeneous Ignition Delay

Homogenous ignition delay results for stoichiometric wet, dry and intermediate NG with 0 to 30% R-EGR addition at compressed pressures and temperatures of 30.2 to 34.0 bar and 667 to 980 K are plotted in figure 13.

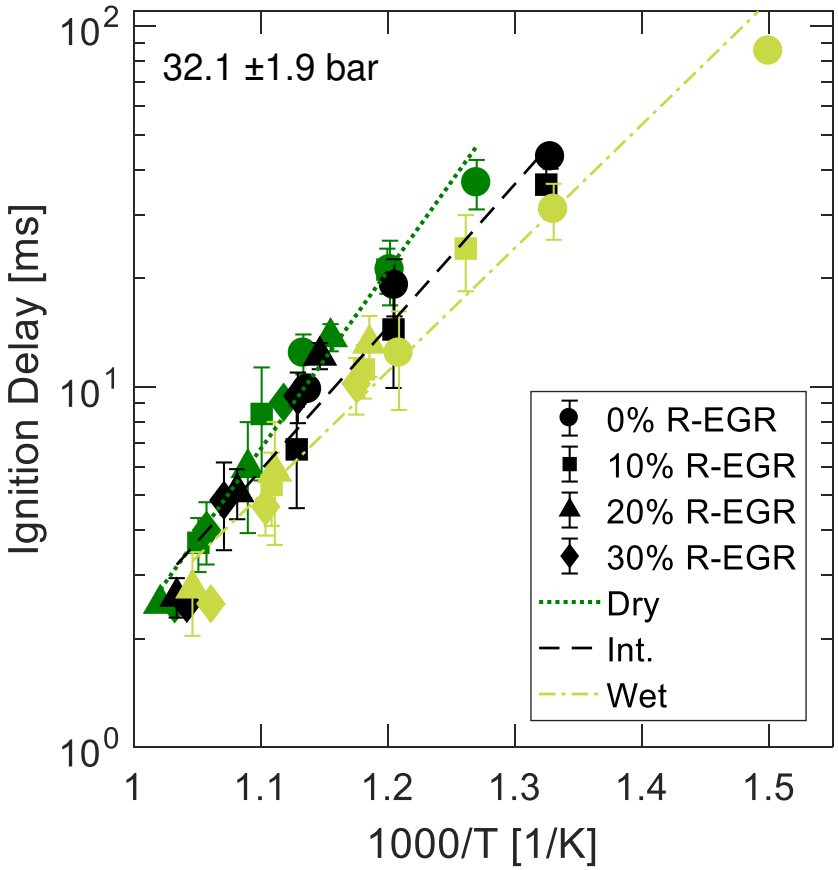

Figure 13: Homogeneous ignition delay plot of all three fuel blends with 0-30% R-EGR substitution. Marker shape indicates percentage of R-EGR and color indicates fuel blend. The linear regressions are fit to each fuel blend and include all the R-EGR percentages for each. Note error bars are statistical 95% confidence intervals.

The ignition delay period for each fuel type with and without R-EGR substitution follows a linear trend on an Arrhenius plot with minimal negative temperature coefficient (NTC) behavior.

The trends shown on this plot are expected the fuel blends that have larger and more reactive hydrocarbons are, in fact, more reactive and have shorter ignition delays as a result. As temperature increases (moving right to left on an Arrhenius plot) the ignition delay decreases in the previously mentioned linear trend. The ignition delay period did not vary substantially between the wet, intermediate and dry fuel blends, suggesting that the ignition kinetics are dominated by the low reactivity CH_4 kinetics for even the wet NG blend that contains 82% CH_4. The chemistry of CH_4, C_2H_6, and C_3H_8 blends are well studied. However, the interaction of the NG blends with the R-EGR mixture is a main goal of this project. In order to learn more about the interaction of the NG blends with R-EGR, figure 13 was remade with the fuels separated and linear regression line of best fits were calculated for the experiments with 0% R-EGR then for the experiments with 10-30% R-EGR substitution (figure 14).

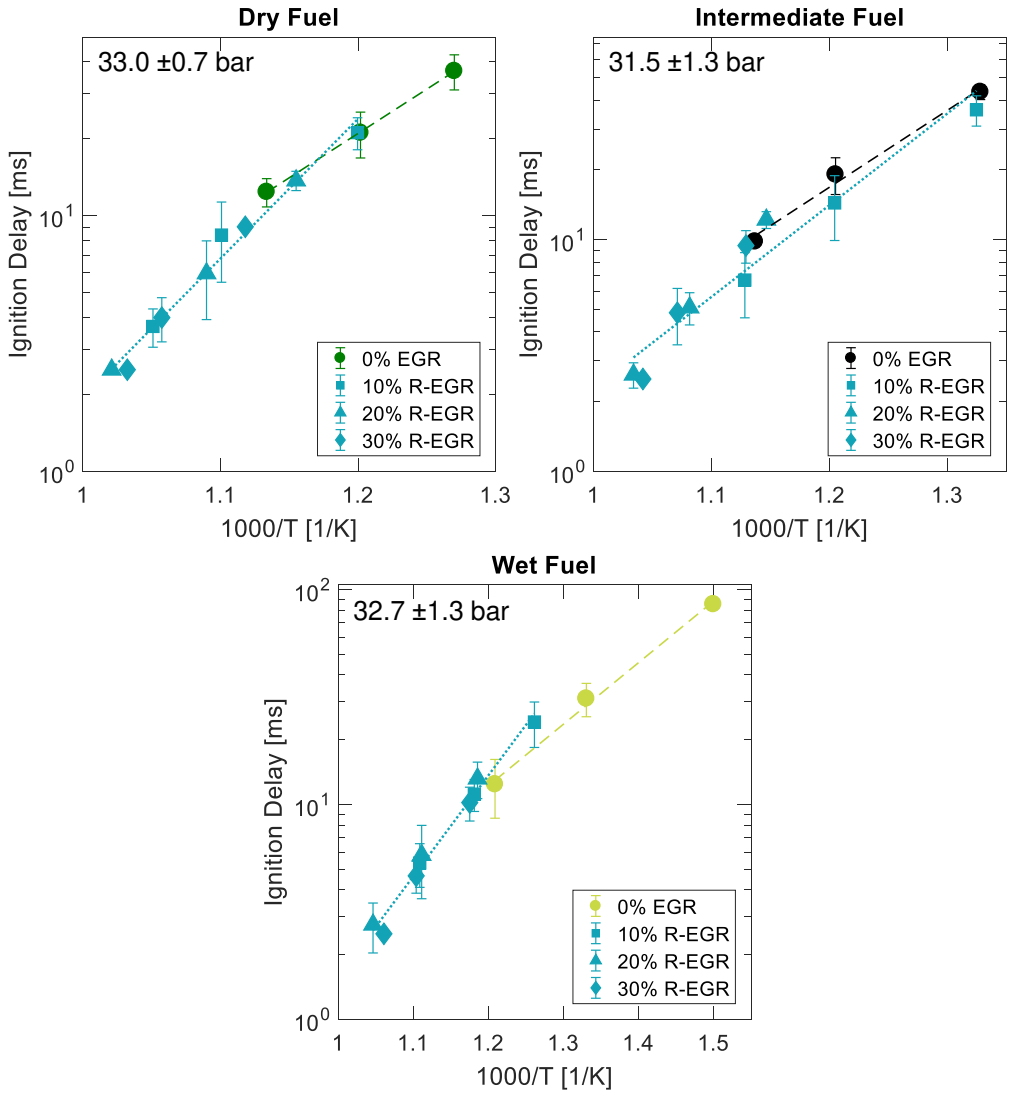

Figure 14: Homogeneous ignition delay of dry, intermediate, and wet fuel blends with 10-30% R-EGR substitution by mass. Marker shape indicates R-EGR substitution percentage. In order to highlight the difference between 0% EGR and R-EGR substitution the experiments with 10-30% R-EGR substitution are colored blue. Note error bars are statistical 95% confidence intervals.

The results shown in figure 14 are insufficient for characterization of the effect of R-EGR substitution. The individual points where the 0% EGR experiments and 10-30% EGR experiments are at the same temperature the ignition delays do not vary significantly. For example, the points above 1000/T of 1.2 on the dry fuel plot are essentially the same point. On both the dry and intermediate fuel experiments the experiments with 10-20% R-EGR are on or close to the linear

fit line of the 0% R-EGR experiments. These results suggest that the addition of R-EGR to the NG did not substantially affect the ignition delay period for a given compressed temperature. Since all experiments were conducted at a fixed initial pressure (1 bar), as EGR gas is added to the mixture the concentration of fuel and oxidizer decreases, which should result in a slight increase in ignition delay for a given temperature. However, this effect is counterbalanced by a slight increase in reactivity from the additional reactive species in the R-EGR. The net result is that the ignition delays are not statistically different at a given single compressed temperature. However, the difference of slope in the linear fit lines that include the results across the full temperature range suggest that there is a difference in the 0% EGR and the experiments with R-EGR substitution. Many R-EGR substitution experiments are at a higher temperature than the 0% EGR experiments. These experiments were run at a constant initial pressure and the same three initial temperatures (308, 318, 328K). Thermodynamically the ratio of specific heats minimally increases with EGR substitution which contributes to the increase compressed temperature. At these higher temperatures the slope of the experiments with R-EGR substitution are larger than the slopes of the 0% EGR experiments. This is most largely visible in the dry and wet fuel results in figure 14. Which indicates that the R-EGR potentially cause a significant change in reactivity of the total mixture. However, it is unclear if the reduced ignition delays are due to the increased temperatures or increased reactivity due to the R-EGR. In a more ideal experiment, the results would look similar to the intermediate fuel results where there is significant overlap in the compressed temperatures between the 0%EGR and R-EGR experiments. In the intermediate fuel blend the slope of the 0% EGR experiments (black-dashed line) and the R-EGR experiments (blue-dotted line) are much closer indicating only a minor increase in reactivity due to R-EGR substitution. With the information that is available above it is difficult to form an effective conclusion whether

R-EGR changes the reactivity of the total mixture because the different fuels types show different conclusions and it is unclear if the observed effects are due to temperature differences or reactivity differences. Therefore, experiments of the intermediate fuel blend with NR-EGR substitution were run to see if homogeneous autoignition delay changes without the reactive NO and CO species (figure 15).

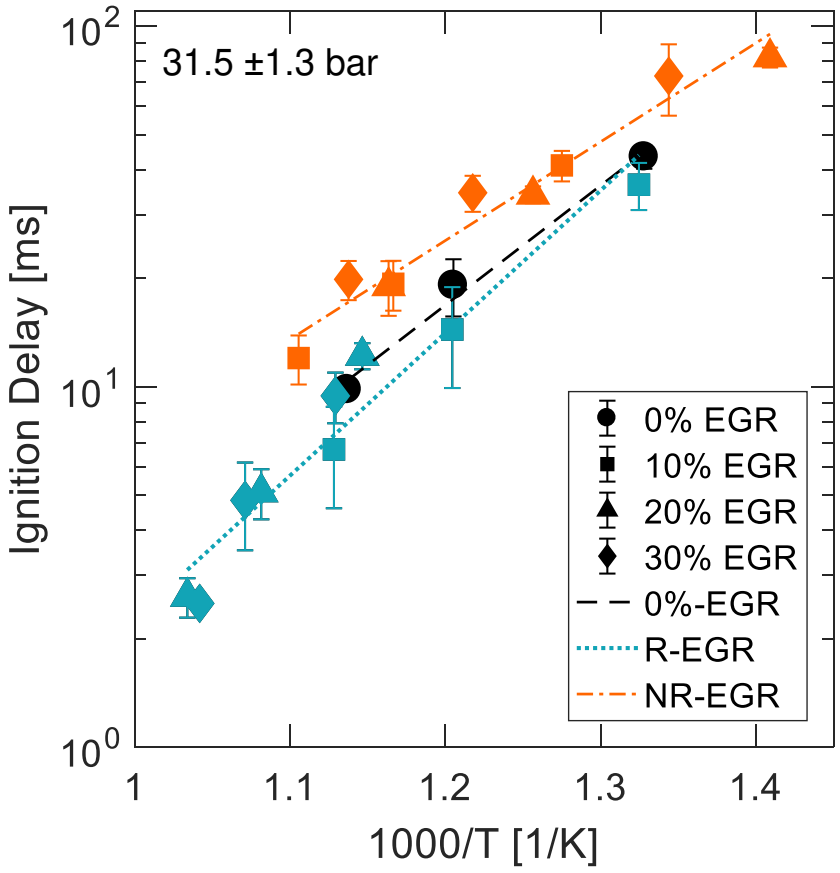

Figure 15: Intermediate fuel blend with both NR-EGR and R-EGR substitution. Marker shape indicates the percentage of EGR substitution. Color indicates NR-EGR (Orange) and R-EGR (Blue). Note error bars are statistical 95% confidence intervals.

The results shown in figure 15 allow the formation of a much stronger conclusion. Figure 15 is a plot of ignition delay period of the intermediate reactivity fuel blend, with R-EGR and NR-EGR substitution. As shown in the figure, a statistically significant increase in ignition delay was, indeed, observed between the cases with R-EGR and NR-EGR substitution. The majority of 95%

confidence intervals do not overlap between any of the NR-EGR and R-EGR ignition delays. These results suggest that the reactive species present in the EGR gas do in fact, affect the homogeneous ignition delay. Therefore, NO and CO concentration in EGR is important to the total reactivity of the mixture. Although a small change (~ 2-4 ms) in homogeneous ignition delay may not seem large, a pronounced change is seen in EGAI propensity of the entire mixture. As discussed in the next section, the effect of the reactive species has a more pronounced effect on EGAI propensity because of the combined effects of reduced flame speed and increased chemical kinetic induction period in the end gas.

4.2 Flame Propagation Rate and EGAI Results

Although homogeneous ignition delay was found to be insensitive to EGR substitution, the flame propagation rate and f_{EGAI} were both found to vary dramatically with EGR substitution. figure 16 shows the flame propagation rate and f_{EGAI} for stoichiometric dry, intermediate and wet NG blends with 0 to 30% R-EGR substitution rates. As shown in figure. 16 (left), the measured flame propagation rates decreased with increasing R-EGR substitution rate. This result is expected given the decrease in adiabatic flame temperature with increasing EGR rate. The flame propagation rates did not statistically significantly vary with fuel reactivity and were substantially higher than the expected 1-D premixed laminar flame speed. The presence of turbulence in the system caused by roll-up vortices (from the non-creviced pistons) and slight asymmetry in the piston timing effectively increased flame propagation rates. Although the turbulence intensity was not quantified, the presence of fluid motion upstream of the expanding flames is apparent in figure 12 (right). The stochastic nature of the turbulence results in large variation in measured flame propagation rate for a fixed set of initial conditions as evidenced by the wide error bars in figure.

16 (left). However, even with the large variation, the decrease in flame propagation rate with R-EGR substitution is clear.

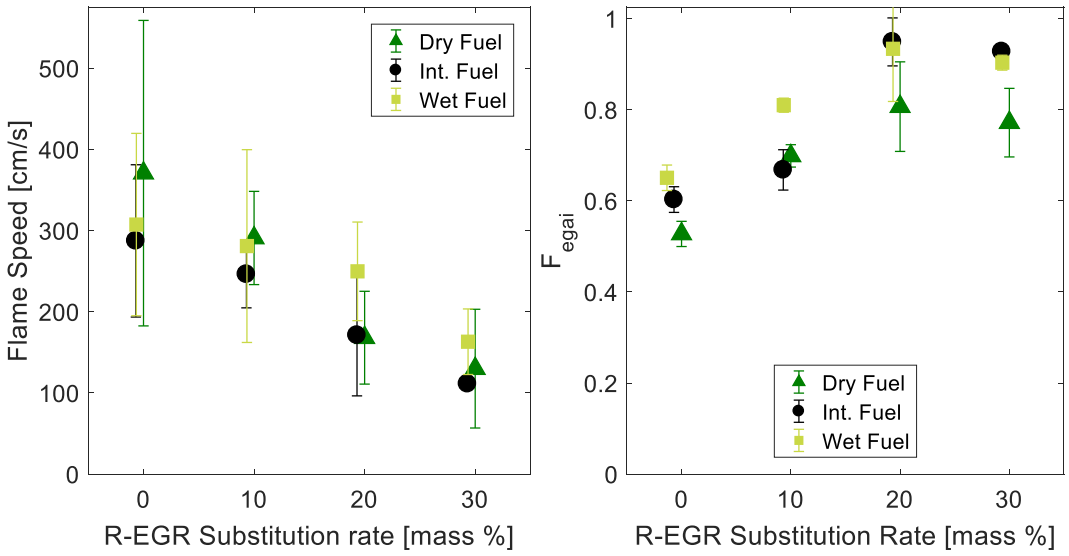

Figure 16: (Left) Flame propagation rate for stoichiometric dry, intermediate and wet NG blends with R-EGR substitution at spark pressure and temperature of 31.7 ± 1.0 bar and 751 to 795 K and **(Right)** end-gas autoignition fraction for stoichiometric dry, intermediate and wet NG blends with R-EGR substitution at spark pressure of 31.7 ± 1.0 bar and time-integrated temperature of 8.55 ± 0.35 Ks. Error bars are statistical 95% confidence intervals and markers have been jittered for visual clarity.

As shown in figure 16 (Right), f_{EGAI} was found to increase with increasing fuel reactivity and increasing R-EGR addition. The increase in f_{EGAI} with increasing fuel reactivity has been observed previously for primary reference fuels and, in fact, the f_{EGAI} parameter has been proposed as a metric to quantify fuel reactivity and knock propensity for SI engines [31]. The increase in f_{EGAI} with increasing R-EGR addition is a consequence of the decreased flame propagation rate combined with the presence of the reactive species in the end-gas. Since the ratio of specific heats does not vary substantially with EGR addition, the end-gas temperature upstream of the propagating flame is relatively insensitive to EGR addition. Therefore, even if the end-gas chemical kinetic induction period were insensitive to EGR addition (as implied in figure 14), the

decrease in flame speed with increasing EGR addition would result in increased f_{EGAI} due to the increased mass of end-gas that autoignites as flame speed decreases. The results of figure 17 show that the effect of EGR addition on f_{EGAI} is greatly enhanced due to the reactive species in the end-gas. Figure 17 contains plots of flame propagation rate and f_{EGAI} for the intermediate NG blend with 0 to 30% R-EGR and NR-EGR. While the flame propagation rate is not affected by the removal of the reactive species from the synthetic EGR blend, the f_{EGAI} for the R-EGR blends differs dramatically from that observed in the NR-EGR blends. This result strongly suggests that reactive species decrease the chemical kinetic induction period (ignition delay) resulting in earlier autoignition of the end-gas than would occur from the decreased flame speed alone.

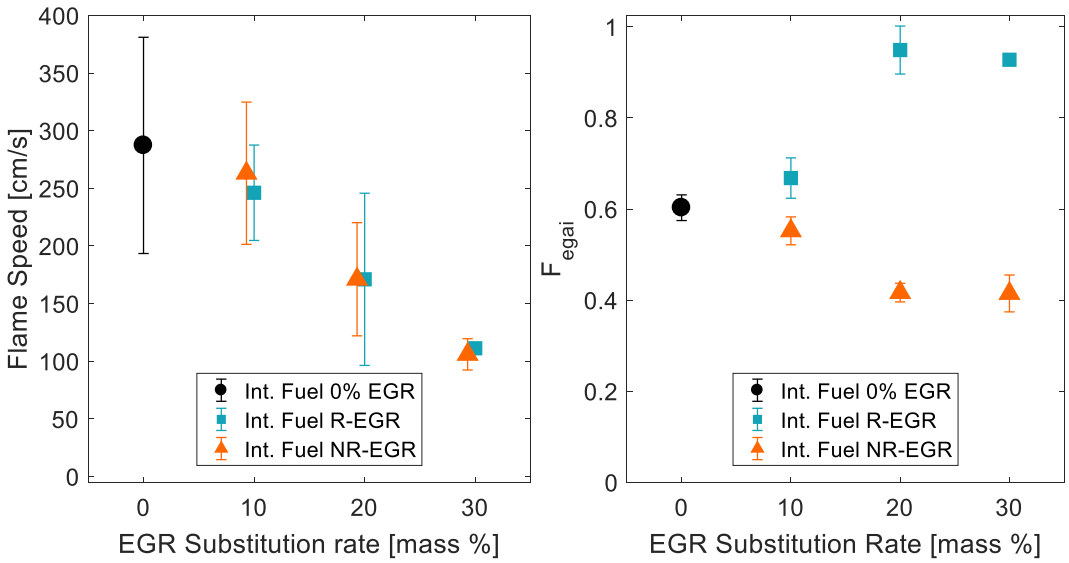

Figure 17: (Left) Flame propagation rate and **(Right)** end-gas autoignition fraction for stoichiometric intermediate NG blend with 0 to 30% R-EGR and NR-EGR at spark pressure of 3.17 ± 0.1 MPa and time-integrated temperature of 8.55 ± 0.35 Ks. Error bars are statistical 95% confidence intervals and markers have been jittered for visual clarity.

To further investigate the effect of the reactive species NO and CO on the chemical kinetic induction period in the end-gas with increasing EGR substitution rate, 0-dimensional (0-D), constant volume, homogenous ignition delay period was computed for stoichiometric intermediate

NG blend with 0 to 30% R-EGR and NR-EGR at initial temperature and pressure of 1000 K and 31.7 bar were run in Chemkin Pro 17.2. A mechanism developed at Lawrence Livermore National Laboratory by Marinov, et al., which consists of 126 species and 637 reactions and includes detailed NO_x chemistry, was used for these simulations [37]. Figure 18 shows that R-EGR addition decreases the ignition delay period of the mixture, whereas the NR-EGR addition results in a substantial increase in ignition delay period.

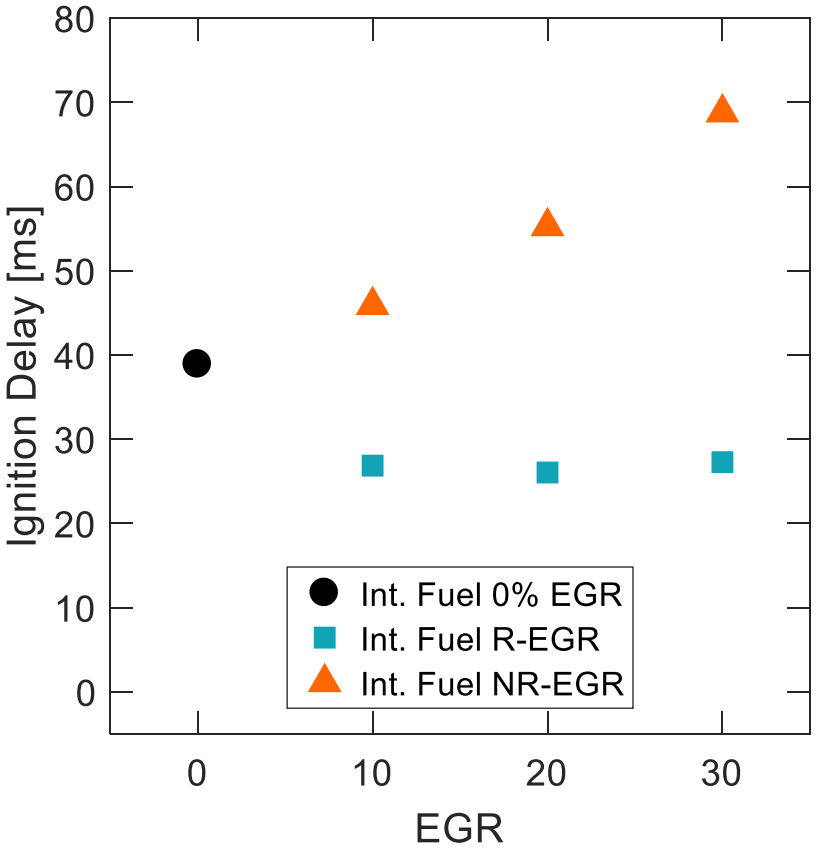

Figure 18: Computed 0-dimensional, constant volume, homogenous ignition delay period for stoichiometric intermediate NG blend with 0 to 30% R-EGR and NR-EGR at initial temperature and pressure of 1000K and 31.7 bar, respectively.

Figure 18 shows that the substitution of R-EGR decreases the ignition delay of the mixture as consistent with the f_{EGAI} results seen in figure 17. The NR-EGR substitution increases the ignition delay of the mixture which is also consistent with the f_{EGAI} results and theory. Further investigation

was also done to understand if NO or CO had a larger impact on homogeneous ignition delay and therefore f_{EGAI}. For these simulations the same conditions as seen in figure 18 were used but four distinct EGR mixtures were simulated.

Table 4: Composition of four EGR mixtures to test individual impact of NO and CO.

	% Mole Fraction			
Species	**R-EGR**	**NR-EGR**	**CO-EGR**	**NO-EGR**
Argon	79.3%	80.0%	79.48%	79.48%
Carbon Dioxide	20.0%	20.0%	20.17%	20.17%
Carbon Monoxide	0.35%	-	0.35%	-
Nitrogen Monoxide	0.35%	-	-	0.35%

Each of these four EGR mixtures were blended with the middle air/fuel blend to stoichiometric mixtures and tested at the same condition as figure 18. The results are shown below in figure 19.

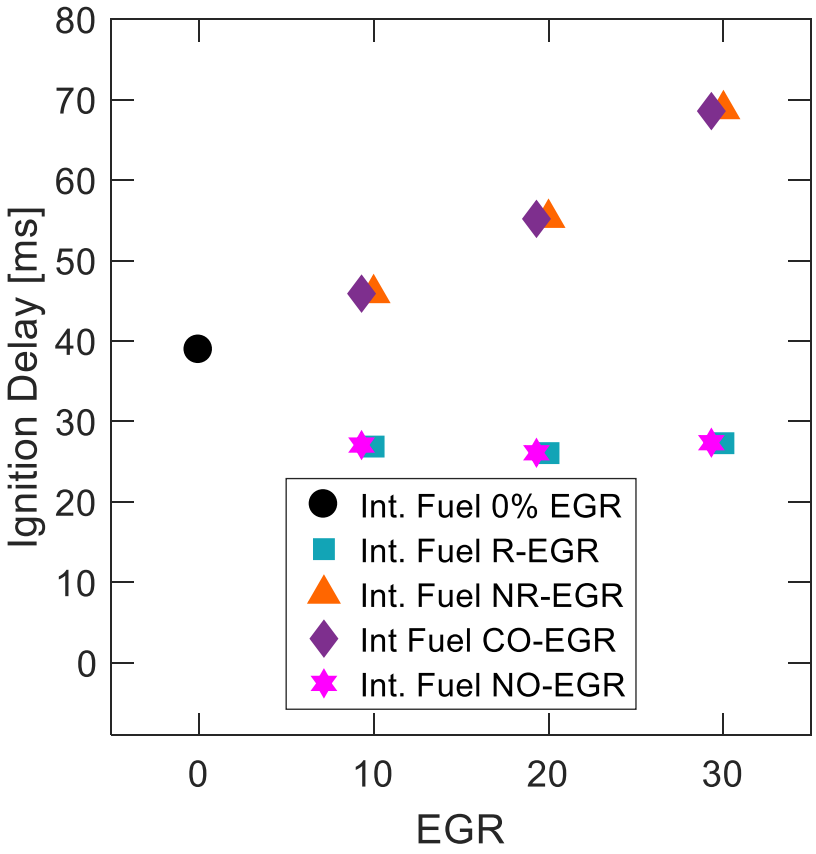

Figure 19: Computed 0-dimensional, constant volume, homogeneous ignition delay period for stoichiometric intermediate natural gas blend with 0 to 30% R-EGR (Blue square symbols), NR-EGR (Orange triangle symbols), EGR containing only CO as the reactive species (Violet diamond symbols) and EGR containing only NO as the reactive species (Magenta star symbols) at initial temperature and pressure of 1000K and 31.7 bar, respectively. Note markers are jittered for visual clarity.

From figure 19, the simulations indicate that NO has the largest and only impact on reactivity. The CO-EGR has similar ignition delay to the NR-EGR blend. Therefore, according to these simulations, the NO species is the most important consideration for knock mitigation in SI-NG engines according to these simulations. However, there are a lot of other factors to consider. A study of NO and primary reference fuel ignition in a motored engine showed that low NO substitution less than 100 ppm increased reactivity and at high substitution 100-300 ppm reduced

reactivity [28]. This study indicates that quantity of NO in EGR could have a non-linear effect of knock mitigation. Future work researching how different levels of NO in the reactant mixture using the CSU RCM could provide insight on what an acceptable range of NO in EGR could be that would still mitigate knock. Therefore, the composition of the EGR may be just as important as the quantity of EGR used for knock suppression and engine control.

The importance of the above results is the indication that engine knock is essentially a competition between the consumption of the reactants by flame propagation against the volumetric autoignition (homogeneous ignition delay) of the end-gas. There are many ways to change combustion characteristics to favor flame propagation over EGAI. For example, maintaining total charge mixture reactivity but increasing flame speed using increased turbulence would reduce f_{EGAI} and the likelihood of knock in the engine. The mechanism by which EGR reduces knock is by decreasing the reactivity of the total charge mixture allowing more time for the flame to consume the mixture before EGAI occurs. However, as seen in this study EGR substitution also decreases adiabatic flame temperature which also decreases flame speed. Therefore, it is important that the composition of the EGR be inert and contain as few reactive species as possible. Similar effects have also been observed in engines in references [28,29]. Although both tests are in engines and the exact chemical kinetics cannot be well separated both studies demonstrated the effect of EGR is non-linear in the mitigation of engine knock. The results of the CSU RCM studies are not extensive enough to confirm these theories, but the experiments could be expanded in the future to better understand the non-linear effects of NO in EGR in the RCM. Lastly, this study was not able to include H_2O in the study. Depending on if the EGR is wet or dry the water content in EGR could be as high as 20% by mole fraction. Although the CSU RCM is not currently configured to

be able to utilize water vapor, modifications could be made to allow some water vapor substitution which could also have significant impacts on EGR's ability to mitigate knock in engines.

5. CHEMICAL KINETIC MECHANISM DEVELOPMENT

5.1 Chemical Kinetic Overview

Chemical kinetic mechanisms are used to model combustion events. On a basic level combustion is a series of exothermic chemical reactions. During a combustion event, hundreds of thousands of these reactions are happening simultaneously. Each one of these reactions can be modeled as an Arrhenius equation. Each one of these equations can then be simultaneously solved and this list of equations is known as a chemical kinetic model. In the most basic modeling, 0-dimensional (0-D), the point values of specific parameters can be calculated with time. For example, homogeneous autoignition delay can be modeled as a 0-D simulation. In a homogeneous autoignition simulation a single point is maintained at a temperature and pressure. The reactions start to be calculated and after a certain amount of time a cascade reaction occurs and the temperature of that point increases (combustion). The homogeneous autoignition delay is defined as the time from the start of the simulation until the point temperature increases a certain amount (400 K in the case of Chemkin Pro 17.2). Therefore, to increase accuracy, the highest number of species and reactions possible is desirable. It is not uncommon for chemical kinetic mechanisms intended for 0-D simulation to contain 300-1500 species. However, in order to develop and model engines and combination of 0-D and 3-D simulation is used. In the case of 3-D simulation, a grid matrix is made to mimic the combustion chamber of the engine (piston, cylinder wall, cylinder head, and intake and exhaust valves). This grid can contain in excess of a million of cells and the series of equations for the chemical kinetic mechanism must be calculated for each grid cell. If the chemical kinetic mechanism consists of 500 or more species the computing power required to complete a 3-D simulation is substantial and single engines cycles could take weeks to run. In order to reduce the required computing power, smaller chemical kinetic mechanisms are desirable.

Therefore, this project also developed a reduced chemical kinetic mechanism (~80 species) that accurately models NG blend combustion at pressures and temperatures in the range of 1-100 bar and 500-1000 K respectively. The methods used to develop the reduced mechanisms are discussed in the following sections.

5.2 Selection of the Parent Mechanism

Development of detailed chemical kinetic mechanisms is time intensive and requires significant trial and error. By starting with a pre-developed detailed mechanism, a reduced mechanism can be extracted that contains the desired number of species and accuracy for a specific project. A total of seven "parent" mechanisms were characterized for their performance and accuracy. A table containing a description and source for each of the parent mechanisms is below.

Table 5: Detailed mechanisms selected for evaluation as parent mechanism.

Detailed Mechanism	Origin	Species	Reactions
Aramco 3.0	National University Ireland Galway [38]	581	3,034
Aramco 2.0	National University Ireland Galway [39]	493	2,714
NUIG NGM II	National University Ireland Galway [40]	229	1,359
Ranzi V1412	Polytechnic University of Milan [41]	115	2,141
GRI Mech 3.0	University California Berkeley [42]	53	325
San Diego	University California San Diego [43]	57	268
USC Mech Version II	University Southern California [44]	111	784

Each of the mechanisms were evaluated for homogenous autoignition data that was found in published data [45–47] using 0-D simulation in Chemkin Pro 17.2. The published data consists of various methane, ethane, and propane blends. The goal of these comparisons was to focus on

methane accuracy but also to check if the chemical kinetic mechanisms has provisions for ethane and propane content. The results of these simulations are shown below in figures 20-22.

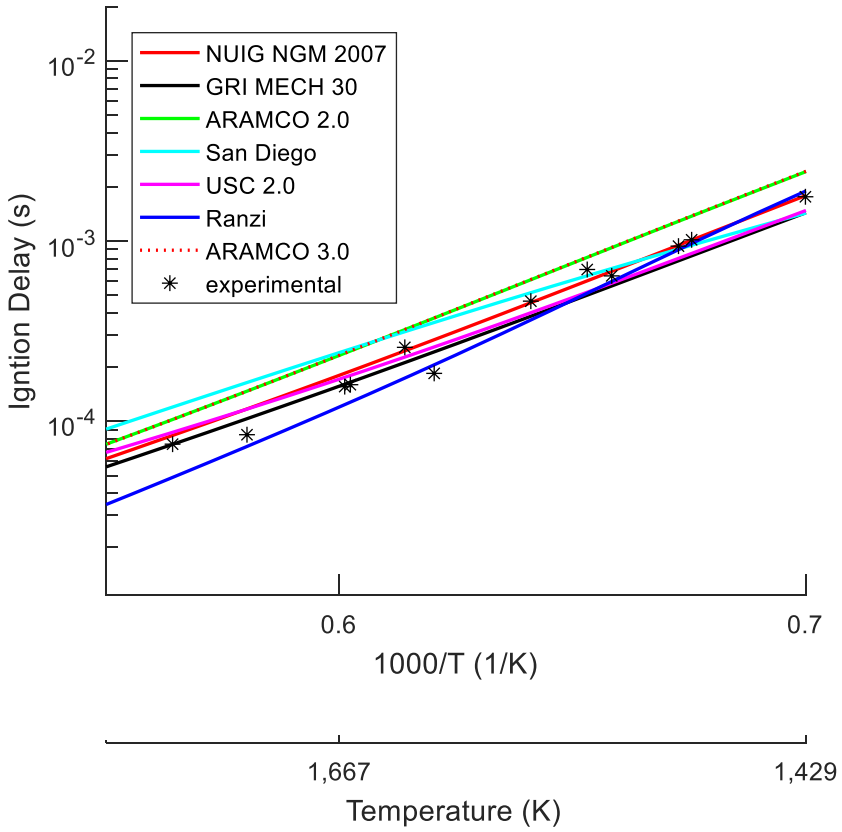

Figure 20: Homogeneous ignition delay prediction of mechanisms (Lines) compared to experimental data (Stars). The Experiments and simulations are stoichiometric CH4/AR/O2 mixtures at 1.95 bar [45].

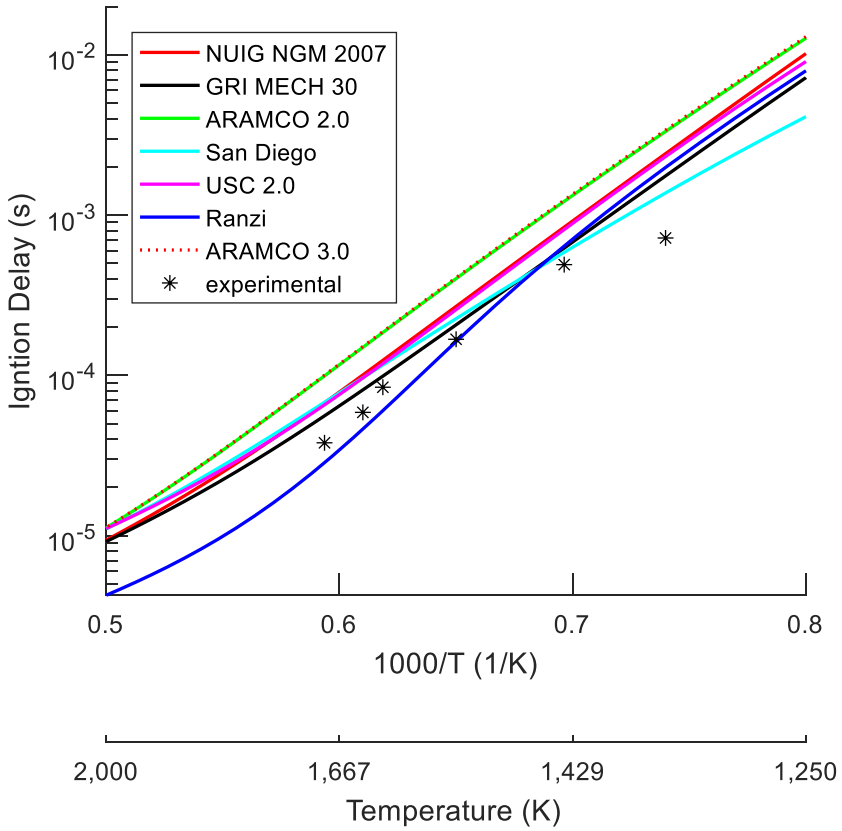

Figure 21: Homogeneous ignition delay prediction of mechanisms (Lines) compared to experimental data (Stars). The Experiments and simulations are stoichiometric CH4/C3H8/AR/O2 mixtures at 7.18 bar [47]

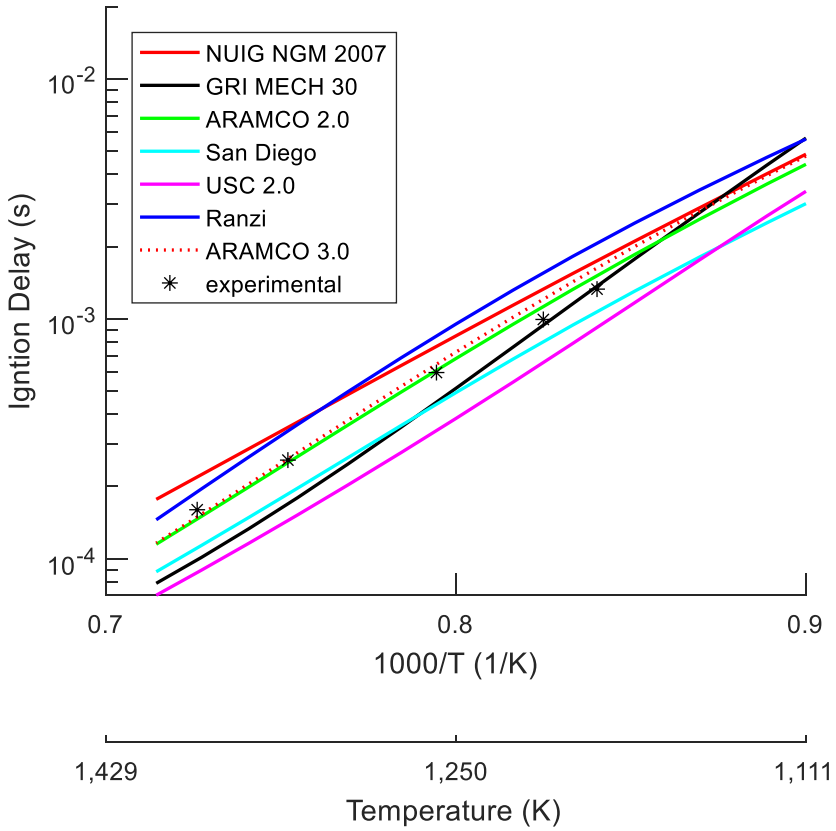

Figure 22: Homogeneous ignition delay prediction of mechanisms (Lines) compared to experimental data (Stars). The Experiments and simulations are stoichiometric CH4/C2H6/AR/O2 mixtures at 30.4 bar [46].

For the homogeneous results, a different mechanism has the most accurate prediction for each experimental data case. The performance in figure 22 was decided to be the most important for the ignition delay cases. Due to its high pressure (30.4 bar) the performance of the mechanisms at the high pressure was desired. Therefore, Aramco 2.0 and 3.0 were the highest performing mechanisms at elevated temperature and pressure ranges that are expected in the CSU RCM. However, since knock prediction is essentially the race between flame speed and homogeneous ignition delay. Flame speed was also an important consideration for parent mechanism selection. Therefore, the accuracy of the flame speed was also desired.

Laminar flame speed simulations were also run in Chemkin Pro 17.2 using the 1-D solver. Laminar flame speed prediction was compared with experimental data when available. However, above 20 bar laminar flame speed is difficult to measure. Therefore, at the higher pressures the numerical robustness of the chemical kinetic models was tested. A mechanism that could converge at high pressure is very important for this project because engine relevant pressures are in the 30 – 100 bar range and a mechanism that can numerically converge at these elevated pressures in desirable.

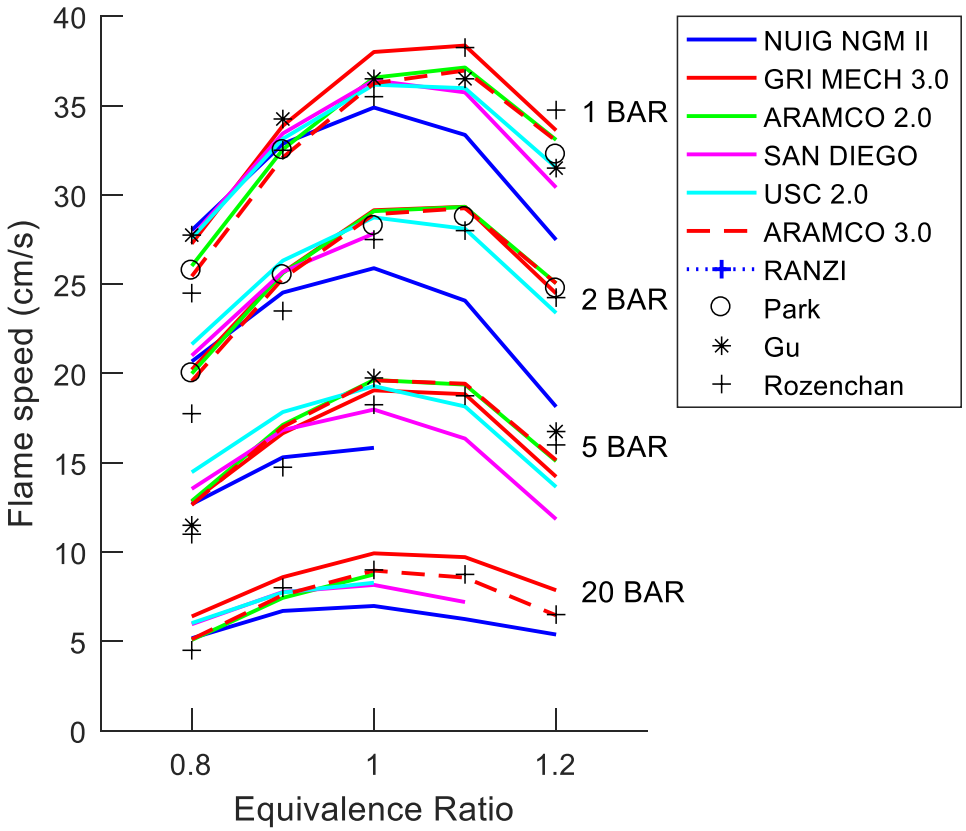

Figure 23: Laminar flame speed prediction of mechanisms (Lines) compared to experimental data (Markers). The simulation and experiments were run for 300 K initial temperatures for CH4/air at equivalence ratios of 0.8-1.2 and pressures from 1-20 bar [48–50].

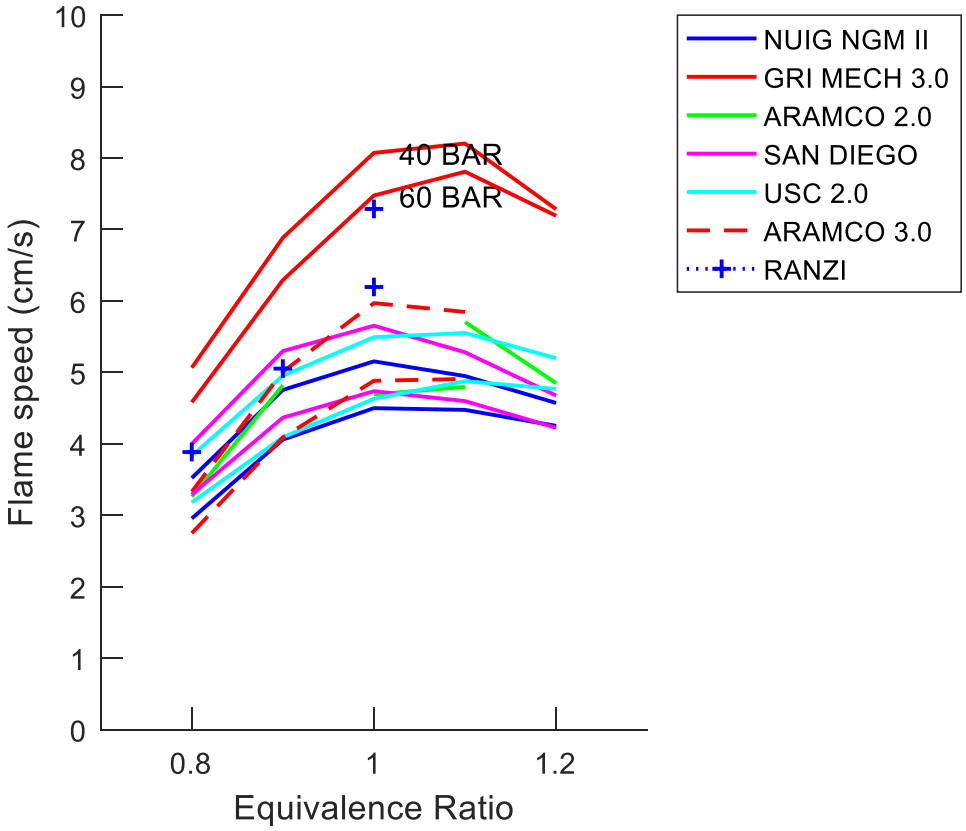

Figure 24: Laminar flame speed prediction of mechanisms. The simulation and experiments were run for stoichiometric CH4/air from 40-60 bar. Note as pressure increases flame speed decreases therefore for all mechanisms the top line is 40 bar and the bottom line is 60 bar. Due to the high pressures experimental data is not reliable at these pressures the main concern is not the value that the mechanism predicts but how reliably the numerical solver can solve the mechanism.

For the flame speed data Aramco 3.0 most closely matches the experimental data at 20 bar. At 40-60 bar Aramco 3.0 numerically solves for the stoichiometric conditions and is acceptable for this project. Therefore, Aramco 3.0 [38] was selected for it numerically robust convergence and good accuracy with the homogeneous autoignition and laminar flame speed published values.

Unfortunately, Aramco 3.0 does not have NO_x chemistry and is therefore missing the NO_x species. Due to time constraints a NO_x was not added to the reduced mechanism. Single cylinder engine testing in future work will determine if NO_x is necessary for accurate knock prediction. Although there is a large effect seen in the RCM experiments with NO the concentration of 3500

pm NO in the exhaust gas would only be seen at normal operating conditions with 0% EGR substitution. In a real engine as EGR is substituted the maximum in-cylinder pressure and temperatures decrease resulting in a sharp decrease in NO concentration in the EGR. Furthermore, there are many other sub-models such as turbulence and heat transfer models that also influence knock in actual engine simulations. Therefore, it is possible that accurate engine modeling could be achieved without NO_x in the mechanism, but single cylinder testing will need to be completed to confirm or reject the importance of NO_x modeling in an actual engine. Aramco 3.0 was selected as the detailed chemical kinetic mechanism and mechanism reduction was completed as discussed in the next section.

5.3 Mechanism reduction

To reduce the mechanism to the desired size (50-90 species) Chemkin Pro 17.2 and Reaction Workbench were used. Reaction workbench reduces mechanisms using Directed Relation Graph with Error Propagation (DRGEP) method. This method tracks the relations between species and weights each species by the number of relations it has to the other species. If a species has the least reactions to other species that species has a low weight and it removed from the mechanism. The resulting mechanism is then tested, and error is measured. If the resulting mechanism has a large error the removed species are re-integrated to minimize total error. Reaction workbench compares the performance of the reduced mechanism and maintains the user specified error for the user specified test runs of the detailed parent mechanism. The table below outlines the resulting mechanisms and the temperature, pressure, and fuel range they were reduced with.

Table 6: Pressure and temperature ranges used to reduce Aramco 3.0. The resulting size of the reduced mechanism is also shown.

Reduction Name	Fuel Type	Pressure [bar]	Temperature [K]	Number of Species	Number of Reactions
ARIES 51	Wet	30-100	700-1000	51	320
ARIES 67	Wet	20-100	500-1000	67	443
ARIES 82	Wet	1-100	500-1000	82	519
IG Blend	Methane, Ethane, Propane*	1-100	500-1000	91	565

*three reduced mechanisms were made for each pure fuel species then re-blended into IG Blend mechanism

5.4 RCM Experiment Modeling

After the reduced mechanisms were made in Reaction Workbench a comparison to the experimental homogeneous autoignition delays measured in the CSU RCM was made. In order to model the RCM in Chemkin Pro a 0-D variable volume model was used. Since the RCM pressure and temperature varies with time matching the pressure and temperature measurements for each experiment is important for accurate modeling. This is accomplished by a user defied volume/time history that matches the temperature and pressure of each experiment. Since the RCM is not an isentropic system the heat loss and mass loss must be accounted for by using the actual measured pressure trace from the experiments.

A MATLAB code is used to calculate the volume/time user defined function for the simulations. Since each set of experiments consisted of three initial temperatures for each fuel/EGR blend. The middle temperature (318 K) tests at each fuel/EGR blend to make the volume trace for the simulations. In the simulations the resulting volume/time history is used at all three

of the initial temperatures for each fuel/EGR blend. This method allows for accurate modeling with the variable mass and heat loss associated with the RCM experiments. A general description of the code is made in below in figure 25.

The MATLAB code receives the experimental data for a specific fuel/EGR blend at an initial temperature of 318 K. The experiments are selected in the same manner as section 3.3, when the compressed temperature (averaged between TDC and ignition of each replicate) was within +/- 10 K of the weighted average compressed temperature of five replicates. The mean of the pressure of the resulting filtered cases was taken (bold blue line). A second order exponential fit is fit to the pressure of the mean of the experimental data between TDC and the first ignition rise. A line of fit is then stitched together using the experimental mean from experiment start until TDC then the second order exponential fit line from TDC to the end of the experiment. The resulting fit line (bold red line) is an estimated pressure trace of the experiment as if combustion did not occur. The line of fit is then inserted into Engineering Equation Solver (EES) were the line of fit of pressure is used to calculate a volume/time history using isentropic compression and expansion assumptions. The resulting volume/time was then used to model the compression and heat loss of the RCM experiment. Chemkin uses the volume trace and inputted mechanism to calculate a pressure/time result (bold black line).

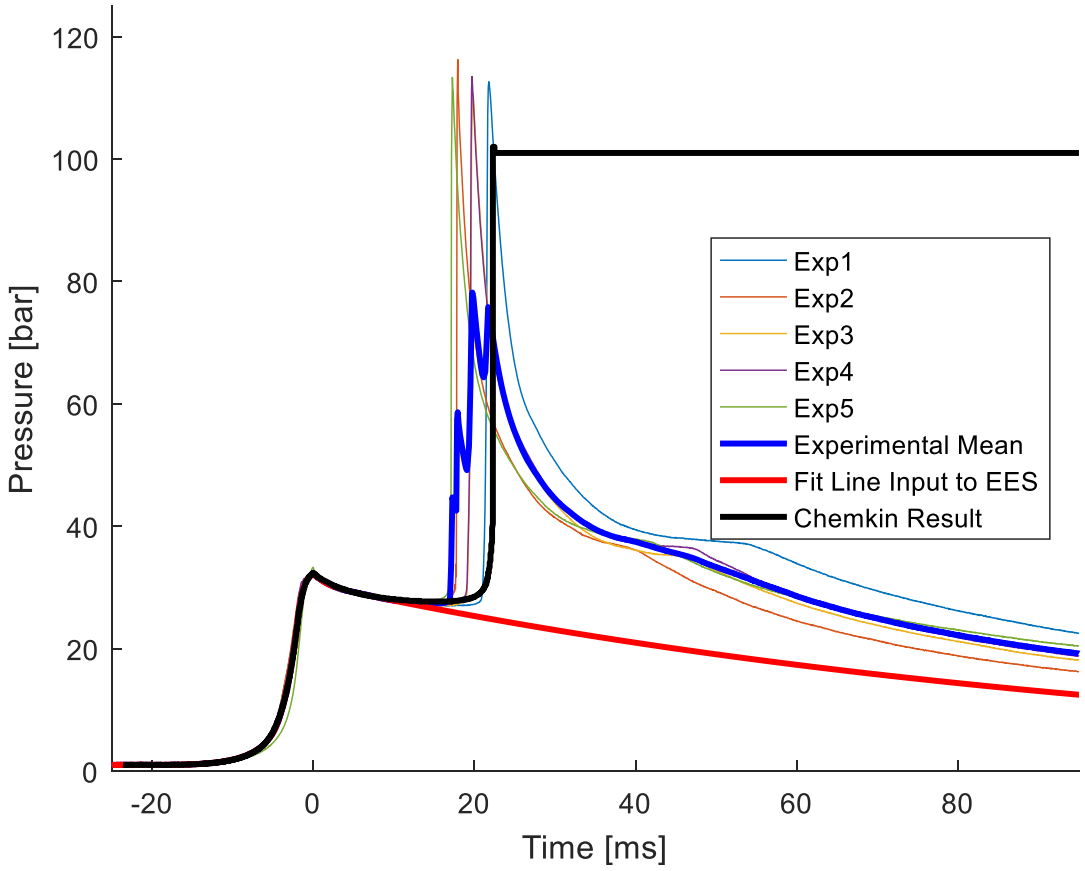

Figure 25: Experimental data compared to simulation model for intermediate fuel experiments starting at an initial pressure and temperature of 1 bar and 318 K respectively. Exp1-5 are the experimental replicates that have been selected using the selection methods in section 3.3. The bold blue line is the mean of all the experimental data. The bold red line is the line of fit that simulates the pressure of a compression event where combustion did not occur. The bold black line is the Chemkin pressure output. The chemical mechanism used in this case was Aramco 3.0.

5.5 Reduced Mechanism Evaluation

All four of the reduced mechanisms and Aramco 3.0 were used to simulate homogenous ignition delay of the RCM experiments. The results for each of the four reduced mechanisms and Aramco 3.0 were then plotted against the experimental data from the RCM. The results are shown below in figure 26.

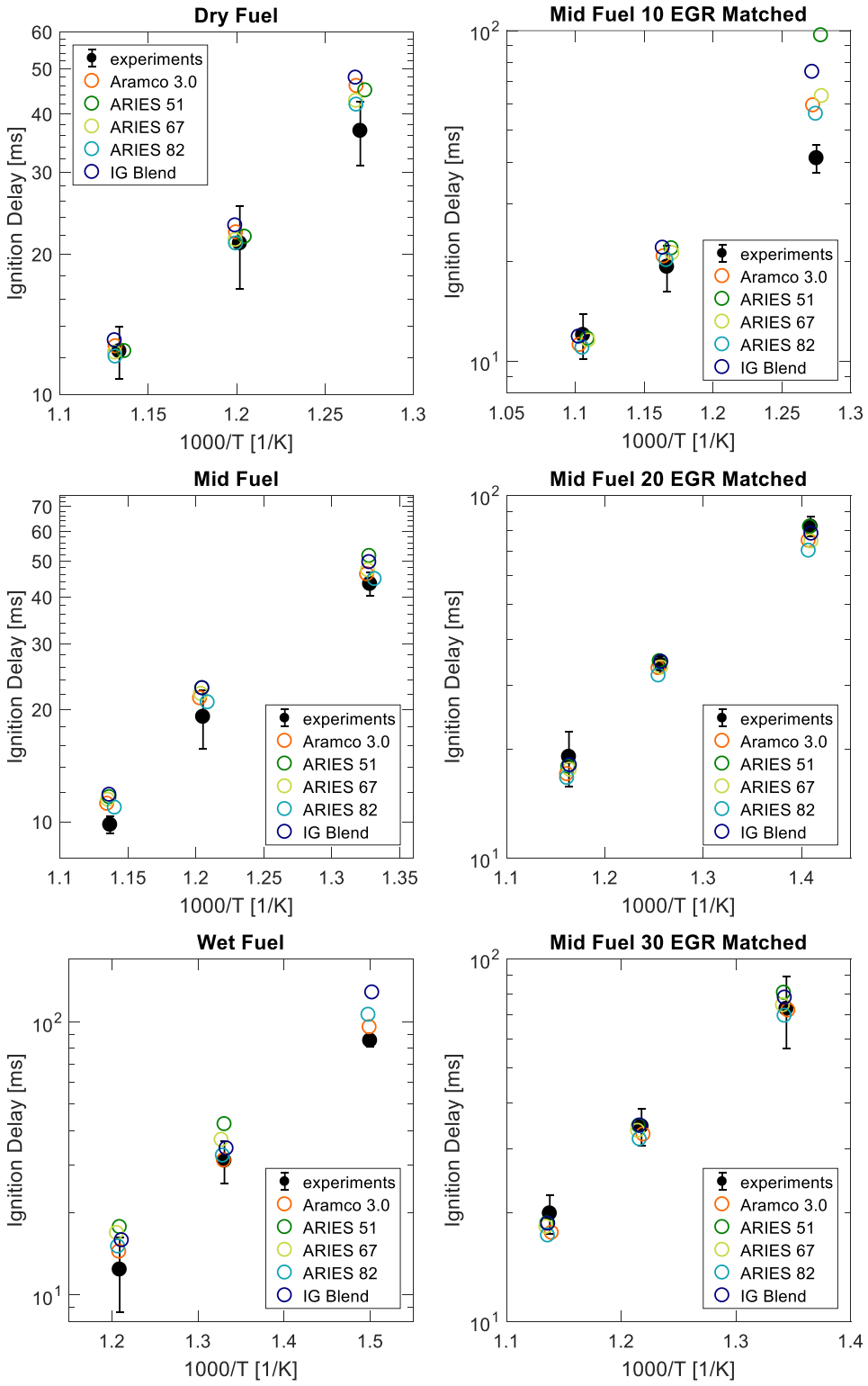

Figure 26: Comparison of reduced mechanism (open circles) homogeneous ignition delay prediction compared to experimental measurements in CSU RCM (closed black circles). Note the markers have been jittered for visual clarity and error bars are statistical 95% confidence intervals.

The average relative error between the experiments and simulations was calculated for each experimental point using the following equation.

$$RE = \frac{S-E}{E} * 100 \quad (8)$$

Where RE is relative error in percent, S is the simulation result, and E is the experimental result.

The error was then averaged for each experimental condition. The results are shown below in table 7.

Table 7: Average relative error of simulations with respect to experimental conditions.

Fuel	NR-EGR Substitution	Aramco 3.0	ARIES 51	ARIES 67	ARIES 82	IG Blend
Dry	**0**	10.9	8.5	5.7	3.7	14.9
Intermediate	**0**	10.7	18.9	13.6	7.8	18.0
Intermediate	**10**	15.1	48.9	20.1	10.8	31.9
Intermediate	**20**	-7.0	-1.4	-6.2	-11.1	-2.6
Intermediate	**30**	-5.9	1.6	-2.9	-8.4	0.6
Wet	**0**	9.5	-5.5	-13.4	16.7	29.6
	Total*	10.6	24.1	17.2	11.0	17.3

*Total relative error is calculated as the average of the absolute value of equation 8.

Of the reduced mechanisms ARIES 82 has the lowest total error at 11.0% which is comparable with the average relative error of Aramco 3.0 at 10.6%.

6. CONCLUSION

6.1 Experimental Conclusions

This study measured the homogeneous ignition delay, flame propagation rate, and f_{EGAI} of pipeline quality natural gas mixtures at various reactive and non-reactive EGR substitution rates. Conventional homogeneous ignition delay plots did not effectively demonstrate reactivity changes between the base fuel mixture and R-EGR substitution. A small but significant difference in homogeneous ignition delay between the R-EGR and NR-EGR substitution was observed. Therefore, a small but significant different in bulk reactivity of the mixtures is observed between the R-EGR and NR-EGR experiments. The NR-EGR bulk mixtures were less reactive than the R-EGR mixtures. This difference is largely attributed to the relatively large amount of NO in the R-EGR as demonstrated in both the homogeneous ignition delay experiments and the simulations shown in figure 19.

Flame propagation decreased with both R-EGR and NR-EGR substitution. As EGR is substituted the adiabatic flame temperature of the propagating flame decreases which in turn decreases the flame propagation rate. F_{EGAI} increased with R-EGR substitution but decreased with NR-EGR substitution. This demonstrated the competition between the flame propagation consuming the reactant charge and the ignite on delay of the end-gas. If the reactivity of the bulk mixture is maintained slower flame speeds consume less fuel leaving a larger quantity of end-gas increasing f_{EGAI}. If the reactivity of the mixture decreases enough f_{EGAI} decreases even though flame speed decreases because there is enough time for the flame to consume the end-gas before the end-gas volumetrically autoignites. This theory was also observed with 0-D Chemkin simulations that showed the relative difference in homogeneous autoignition delay times of the mixtures with R-

EGR decreased and NR-EGR increased. For the same reasons NO was suspected as being the largest influence on homogeneous ignition delay, NO is also the likely cause of the differences observed in $f_{EGAI.}$ Since NO causes homogeneous ignition delay to be shorter there is less time for the flame to consume the end-gas resulting in a larger f_{EGAI}. In the NR-EGR cases the homogeneous ignition delay was increased due to the lack of NO in the mixture. This increased the amount of time for the flame to consume the end-gas resulting in a lower f_{EGAI}.

6.2 Chemical Kinetic Model Conclusions

A reduced chemical kinetic mechanism was also developed. Seven detailed "parent" mechanisms were benched marked for accuracy against published data. Aramco 3.0 [38] was selected due to its homogeneous ignition delay accuracy it higher pressures ~30 bar and its ability to numerically solve for pressures up to 60 bar. Four reduced mechanisms were developed with a species number range of 52 – 91 for mixtures of CH_4, C_2H_6, and C_3H_8. The mechanisms were designed for pressure and temperature range of 500 – 1000 K and 1 – 100 bar respectively. In order to validate the reduced mechanism a variable volume 0-D RCM model was constructed that used adiabatic compression and expansion to mimic the compression cycle and resulting heat loss after TDC in the RCM experiments. Using this model, the mechanisms were compared to homogeneous ignition delays measured in the RCM of NG fuel blends with methane numbers ranging from 68 – 95 and NR-EGR concentrations of 0 – 30% by mass. For the six experimental cases tested in the RCM the detailed mechanism (Aramco 3.0) demonstrated a total average relative error of 10.6%. the best performing reduced mechanism (ARIES 82) demonstrated a similar total average relative error of 11.0%.

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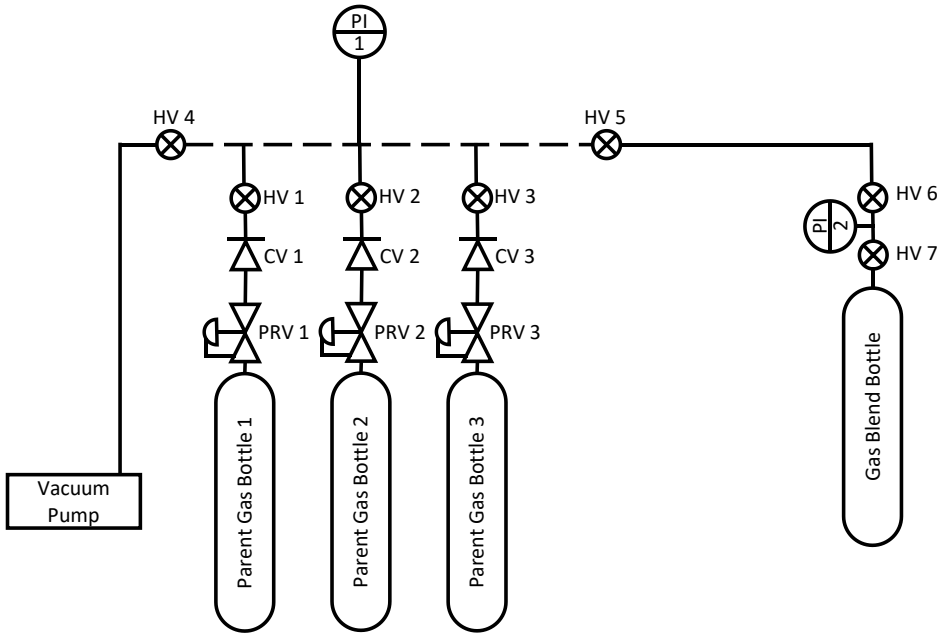
APPENDIX A

Mixing Reactant Mixtures for RCM Experiments

When running RCM experiments a considerable amount of time is spent on mixing the reactants to be tested. Great care must be taken to insure accurate and repeatable mixtures are created. Therefore, it is recommended that RCM users create a procedure that not only maintains accuracy but also maintains consistency in error. The gas mixing procedure that was used for this project is described in detail below. These methods demonstrated an accuracy of 0.25% by mole fraction for a working pressure of 3 bar for the natural gas blends. There are two procedures described below. The first being the mixing procedure to mix the natural gas blends in a 300-size standard gas cylinder. The second being the procedure to mix the total reactant mixture in the liquid mixing tank.

Mixing Natural Gas Fuel Blends

CH_4, C_2H_6, and C_3H_8 were mixed separately in a size 300, CGA 350 gas cylinder (gas blend bottle) to a total pressure of 3 bar. Partial pressure was measured using an OMEGA DPGM409-3.5BA pressure transducer. The procedure was adapted from ASTM Standard D4051-10. The following image contains the piping and instrumentation diagram that displays the configuration of the gas mixing system to mix the NG gas blend bottle. The step by step procedure is listed below the image.



Piping and instrumentation diagram of gas manifold system to utilize NG gas blend bottle. Where: PI = pressure indicator, HV = hand valve, PRV = pressure regulated valve, CV = check valve, dotted lines indicate temperature-controlled section of the system.

1. Start with a system where all hand valves and parent gas bottles are closed, and the vacuum pump is on.

2. Open HV 4-7 to begin vacuuming the gas blend bottle empty. After PI 2 indicates it lowest pressure (-0.00 for the case of OMEGA DPGM409-3.5BA) close HV 6 and HV 4.

3. Open parent gas bottle 1 and set PRV 1 to an appropriate pressure that is above the desired partial pressure of species 1.

4. Open HV 1 and allow species 1 to full the gas manifold between HV 4 and HV 6. Open HV 4 for 5-10 second to allow flow of species 1. This insures only species 1 is present in the gas manifold.

5. Open HV 6 slowly and allow species 1 to begin filling the gas blend bottle. The fill rate should be slow enough to minimize a temperature increase in the gas blend bottle. The goal should be to fill at a rate that the heat into the system is equivalent to the heat out of the system through heat transfer.

6. Once species 1 reaches the desired partial pressure close HV 6

7. Wait at least 5 minutes to allow pressure in gas blend tank to equalize. The pressure will drop do to heat transfer of species 1 to the gas bottle walls and the gas bottle walls to the room. Wait until the pressure has stopped changing before moving to next step.

8. Repeat steps 5-7 until the desired partial pressure is achieved without a pressure drop after step 7.

9. Ensure HV 6 is closed. Close parent gas bottle 1 and open HV 4 to vacuum gas manifold empty. Note some PRV's can be damaged if exposed to vacuum. If this is the case, close HV 1 before vacuuming the gas manifold.

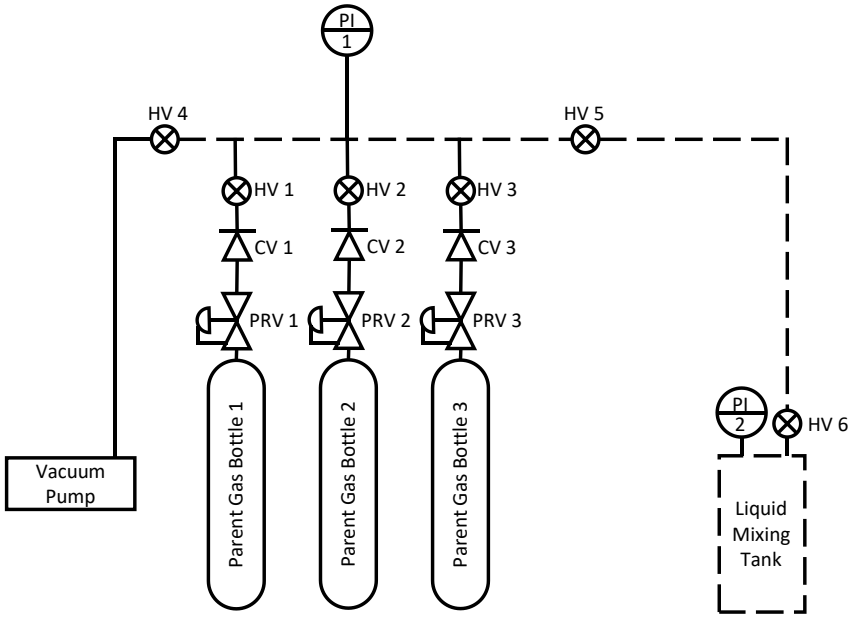
10. After the gas manifold is empty (indicated on PI 1) close HV 4.

11. Repeat steps 3-10 with remaining species until desired mixture is blended.

12. Once the total desire mixture is mixed close the gas blend bottle (HV 7) and any open parent bottles. Evacuate the gas manifold completely by opening HV 4. It is recommended to leave the gas mixture overnight to allow diffusive mixing to create a homogeneous gas mixture. If faster mixing is desired the mixing procedure in ASTM Standard D4051-10 recommends carefully heating alternating ends of the gas cylinder to promote convective mixing however every reasonable safety precaution must be made to avoid accidental ignition with flammable mixtures.

Mixing Full Oxidized Reactant Blends

Similar to the NG gas blend mixing techniques the procedure to mix the oxidized fuel blends was adapted from ASTM Standard D4051-10. Partial pressure was measured using an OMEGA DPGM409-3.5BA pressure transducer. The procedure was adapted from ASTM Standard D4051-10. The procedure is largely the same as the NG gas blend mixing procedure with the only difference being the total fill pressure and that the mixture is mixed in the liquid mixing tank instead of a DOT size 300 gas cylinder. The liquid mixing tank does have provisions for in cylinder gas temperature measurements which greatly increases the accuracy of the mixing system. The following image is the piping and instrumentation diagram that demonstrates the desired gas manifold configuration for mixing reactants in the liquid mixing tanks.



Piping and instrumentation diagram of gas manifold configuration to utilize liquid mixing tank. Where: PI = pressure indicator, HV = hand valve, PRV = pressure regulated valve, CV = check valve, dotted lines indicate temperature-controlled section of the system.

1. Start with a system where all hand valves and parent gas bottles are closed, and the vacuum pump is on. Turn on PID and heater system for liquid mixing tanks and turn on magnetic stir bar.

2. Open HV 4-6 to begin vacuuming the liquid mixing tank empty. After PI 2 indicates it lowest pressure (-0.00 for the case of OMEGA DPGM409-3.5BA) close HV 6 and HV 4. Note, this step can be completed at the same time the liquid mixing tank is warming to operating temperature. For the tests in this study the liquid mixing tank was heated to 298 K.

3. Open parent gas bottle 1 and set PRV 1 to an appropriate pressure that is above the desired partial pressure of species 1.

4. Open HV 1 and allow species 1 to full the gas manifold between HV 4 and HV 6. Open HV 4 for 5-10 second to allow flow of species 1. This insures only species 1 is present in the gas manifold.

5. Open HV 6 slowly and allow species 1 to begin filling the liquid mixing tank. The fill rate should be slow enough to minimize a temperature increase in the liquid mixing tanks. The goal should be to fill at a rate that the heat into the system is equivalent to the heat out of the system through heat transfer.

6. Once species 1 reaches the desired partial pressure close HV 6

7. Wait until the temperature of the gas in the liquid mixing tank returns to operating temperate (298 K). Allow pressure in gas blend tank to equalize. The pressure will drop do to heat transfer of species 1 to the tank walls and tank walls to the room. Wait until the pressure has stopped changing before moving to next step.

8. Repeat steps 5-7 until the desired partial pressure is achieved at operating temperature.

9. Ensure HV 6 is closed. Close parent gas bottle 1 and open HV 4 to vacuum gas manifold empty. Note some PRV's can be damaged if exposed to vacuum. If this is the case, close HV 1 before vacuuming the gas manifold.

10. After the gas manifold is empty (indicated on PI 1) close HV 4.

11. Repeat steps 3-10 with remaining species until desired mixture is blended.

12. Once the total desire mixture is mixed close HV 6 and any open parent bottles. Evacuate the gas manifold completely by opening HV 4. The magnetic stir bar speeds mixing, and the tank can be assumed homogeneous after 2 hours.

Gas mixing notes:

1. In order to ensure accurate mixing, it is recommended to start with the species that has the lowest mole fraction of the total mixture. However, care should be taken to avoid hazardous conditions when mixing. For example, do not mix hydrocarbons with pure oxygen as this mixture may spontaneously autoignite. First mix the hydrocarbon fuel, then inert, then oxygen.

2. This method assumes a leak free manifold. The system should be able to be vacuumed down and this vacuum should be able to be maintained for several hours. If any leaks are in the system significant mixing error can occur

3. In order to maximize accuracy, the distance between the tank and the pressure indicator should be minimized. In the case of the liquid mixing tanks the pressure is read directly from the tank volume. For the NG gas blend bottle the distance between HV 6 and the tank volume should be as short as possible.

4. Use common sense when using flammable and reactive mixtures. It is up to the operator to ensure all reasonable safety precautions have been met before using the system.

   If desired a similar approach to reference [31] can be used. This method assumes ideal gas law and does not require a constant temperature to be maintained in the liquid mixing tanks. Instead, it recalculates the mixtures based on the new temperature. However, keep in mind that the accuracy of the PID temperature measurement is one full degree Celsius and that the chamber heats quicker than it cools. Therefore, appropriate consideration of temperature measurements and mixing error should be considered before using this method.

APPENDIX B

RCM Test Conditions for Homogeneous Ignition Delay

Fuel Type	EGR Type	EGR Substitution	Compressed Temperature [K]	Compressed Pressure [bar]
Dry	R-EGR	0	925-964	32.5-33.3
	R-EGR	10	917-975	32.9-33.0
	R-EGR	20	938-970	32.8-33.7
	R-EGR	30	936-960	32.3-33.7
Intermediate	R-EGR	0	891-951	32.1-32.3
	R-EGR	10	900-928	31.4-32.4
	R-EGR	20	945-977	33.0-34.0
	R-EGR	30	941-950	31.9-33.8
Intermediate	NR-EGR	10	940-973	32.9-33.8
	NR-EGR	20	911-937	31.7-32.8
	NR-EGR	30	935-966	32.6-33.7
Wet	R-EGR	0	857-907	30.2-30.8
	R-EGR	10	903-937	31.7-31.9
	R-EGR	20	912-946	32.0-32.8
	R-EGR	30	907-930	31.4-32.7

APPENDIX C

RCM Test Conditions for Laser Ignited Experiments

Fuel Type	EGR Type	EGR Substitution	Compressed Temperature [K]	Compressed Pressure [bar]
Dry	R-EGR	0	792	32.0
	R-EGR	10	769	31.5
	R-EGR	20	753	32.1
	R-EGR	30	765	30.5
Intermediate	R-EGR	0	765	31.4
	R-EGR	10	750	30.7
	R-EGR	20	797	33.4
	R-EGR	30	839	33.3
Intermediate	NR-EGR	10	773	31.9
	NR-EGR	20	747	30.9
	NR-EGR	30	787	32.0
Wet	R-EGR	0	717	29.8
	R-EGR	10	782	31.6
	R-EGR	20	771	32.8
	R-EGR	30	799	32.0

APPENDIX D

ARIES 51 Mechanism

```
ELEMENTS
C H N O AR
HE
END
SPECIES
AR N2 HE H2 H
O2 O H2O OH OHV
H2O2 HO2 CO CO2 CH4
CH3 CH2 CH2(S) CH CHV
CH3O2H CH3O2 CH3O CH2OH CH2O
HCO HCOH HO2CHO O2CHO HOCHO
OCHO C2H6 C2H5 C2H4 C2H3
CHCHO C2H2 CH3CHO CH2CHO CH2CO
HCCO C3H8 IC3H7 NC3H7 NC3H7O2
IC3H7O2 C3H6 C3H5-A CH3CHCO C3H6OH2-1
CH3COCH3
END

THERMO ALL
  300.000  1000.000  5000.000
AR               G-5-97AR  1             G     200.0    6000.0  1000.0      1
        2.5E0         0.0E0         0.0E0         0.0E0         0.0E0    2
    -7.45375E2   4.37967491E0         2.5E0         0.0E0         0.0E0    3
        0.0E0         0.0E0    -7.45375E2   4.37967491E0                   4
N2               G-8-02N   2             G     200.0    6000.0  1000.0      1
   2.95257637E0   1.3969004E-3 -4.92631603E-7 7.86010195E-11-4.60755204E-15    2
  -9.23948688E2   5.87188762E0   3.53100528E0 -1.23660988E-4 -5.02999433E-7    3
   2.43530612E-9-1.40881235E-12  -1.04697628E3   2.96747038E0                   4
HE               G-5-97HE  1             G     200.0    6000.0  1000.0      1
        2.5E0         0.0E0         0.0E0         0.0E0         0.0E0    2
    -7.45375E2  9.28723974E-1         2.5E0         0.0E0         0.0E0    3
        0.0E0         0.0E0    -7.45375E2  9.28723974E-1                   4
H2               TPIS78H   2             G     200.0    6000.0  1000.0      1
   2.93286575E0  8.26608026E-4 -1.46402364E-7 1.54100414E-11  -6.888048E-16    2
  -8.13065581E2  -1.02432865E0   2.34433112E0  7.98052075E-3  -1.9478151E-5    3
   2.01572094E-8-7.37611761E-12  -9.17935173E2  6.83010238E-1                   4
H                L-6-94H   1             G     200.0    6000.0  1000.0      1
        2.5E0         0.0E0         0.0E0         0.0E0         0.0E0    2
    2.547366E4  -4.4668285E-1         2.5E0         0.0E0         0.0E0    3
        0.0E0         0.0E0    2.547366E4  -4.4668285E-1                   4
O2               RUS-89O   2             G     200.0    6000.0  1000.0      1
   3.66096065E0  6.56365811E-4 -1.41149627E-7 2.05797935E-11-1.29913436E-15    2
  -1.21597718E3   3.41536279E0   3.78245636E0 -2.99673416E-3  9.84730201E-6    3
  -9.68129509E-9 3.24372837E-12  -1.06394356E3   3.65767573E0                   4
O                L-1-90O   1             G     200.0    6000.0  1000.0      1
   2.54363697E0 -2.73162486E-5  -4.1902952E-9 4.95481845E-12-4.79553694E-16    2
    2.9226012E4   4.92229457E0   3.1682671E0 -3.27931884E-3  6.64306396E-6    3
  -6.12806624E-9 2.11265971E-12   2.91222592E4   2.05193346E0                   4
H2O              L-5-89H   2O  1         G     200.0    6000.0  1000.0      1
    2.6770389E0   2.9731816E-3  -7.7376889E-7  9.4433514E-11 -4.2689991E-15    2
   -2.9885894E4      6.88255E0   4.1986352E0  -2.0364017E-3   6.5203416E-6    3
  -5.4879269E-9   1.771968E-12   -3.0293726E4  -8.4900901E-1                   4
OH               IU3-03H   1O  1         G     200.0    6000.0  1000.0      1
   2.83853033E0  1.10741289E-3 -2.94000209E-7 4.20698729E-11 -2.4228989E-15    2
   3.69780808E3   5.84494652E0   3.99198424E0 -2.40106655E-3  4.61664033E-6    3
  -3.87916306E-9 1.36319502E-12   3.36889836E3 -1.03998477E-1                   4
!UB REFIT 13-11-2018
OHV              -THERMH   1O  1         G     300.0    5000.0  1710.0      1
    2.8537604E0  1.02994334E-3 -2.32666477E-7 1.93750704E-11-3.15759847E-16    2
   5.03225473E4   5.76240468E0   3.41896226E0  3.19255801E-4 -3.08292717E-7    3
 3.64407494E-10-1.00195479E-13   5.00756946E4   2.51917016E0                   4
H2O2             T-8-03H   2O  2         G     200.0    6000.0  1000.0      1
   4.57977305E0  4.05326003E-3  -1.2984473E-6   1.982114E-10-1.13968792E-14    2
  -1.80071775E4  6.64970694E-1   4.31515149E0 -8.47390622E-4  1.76404323E-5    3
  -2.26762944E-8 9.08950158E-12  -1.77067437E4   3.27373319E0                   4
HO2              T-1-09H   1O  2         G     200.0    5000.0  1000.0      1
   4.17228741E0  1.88117627E-3 -3.46277286E-7 1.94657549E-11 1.76256905E-16    2
   3.10206839E1   2.95767672E0   4.30179807E0 -4.74912097E-3  2.11582905E-5    3
  -2.42763914E-8 9.29225225E-12   2.64018485E2   3.7166622E0                   4
CO               RUS-79O   1C  1         G     200.0    6000.0  1000.0      1
    3.0484859E0   1.3517281E-3  -4.8579405E-7  7.8853644E-11 -4.6980746E-15    2
   -1.4266117E4   6.0170977E0   3.5795335E0  -6.1035369E-4   1.0168143E-6    3
  9.0700586E-10 -9.0442449E-13   -1.4344086E4   3.5084093E0                   4
CO2              L-7-88O   2C  1         G     200.0    6000.0  1000.0      1
    4.6365111E0   2.7414569E-3  -9.9589759E-7  1.6038666E-10 -9.1619857E-15    2
   -4.9024904E4   -1.9348955E0    2.356813E0   8.9841299E-3  -7.1220632E-6    3
   2.4573008E-9 -1.4288548E-13   -4.8371971E4    9.9009035E0                   4
CH4              G-8-99H   4C  1         G     200.0    6000.0  1000.0      1
   1.65326226E0  1.00263099E-2 -3.31661238E-6 5.36483138E-10-3.14696758E-14    2
  -1.00095936E4   9.90506283E0   5.14911468E0 -1.36622009E-2  4.91453921E-5    3
 -4.84246767E-8 1.66603441E-11  -1.02465983E4  -4.63848842E0                   4
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CH3               IU0702H   3C   1         G    200.0    6000.0  1000.0      1
   2.9781206E0   5.797852E-3   -1.97558E-6   3.072979E-10 -1.7917416E-14    2
   1.6509513E4   4.7224799E0   3.6571797E0   2.1265979E-3   5.4583883E-6    3
 -6.6181003E-9  2.4657074E-12   1.6422716E4   1.6735354E0                   4
CH2               IU3-03H   2C   1         G    200.0    6000.0  1000.0      1
  3.14631886E0  3.03671259E-3 -9.96474439E-7  1.5048358E-10-8.57335515E-15    2
  4.60412605E4   4.72341711E0   3.71757846E0   1.2739126E-3  2.17347251E-6    3
  -3.488585E-9 1.65208866E-12   4.58723866E4   1.75297945E0                 4
CH2(S)            IU6-03H   2C   1         G    200.0    6000.0  1000.0      1
  3.13501686E0  2.89593926E-3  -8.1666809E-7 1.13572697E-10-6.36262835E-15    2
  5.05040504E4   4.06030621E0   4.19331325E0 -2.33105184E-3  8.15676451E-6    3
 -6.62985981E-9 1.93233199E-12   5.03662246E4  -7.4673431E-1                 4
CH                IU3-03H   1C   1         G    200.0    6000.0  1000.0      1
   2.5209369E0   1.7653639E-3   -4.614766E-7  5.9289675E-11 -3.3474501E-15    2
   7.0946769E4   7.4051829E0   3.4897583E0   3.243216E-4  -1.6899751E-6    3
  3.162842E-9 -1.4061803E-12   7.0612646E4   2.0842841E0                   4
!UB REFIT 13-11-2018
CHV               -THERMH   1C   1         G    300.0    5000.0  1365.0      1
  2.21703785E0  2.15314038E-3 -5.71569209E-7 6.54441183E-11-2.66374894E-15    2
  1.04414085E5   9.18247549E0   3.50775836E0 -4.57470019E-4  1.32602633E-6    3
 -5.1421376E-10 5.82219975E-14   1.03920991E5   2.09911232E0                 4
CH3O2H            A-7-05H   4O   2C   1    G    200.0    6000.0  1000.0      1
  7.76538058E0  8.61499712E-3 -2.98006935E-6 4.68638071E-10-2.75339255E-14    2
 -1.82979984E4  -1.43992663E1   2.90540897E0  1.74994735E-2   5.2824363E-6    3
 -2.52827275E-8 1.34368212E-11  -1.68894632E4   1.13741987E1                 4
CH3O2               H   3O   2C   1    G    300.0    5000.0  1374.0      1
  6.47970487E0   7.4440108E-3 -2.52348555E-6 3.89577296E-10-2.25182399E-14    2
 -1.56285441E3  -8.19477074E0   1.97339205E0   1.5354234E-2 -6.37314891E-6    3
 3.19930565E-10 2.82193915E-13   2.54278835E2   1.69194215E1                 4
CH3O              IU1-03H   3O   1C   1    G    200.0    6000.0  1000.0      1
  4.75779238E0  7.44142474E-3 -2.69705176E-6 4.38090504E-10-2.63537098E-14    2
   3.7811194E2  -1.96680028E0   3.71180502E0 -2.80463306E-3  3.76550971E-5    3
 -4.73072089E-8  1.8658842E-11   1.2956976E3   6.57240864E0                 4
CH2OH             IU2-03H   3O   1C   1    G    200.0    6000.0  1000.0      1
   5.0931437E0   5.9476126E-3  -2.0649746E-6 3.23008173E-10-1.88125902E-14    2
  -4.0340964E3  -1.84691493E0   4.47834367E0  -1.3507031E-3   2.7848498E-5    3
  -3.6486906E-8  1.4790745E-11   -3.5007289E3    3.309135E0                 4
CH2O              T-5-11H   2O   1C   1    G    200.0    6000.0  1000.0      1
  3.16952665E0   6.1932056E-3 -2.25056366E-6  3.6597566E-10-2.20149458E-14    2
 -1.45486831E4   6.04207898E0   4.79372312E0 -9.90833322E-3   3.7321999E-5    3
 -3.79285237E-8 1.31772641E-11  -1.43791953E4  6.02798058E-1                 4
HCO               T-5-03H   1O   1C   1    G    200.0    6000.0  1000.0      1
  3.92001542E0  2.52279324E-3 -6.71004164E-7 1.05615948E-10-7.43798261E-15    2
  3.65342928E3   3.58077056E0   4.2375461E0 -3.32075257E-3  1.40030264E-5    3
 -1.34239995E-8 4.37416208E-12   3.87241185E3   3.30834869E0                 4
HCOH              -MAR94H   2O   1C   1    G    300.0    5000.0  1398.0      1
  9.18749272E0  1.52011152E-3 -6.27603516E-7 1.09727989E-10-6.89655128E-15    2
  7.81364593E3  -2.73434214E1  -2.82157421E0  3.57331702E-2  -3.8086158E-5    3
 1.86205951E-8-3.45957838E-12   1.12956672E4   3.48487757E1                 4
HO2CHO            -THERMH   2O   3C   1    G    300.0    5000.0  1378.0      1
  9.87503878E0  4.64663708E-3 -1.67230522E-6 2.68624413E-10-1.59595232E-14    2
 -3.80502496E4  -2.24939155E1   2.42464726E0   2.1970638E-2 -1.68705546E-5    3
  6.25612194E-9-9.11645843E-13  -3.54828006E4   1.75027796E1                 4
O2CHO             -THERMH   1O   3C   1    G    300.0    5000.0  1368.0      1
  7.24075139E0  4.63312951E-3 -1.63693995E-6 2.59706693E-10-1.52964699E-14    2
 -1.87027618E4  -6.49547212E0   3.96059309E0  1.06002279E-2 -5.25713351E-6    3
  1.01716726E-9-2.87487602E-14  -1.73599383E4   1.17807483E1                 4
HOCHO             L-8-88H   2O   2C   1    G    200.0    6000.0  1000.0      1
   4.6138316E0   6.4496364E-3  -2.2908251E-6  3.6716047E-10 -2.1873675E-14    2
   -4.751485E4   8.4788383E-1    3.8983616E0  -3.5587795E-3   3.5520538E-5    3
  -4.3849959E-8  1.7107769E-11   -4.6770609E4   7.3495397E0                 4
OCHO              ATCT-AH   1O   2C   1    G    200.0    6000.0  1000.0      1
  4.14394211E0  5.59738818E-3 -1.99794019E-6 3.16179193E-10-1.85614483E-14    2
 -1.72459887E4   5.07778617E0   4.68825921E0 -4.14871834E-3   2.5506601E-5    3
  -2.844739E-8  1.04422559E-11  -1.69867041E4   4.2842648E0                 4
C2H6              G-8-88H   6C   2         G    200.0    6000.0  1000.0      1
  4.04666411E0  1.53538802E-2 -5.47039485E-6 8.77826544E-10-5.23167531E-14    2
 -1.24473499E4 -9.68698313E-1   4.29142572E0 -5.50154901E-3  5.99438458E-5    3
 -7.08466469E-8 2.68685836E-11  -1.15222056E4   2.66678994E0                 4
C2H5              -THERMH   5C   2         G    300.0    5000.0  1387.0      1
   5.8878439E0  1.03076793E-2 -3.46844396E-6 5.32499257E-10-3.06512651E-14    2
  1.15065499E4  -8.49651771E0   1.32730217E0  1.76656753E-2 -6.14926558E-6    3
-3.01143466E-10 4.38617775E-13   1.34284028E4   1.71789216E1                 4
C2H4                H   4C   2         G    300.0    5000.0  1392.0      1
  5.07061289E0  9.11140768E-3 -3.10506692E-6 4.80733851E-10-2.78321396E-14    2
  3.66391217E3  -6.64501414E0  4.81118223E-1   1.8377806E-2 -9.99633565E-6    3
  2.73211039E-9-3.01837289E-13   5.44386648E3   1.85867157E1                 4
C2H3                H   3C   2         G    300.0    5000.0  1400.0      1
  4.99675415E0  6.55838271E-3 -2.20921909E-6 3.39300272E-10-1.95316926E-14    2
  3.34604382E4  -3.01451097E0   1.25545094E0  1.57481597E-2 -1.12218328E-5    3
  4.50915682E-9-7.74861577E-13   3.47435574E4   1.69664043E1                 4
CHCHO               H   2O   1C   2    G    298.15   2000.0  1000.0      1
   4.9263291E0  9.71712147E-3  -5.5485598E-6  1.53068537E-9-1.64742462E-13    2
  2.89499494E4  5.27874677E-1   2.33256751E0  1.62952986E-2 -9.72052177E-6    3
 5.15124155E-10 1.03836514E-12   2.96585452E4   1.39904923E1                 4
C2H2              G-1-91H   2C   2         G    200.0    6000.0  1000.0      1
  4.65878489E0  4.88396667E-3 -1.60828888E-6 2.46974544E-10-1.38605959E-14    2
  2.57594042E4  -3.99838194E0  8.08679682E-1  2.33615762E-2 -3.55172234E-5    3
  2.80152958E-8-8.50075165E-12   2.64289808E4   1.39396761E1                 4
CH3CHO            L-8-88H   4O   1C   2    G    200.0    6000.0  1000.0      1
   5.4041108E0   1.1723059E-2  -4.2263137E-6  6.8372451E-10 -4.0984863E-14    2
  -2.2593122E4   -3.4807917E0    4.7294595E0  -3.1932858E-3   4.7534921E-5    3
  -5.7458611E-8  2.1931112E-11   -2.1572878E4    4.1030159E0                 4
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CH2CHO            T03-10H   3O   1C   2     G     200.0    6000.0  1000.0      1
  6.53928338E0  7.80238629E-3 -2.76413612E-6 4.42098906E-10 -2.6295429E-14    2
 -1.18858659E3  -8.72091393E0     2.795026E0  1.01099472E-2  1.61750645E-5    3
 -3.10303145E-8 1.39436139E-11   1.62944975E2   1.23646657E1                   4
!UB REFIT 13-11-2018
CH2CO             -THERMH   2O   1C   2     G     300.0    5000.0  1400.0      1
  6.32896692E0  5.44012978E-3 -1.82687969E-6 2.80010787E-10 -1.6096416E-14    2
 -8.36526176E3  -9.53528539E0   2.35724171E0  1.62213064E-2 -1.34812364E-5    3
  6.11939897E-9-1.13613089E-12  -7.11393356E3   1.12990053E1                   4
HCCO              T-4-09H   1O   1C   2     G     200.0    6000.0  1000.0      1
  5.91479333E0   3.7140873E-3  -1.3013701E-6 2.06473345E-10-1.21476759E-14    2
  1.93596301E4  -5.50567269E0   1.87607969E0  2.21205418E-2 -3.58869325E-5    3
  3.05402541E-8-1.01281069E-11    2.0163384E4    1.3696829E1                   4
C3H8                H   8C   3         G     300.0    5000.0  1390.0      1
   9.1554131E0  1.72574139E-2 -5.85614868E-6 9.04190155E-10-5.22523772E-14    2
 -1.75762439E4   -2.7741851E1   2.4087847E-1  3.39548599E-2 -1.60930874E-5    3
  2.83480628E-9 2.78195172E-14  -1.40362853E4    2.165008E1                   4
IC3H7               H   7C   3         G     298.0    6000.0  1000.0      1
  6.70775549E0  1.74048076E-2 -6.07615926E-6 9.60084351E-10 -5.6565649E-14    2
  7.55377821E3  -1.03686516E1 -8.97467137E-1  4.15744022E-2 -4.94778349E-5    3
  4.56493655E-8-1.79085437E-11   9.93950407E3   2.92641758E1                   4
NC3H7               H   7C   3         G     298.0    6000.0  1000.0      1
  7.48614243E0  1.65769478E-2 -5.74876481E-6 9.04103694E-10-5.30867231E-14    2
  8.93710008E3  -1.42595379E1  -2.20120865E0  5.29641653E-2 -7.23640506E-5    3
  6.3699694E-8-2.29332581E-11   1.15130744E4   3.43669174E1                   4
NC3H7O2               H   7O   2C   3     G     300.0    5000.0  1390.0      1
  1.32753283E1  1.61303126E-2 -5.52348308E-6 8.58197168E-10-4.98172586E-14    2
 -1.16032968E4  -4.15091215E1  2.13311681E0  3.96692045E-2 -2.37570127E-5    3
  6.96020417E-9-7.82576856E-13  -7.46687112E3   1.92444565E1                   4
IC3H7O2               H   7O   2C   3     G     300.0    5000.0  1407.0      1
   1.3526812E1  1.54306581E-2 -5.17464218E-6 7.92548669E-10-4.55415379E-14    2
 -1.33946348E4  -4.40461451E1   2.58517502E0  4.16107259E-2 -2.92193877E-5    3
  1.08614807E-8-1.66312005E-12  -9.67013161E3    1.447313E1                   4
C3H6                H   6C   3         G     298.0    6000.0  1000.0      1
  6.59032304E0  1.52592866E-2 -5.30369441E-6 8.35510888E-10-4.91215549E-14    2
 -2.47481113E2  -1.15748238E1  -1.54606737E0  4.36553128E-2 -5.61392417E-5    3
  4.98421927E-8-1.84798923E-11   2.07056233E3   2.99232495E1                   4
C3H5-A              H   5C   3         G     298.0    6000.0  1000.0      1
  7.37604097E0  1.23449782E-2 -4.26463882E-6 6.69045835E-10-3.92202554E-14    2
   1.7733296E4  -1.61758204E1  -3.32899442E0  5.38423469E-2 -7.65500752E-5    3
  6.35512285E-8-2.14283003E-11   2.03420628E4   3.68038362E1                   4
CH3CHCO           -THERMH   4O   1C   3     G     300.0    5000.0  1400.0      1
  1.00219123E1   9.569663E-3 -3.26221644E-6 5.05231706E-10-2.92593257E-14    2
 -1.42482738E4  -2.77829973E1   1.48380119E0  3.22203013E-2 -2.70250033E-5    3
  1.20499164E-8-2.18365931E-12   -1.1527654E4   1.71552068E1                   4
C3H6OH2-1         -THERMH   7O   1C   3     G     300.0    5000.0  1392.0      1
  1.12222277E1  1.36444398E-2 -4.51406709E-6 7.10523275E-10-4.22690392E-14    2
 -1.75350136E4  -3.18911926E1   1.0967036E0  3.80727565E-2 -2.75022497E-5    3
  1.07477493E-8-1.74895773E-12  -1.40764487E4   2.22475799E1                   4
CH3COCH3            H   6O   1C   3     G     300.0    5000.0  1394.0      1
  8.87619308E0  1.45700263E-2  -4.8482328E-6 7.38614777E-10-4.22831194E-14    2
 -3.06046242E4  -2.12730484E1   2.20008426E0  2.74019559E-2 -1.31342003E-5    3
  2.57150371E-9-6.21509091E-14  -2.79933966E4   1.55883508E1                   4
END

TRANSPORT
AR 0 136.5 3.33 0.0 0.0 0.0
N2 1 97.53 3.621 0.0 1.76 4.0
HE 0 10.2 2.576 0.0 0.0 0.0
H2 1 38.0 2.92 0.0 0.79 280.0
H 0 145.0 2.05 0.0 0.0 0.0
O2 1 107.4 3.458 0.0 1.6 3.8
O 0 80.0 2.75 0.0 0.0 0.0
H2O 2 572.4 2.605 1.844 0.0 4.0
OH 1 80.0 2.75 0.0 0.0 0.0
OHV 1 80.0 2.75 0.0 0.0 0.0
H2O2 2 107.4 3.458 0.0 0.0 3.8
HO2 2 107.4 3.458 0.0 0.0 1.0
CO 1 98.1 3.65 0.0 1.95 1.8
CO2 1 244.0 3.763 0.0 2.65 2.1
CH4 2 141.4 3.746 0.0 2.6 13.0
CH3 1 144.0 3.8 0.0 0.0 0.0
CH2 1 144.0 3.8 0.0 0.0 0.0
CH2(S) 1 144.0 3.8 0.0 0.0 0.0
CH 1 80.0 2.75 0.0 0.0 0.0
CHV 1 80.0 2.75 0.0 0.0 0.0
CH3O2H 2 481.8 3.626 0.0 0.0 1.0
CH3O2 2 481.8 3.626 0.0 0.0 1.0
CH3O 2 417.0 3.69 1.7 0.0 2.0
CH2OH 2 417.0 3.69 1.7 0.0 2.0
CH2O 2 498.0 3.59 0.0 0.0 2.0
HCO 2 498.0 3.59 0.0 0.0 0.0
HCOH 2 498.0 3.59 0.0 0.0 1.0
HO2CHO 2 436.0 3.97 0.0 0.0 2.0
O2CHO 2 436.0 3.97 0.0 0.0 2.0
HOCHO 2 436.0 3.97 0.0 0.0 2.0
OCHO 2 498.0 3.59 0.0 0.0 2.0
C2H6 2 247.5 4.35 0.0 0.0 1.5
C2H5 2 247.5 4.35 0.0 0.0 1.5
C2H4 2 238.4 3.496 0.0 0.0 1.5
C2H3 2 265.3 3.721 0.0 0.0 1.0
CHCHO 2 436.0 3.97 0.0 0.0 2.0
C2H2 1 265.3 3.721 0.0 0.0 2.5
```

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CH3CHO 2 436.0 3.97 0.0 0.0 2.0
CH2CHO 2 436.0 3.97 0.0 0.0 2.0
CH2CO 2 436.0 3.97 0.0 0.0 2.0
HCCO 2 150.0 2.5 0.0 0.0 1.0
C3H8 2 303.4 4.81 0.0 0.0 1.0
IC3H7 2 303.4 4.81 0.0 0.0 1.0
NC3H7 2 303.4 4.81 0.0 0.0 1.0
NC3H7O2 2 481.5 4.997 1.7 0.0 1.0
IC3H7O2 2 459.5 5.036 1.7 0.0 1.0
C3H6 2 307.8 4.14 0.0 0.0 1.0
C3H5-A 2 316.0 4.22 0.0 0.0 1.0
CH3CHCO 2 443.2 4.12 0.0 0.0 1.0
C3H6OH2-1 2 487.9 4.82 0.0 0.0 1.0
CH3COCH3 2 435.5 4.86 0.0 0.0 1.0
END

REACTIONS MOLES CAL/MOLE
H2+M=2H+M    4.577E19 -1.4 1.044E5
   H2/2.5/
   H2O/12.0/
   CO/1.9/
   CO2/3.8/
   HE/0.83/
   CH4/2.0/
   C2H6/3.0/
H2+O=H+OH    5.08E4 2.67 6.292E3
H2+OH=H+H2O    4.38E13 0.0 6.99E3
2O+M=O2+M    6.165E15 -0.5 0.0E0
   H2/2.5/
   H2O/12.0/
   AR/0.83/
   CO/1.9/
   CO2/3.8/
   HE/0.83/
   CH4/2.0/
   C2H6/3.0/
O2+H=O+OH    1.04E14 0.0 1.5286E4
H+OH+M=H2O+M    3.5E22 -2.0 0.0E0
   H2/0.73/
   H2O/3.65/
   CH4/2.0/
   C2H6/3.0/
   AR/0.38/
O+H2O=2OH    6.7E7 1.704 1.49868E4
O+H+M=OH+M    4.714E18 -1.0 0.0E0
   H2/2.5/
   H2O/12.0/
   AR/0.75/
   CO/1.5/
   CO2/2.0/
   HE/0.75/
   CH4/2.0/
   C2H6/3.0/
H+O+M=OHV+M    1.5E13 0.0 5.975E3
   H2/1.0/
   H2O/6.5/
   O2/0.4/
   N2/0.4/
   AR/0.35/
OHV+H2O=OH+H2O    5.93E12 0.5 -8.6E2
OHV+H2=OH+H2    2.95E12 0.5 -4.44E2
OHV+N2=OH+N2    1.08E11 0.5 -1.242E3
OHV+OH=2OH    6.01E12 0.5 -7.64E2
OHV+H=OH+H    1.31E12 0.5 -1.67E2
OHV+AR=OH+AR    1.69E12 0.0 4.135E3
OHV=OH    1.45E6 0.0 0.0E0
OHV+O2=OH+O2    2.1E12 0.5 -4.78E2
OHV+CO2=OH+CO2    2.75E12 0.5 -9.68E2
OHV+CO=OH+CO    3.23E12 0.5 -7.87E2
OHV+CH4=OH+CH4    3.36E12 0.5 -6.35E2
H2O2(+M)=2OH(+M)    2.0E12 0.9 4.8749E4
   H2O/7.65/
   CO2/1.6/
   N2/1.5/
   O2/1.2/
   HE/0.65/
   H2O2/7.7/
   H2/3.7/
   CO/2.8/
   LOW/2.49E24 -2.3E0 4.8749E4/
   TROE/4.3E-1 1.0E-30 1.0E30/
H2O2+H=H2O+OH    2.41E13 0.0 3.97E3
H2O2+H=H2+HO2    2.15E10 1.0 6.0E3
H2O2+O=OH+HO2    9.55E6 2.0 3.97E3
H2O2+OH=H2O+HO2    1.74E12 0.0 3.18E2
   DUP
H2O2+OH=H2O+HO2    7.59E13 0.0 7.269E3
   DUP
HO2+H=2OH    7.079E13 0.0 2.95E2
HO2+H=H2+O2    1.1402E10 1.0827 5.5378E2
HO2+O=OH+O2    3.25E13 0.0 0.0E0
HO2+OH=H2O+O2    2.456E13 0.0 -4.97E2
2HO2=H2O2+O2    1.0E14 0.0 1.1040883E4
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   DUP
2HO2=H2O2+O2    1.9E11 0.0 -1.4089248E3
   DUP
H+O2(+M)=HO2(+M)    4.65E12 0.44 0.0E0
   H2/1.3/
   CO/1.9/
   CO2/3.8/
   HE/0.64/
   H2O/10.0/
   AR/0.5/
   CH4/2.0/
   C2H6/3.0/
   LOW/1.737E19 -1.23E0 0.0E0/
   TROE/6.7E-1 1.0E-30 1.0E30 1.0E30/
CO+O(+M)=CO2(+M)    1.362E10 0.0 2.384E3
   H2/2.0/
   H2O/12.0/
   CO/1.75/
   CO2/3.6/
   AR/0.7/
   HE/0.7/
   LOW/1.173E24 -2.79E0 4.191E3/
CO+OH=CO2+H    7.015E4 2.053 -3.557E2
   DUP
CO+OH=CO2+H    5.757E12 -0.664 3.318E2
   DUP
CO+HO2=CO2+OH    1.57E5 2.18 1.794E4
CO+O2=CO2+O    1.119E12 0.0 4.77E4
H+CO2=OCHO    7.5E13 0.0 2.9E4
CH3+H(+M)=CH4(+M)    1.27E16 -0.63 3.83E2
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/2.477E33 -4.76E0 2.44E3/
   TROE/7.83E-1 7.4E1 2.941E3 6.964E3/
CH4+H=CH3+H2    6.14E5 2.5 9.587E3
CH4+O=CH3+OH    1.02E9 1.5 8.6E3
CH4+OH=CH3+H2O    5.83E4 2.6 2.19E3
CH4+HO2=CH3+H2O2    1.13E1 3.74 2.101E4
CH4+CH3O2=CH3+CH3O2H    9.6E-1 3.77 1.781E4
CH3+HO2=CH4+O2    1.16E5 2.23 -3.022E3
CH4+CH2=2CH3    2.46E6 2.0 8.27E3
CH2(S)+N2=CH2+N2    1.5E13 0.0 6.0E2
CH2(S)+AR=CH2+AR    9.0E12 0.0 6.0E2
CH2(S)+H2O=CH2+H2O    3.0E13 0.0 0.0E0
CH2(S)+CO=CH2+CO    9.0E12 0.0 0.0E0
CH2(S)+CO2=CH2+CO2    7.0E12 0.0 0.0E0
CH2(S)+O2=>H+OH+CO    2.8E13 0.0 0.0E0
CH2(S)+O2=CO+H2O    1.2E13 0.0 0.0E0
CH2(S)+O=CO+H2    1.5E13 0.0 0.0E0
CH2(S)+O=HCO+H    1.5E13 0.0 0.0E0
CH2(S)+H2=CH3+H    7.0E13 0.0 0.0E0
CH2(S)+H=CH+H2    3.0E13 0.0 0.0E0
CH2(S)+OH=CH2O+H    3.0E13 0.0 0.0E0
CH2(S)+CO2=CH2O+CO    1.4E13 0.0 0.0E0
CH2+H(+M)=CH3(+M)    2.5E16 -0.8 0.0E0
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/3.2E27 -3.14E0 1.23E3/
   TROE/6.8E-1 7.8E1 1.995E3 5.59E3/
CH2+O2=HCO+OH    1.06E13 0.0 1.5E3
CH2+O2=>CO2+2H    2.64E12 0.0 1.5E3
CH2+O=>CO+2H    5.0E13 0.0 0.0E0
CH2+H=CH+H2    3.0E13 0.0 0.0E0
CH2+OH=CH+H2O    1.13E7 2.0 3.0E3
CHV+AR=CH+AR    4.0E11 0.5 0.0E0
CHV+H2O=CH+H2O    5.3E13 0.0 0.0E0
CHV+CO=CH+CO    2.44E12 0.5 0.0E0
CHV+CO2=CH+CO2    2.41E-1 4.3 -1.694E3
CHV+O2=CH+O2    2.48E6 2.14 -1.72E3
CHV+H2=CH+H2    1.47E14 0.0 1.361E3
CHV+CH4=CH+CH4    1.73E13 0.0 1.67E2
CHV=CH    1.86E6 0.0 0.0E0
CHV+N2=CH+N2    3.03E2 3.4 -3.81E2
CH+O2=CO+OHV    4.04E13 0.0 0.0E0
CH+O2=HCO+O    3.3E13 0.0 0.0E0
CH+O=CO+H    5.7E13 0.0 0.0E0
CH+OH=HCO+H    3.0E13 0.0 0.0E0
CH+H2O=H+CH2O    1.774E16 -1.22 2.38E1
CH+CO2=HCO+CO    1.7E12 0.0 6.85E2
CH3+O2(+M)=CH3O2(+M)    7.812E9 0.9 0.0E0
   LOW/6.85E24 -3.0E0 0.0E0/
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    TROE/6.0E-1 1.0E3 7.0E1 1.7E3/
CH3+O2=CH3O+O    7.546E12 0.0 2.832E4
CH3+O2=CH2O+OH    2.641E0 3.283 8.105E3
CH3+O=CH2O+H    5.54E13 0.05 -1.36E2
CH3+OH=CH2(S)+H2O    4.936E14 -0.669 -4.458E2
    PLOG/1.0E-2 4.936E14 -6.69E-1 -4.458E2/
    PLOG/1.0E-1 1.207E15 -7.78E-1 -1.756E2/
    PLOG/1.0E0 5.282E17 -1.518E0 1.772E3/
    PLOG/1.0E1 4.788E23 -3.155E0 7.003E3/
    PLOG/1.0E2 8.433E19 -1.962E0 8.244E3/
CH3+OH=CH2O+H2    3.502E5 1.441 -3.244E3
    PLOG/1.0E-2 3.502E5 1.441E0 -3.244E3/
    PLOG/1.0E-1 8.854E5 1.327E0 -2.975E3/
    PLOG/1.0E0 1.65E7 9.73E-1 -2.01E3/
    PLOG/1.0E1 5.374E9 2.87E-1 2.8E2/
    PLOG/1.0E2 9.494E18 -2.199E0 9.769E3/
CH3+OH=CH2OH+H    1.621E10 0.965 3.21E3
    PLOG/1.0E-2 1.621E10 9.65E-1 3.214E3/
    PLOG/1.0E-1 1.807E10 9.5E-1 3.247E3/
    PLOG/1.0E0 4.686E10 8.33E-1 3.566E3/
    PLOG/1.0E1 1.525E13 1.34E-1 5.641E3/
    PLOG/1.0E2 3.59E14 -1.86E-1 8.601E3/
CH3+OH=H+CH3O    1.186E9 1.016 1.194E4
    PLOG/1.0E-2 1.186E9 1.016E0 1.194E4/
    PLOG/1.0E-1 1.188E9 1.016E0 1.194E4/
    PLOG/1.0E0 1.23E9 1.011E0 1.195E4/
    PLOG/1.0E1 1.798E9 9.65E-1 1.206E4/
    PLOG/1.0E2 5.242E10 5.51E-1 1.307E4/
CH3+OH=HCOH+H2    8.674E8 0.787 -3.046E3
    PLOG/1.0E-2 8.674E8 7.87E-1 -3.046E3/
    PLOG/1.0E-1 3.115E9 6.3E-1 -2.669E3/
    PLOG/1.0E0 1.557E11 1.56E-1 -1.368E3/
    PLOG/1.0E1 1.704E21 -2.641E0 6.412E3/
    PLOG/1.0E2 7.25E20 -2.402E0 9.639E3/
CH3+OH=CH2+H2O    4.293E4 2.568 3.9978E3
CH3+HO2=CH3O+OH    1.0E12 0.269 -6.875E2
CH3O2+O=CH3O+O2    3.6E13 0.0 0.0E0
CH3O2+H=CH3O+OH    9.6E13 0.0 0.0E0
CH3O2+HO2=CH3O2H+O2    2.47E11 0.0 -1.57E3
CH3O2+H2O2=CH3O2H+HO2    2.41E12 0.0 9.936E3
CH3O2+CH3=2CH3O    5.08E12 0.0 -1.411E3
2CH3O2=>O2+2CH3O    1.4E16 -1.61 1.86E3
H2+CH3O2=H+CH3O2H    1.5E14 0.0 2.603E4
CH3O2H=CH3O+OH    6.31E14 0.0 4.23E4
CH2OH+O2=CH2O+HO2    1.51E15 -1.0 0.0E0
    DUP
CH2OH+O2=CH2O+HO2    2.41E14 0.0 5.017E3
    DUP
CH2OH+H=CH2O+H2    6.0E12 0.0 0.0E0
CH2OH+HO2=CH2O+H2O2    1.2E13 0.0 0.0E0
CH2OH+HCO=2CH2O    1.8E14 0.0 0.0E0
CH2OH+OH=H2O+CH2O    2.4E13 0.0 0.0E0
CH2OH+O=OH+CH2O    4.2E13 0.0 0.0E0
CH3O+O2=CH2O+HO2    4.38E-19 9.5 -5.501E3
CH3O+H=CH2O+H2    2.0E13 0.0 0.0E0
CH3O+HO2=CH2O+H2O2    3.01E11 0.0 0.0E0
CH3O+CH3=CH2O+CH4    1.2E13 0.0 0.0E0
HCOH+O2=>CO2+H+OH    5.0E12 0.0 0.0E0
HCOH+O2=CO2+H2O    3.0E13 0.0 0.0E0
HCOH+O=>CO2+2H    5.0E13 0.0 0.0E0
HCOH+O=>CO+OH+H    3.0E13 0.0 0.0E0
HCOH+H=CH2O+H    2.0E14 0.0 0.0E0
HCOH+OH=HCO+H2O    2.0E13 0.0 0.0E0
HCO+H(+M)=CH2O(+M)    1.09E12 0.48 -2.6E2
    H2/2.0/
    H2O/6.0/
    AR/0.7/
    CO/1.5/
    CO2/2.0/
    CH4/2.0/
    C2H6/3.0/
    HE/0.7/
    LOW/1.35E24 -2.57E0 1.425E3/
    TROE/7.824E-1 2.71E2 2.755E3 6.57E3/
CO+H2(+M)=CH2O(+M)    4.3E7 1.5 7.96E4
    H2/2.0/
    H2O/6.0/
    AR/0.7/
    CO/1.5/
    CO2/2.0/
    CH4/2.0/
    C2H6/3.0/
    HE/0.7/
    LOW/5.07E27 -3.42E0 8.4348E4/
    TROE/9.32E-1 1.97E2 1.54E3 1.03E4/
CH2O+O2=HCO+HO2    8.07E15 0.0 5.342E4
CH2O+O=HCO+OH    6.26E9 1.15 2.26E3
CH2O+H=HCO+H2    5.74E7 1.9 2.74E3
CH2O+OH=HCO+H2O    7.82E7 1.63 -1.055E3
CH2O+HO2=HCO+H2O2    1.88E4 2.7 1.152E4
CH2O+CH3=HCO+CH4    3.83E1 3.36 4.312E3
CH2O+O2CHO=HCO+HO2CHO    1.99E12 0.0 1.166E4
CH2O+OCHO=HCO+HOCHO    5.6E12 0.0 1.36E4
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CH2O+CH3O2=HCO+CH3O2H    1.99E12 0.0 1.166E4
HCO+M=H+CO+M    5.7E11 0.66 1.487E4
   H2/2.0/
   H2O/6.0/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
HCO+O2=CO+HO2    7.58E12 0.0 4.1E2
HCO+O=CO+OH    3.02E13 0.0 0.0E0
HCO+H=CO+H2    7.34E13 0.0 0.0E0
HCO+OH=CO+H2O    3.011E13 0.0 0.0E0
HCO+CH3=CO+CH4    2.65E13 0.0 0.0E0
2HCO=CO+CH2O    1.8E13 0.0 0.0E0
HCO+O=CO2+H    3.0E13 0.0 0.0E0
HCO+HO2=>CO2+H+OH    3.0E13 0.0 0.0E0
2HCO=>H2+2CO    3.0E12 0.0 0.0E0
CH2O+H(+M)=CH2OH(+M)    5.4E11 0.454 3.6E3
   H2/2.0/
   H2O/6.0/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   LOW/1.27E32 -4.82E0 6.53E3/
   TROE/7.187E-1 1.03E2 1.291E3 4.16E3/
CH3O(+M)=CH2O+H(+M)    6.8E13 0.0 2.617E4
   H2/2.0/
   H2O/6.0/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   LOW/1.867E25 -3.0E0 2.4307E4/
   TROE/9.0E-1 2.5E3 1.3E3 1.0E99/
HCO+O2=O2CHO    1.2E11 0.0 -1.1E3
HOCHO=CO+H2O    2.45E12 0.0 6.047E4
HOCHO=CO2+H2    2.95E9 0.0 4.852E4
OCHO+HO2=HOCHO+O2    3.5E10 0.0 -3.275E3
OCHO+H2O2=HOCHO+HO2    2.4E12 0.0 1.0E4
HOCHO+H=>H2+CO2+H    4.24E6 2.1 4.868E3
HOCHO+H=>H2+CO+OH    6.03E13 -0.35 2.988E3
HOCHO+O=>CO+2OH    1.77E18 -1.9 2.975E3
HOCHO+OH=>H2O+CO2+H    2.62E6 2.06 9.16E2
HOCHO+OH=>H2O+CO+OH    1.85E7 1.51 -9.62E2
HOCHO+CH3=>CH4+CO+OH    3.9E-7 5.8 2.2E3
HOCHO+HO2=>H2O2+CO+OH    1.0E12 0.0 1.192E4
OCHO+OH=HO2CHO    2.0E13 0.0 0.0E0
2CH3(+M)=C2H6(+M)    2.277E15 -0.69 1.749E2
   H2O/5.0/
   CO/2.0/
   CO2/3.0/
   LOW/8.054E31 -3.75E0 9.816E2/
   TROE/0.0E0 5.7E2 1.0E30 1.0E30/
C2H5+H(+M)=C2H6(+M)    5.21E17 -0.99 1.58E3
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/1.99E41 -7.08E0 6.685E3/
   TROE/8.42E-1 1.25E2 2.219E3 6.882E3/
2CH3=H+C2H5    4.74E12 0.105 1.06643E4
   PLOG/1.0E-2 4.74E12 1.05E-1 1.06643E4/
   PLOG/1.0E-1 2.57E13 -9.6E-2 1.14061E4/
   PLOG/1.0E0 3.1E14 -3.62E-1 1.33725E4/
   PLOG/1.0E1 2.15E10 8.85E-1 1.35325E4/
   PLOG/1.0E2 1.032E2 3.23E0 1.12361E4/
C2H6+O2=C2H5+HO2    6.03E13 0.0 5.187E4
C2H6+O=C2H5+OH    3.55E6 2.4 5.83E3
C2H6+H=C2H5+H2    1.15E8 1.9 7.53E3
C2H6+OH=C2H5+H2O    1.48E7 1.9 9.5E2
C2H6+HO2=C2H5+H2O2    3.46E1 3.61 1.692E4
C2H6+CH=C2H5+CH2    1.1E14 0.0 -2.6E2
C2H6+CH2(S)=C2H5+CH3    1.2E14 0.0 0.0E0
C2H6+CH3=C2H5+CH4    5.55E-4 4.72 3.231E3
C2H6+CH3O2=C2H5+CH3O2H    1.94E1 3.64 1.71E4
C2H4+H(+M)=C2H5(+M)    9.569E8 1.463 1.355E3
   H2/2.0/
   H2O/6.0/
   CH4/2.0/
   CO/1.5/
   CO2/2.0/
   C2H6/3.0/
   AR/0.7/
   LOW/1.419E39 -6.642E0 5.769E3/
   TROE/-5.69E-1 2.99E2 -9.147E3 1.524E2/
C2H5+H=C2H4+H2    2.0E12 0.0 0.0E0
2C2H4=C2H5+C2H3    4.82E14 0.0 7.153E4
C2H5+CH3=CH4+C2H4    1.18E4 2.45 -2.921E3
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C2H5+O=CH3CHO+H    1.1E14 0.0 0.0E0
C2H5+O2=C2H4+HO2    2.094E9 0.49 -3.914E2
   PLOG/4.0E-2 2.094E9 4.9E-1 -3.914E2/
   PLOG/1.0E0 1.843E7 1.13E0 -7.206E2/
   PLOG/1.0E1 7.561E14 -1.01E0 4.749E3/
C2H5+O2=CH3CHO+OH    4.908E-6 4.76 2.543E2
   PLOG/4.0E-2 4.908E-6 4.76E0 2.543E2/
   PLOG/1.0E0 6.803E-2 3.57E0 2.643E3/
   PLOG/1.0E1 8.265E2 2.41E0 5.285E3/
C2H3+H(+M)=C2H4(+M)    6.08E12 0.27 2.8E2
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/1.4E30 -3.86E0 3.32E3/
   TROE/7.82E-1 2.075E2 2.663E3 6.095E3/
C2H4+O2=C2H3+HO2    4.22E13 0.0 5.76231E4
C2H4+H=C2H3+H2    5.07E7 1.93 1.295E4
C2H4+OH=C2H3+H2O    2.23E4 2.745 2.2155E3
C2H4+CH3O2=C2H3+CH3O2H    8.59E0 3.754 2.7132E4
C2H4+CH3=C2H3+CH4    9.76E2 2.947 1.5148E4
   DUP
C2H4+CH3=C2H3+CH4    8.13E-5 4.417 8.8358E3
   DUP
C2H4+O=CH3+HCO    7.453E6 1.88 1.83E2
C2H4+O=CH2CHO+H    6.098E6 1.88 1.83E2
CH+CH4=C2H4+H    6.0E13 0.0 0.0E0
CH2(S)+CH3=C2H4+H    2.0E13 0.0 0.0E0
C2H4+OH=CH3+CH2O    5.35E0 2.92 -1.7327E3
   PLOG/1.0E-2 5.35E0 2.92E0 -1.7327E3/
   PLOG/2.5E-2 3.19E1 2.71E0 -1.1723E3/
   PLOG/1.0E-1 5.55E2 2.36E0 -1.808E2/
   PLOG/1.0E0 1.78E5 1.68E0 2.0605E3/
   PLOG/1.0E1 2.37E9 5.6E-1 6.0067E3/
   PLOG/1.0E2 2.76E13 -5.0E-1 1.14551E4/
C2H4+OH=CH3CHO+H    2.37E-7 5.3 -2.0506E3
   PLOG/1.0E-2 2.37E-7 5.3E0 -2.0506E3/
   PLOG/2.5E-2 8.73E-5 4.57E0 -6.18E2/
   PLOG/1.0E-1 4.03E-1 3.54E0 1.8817E3/
   PLOG/1.0E0 2.38E-2 3.91E0 1.7227E3/
   PLOG/1.0E1 8.25E8 1.01E0 1.05073E4/
   PLOG/1.0E2 6.8E9 8.1E-1 1.38673E4/
C2H2+H(+M)=C2H3(+M)    1.71E10 1.266 2.709E3
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/6.346E31 -4.664E0 3.78E3/
   TROE/7.88E-1 -1.02E4 1.0E-30/
C2H3+O2=CHCHO+OH    2.84E14 -0.8 7.232E3
   DUP
   PLOG/1.0E-2 3.91E11 -1.1E-1 2.131E3/
   PLOG/1.0E-1 1.13E9 5.5E-1 4.6E1/
   PLOG/3.16E-1 8.46E8 5.6E-1 7.0E-1/
   PLOG/1.0E0 2.75E14 -1.83E0 4.6E0/
   PLOG/3.16E0 2.58E20 -2.84E0 7.53E3/
   PLOG/1.0E1 9.18E14 -2.26E0 -4.0E-1/
   PLOG/3.16E1 6.11E25 -4.21E0 1.305E4/
   PLOG/1.0E2 1.65E30 -5.35E0 1.843E4/
C2H3+O2=CHCHO+OH    2.84E14 -0.8 7.232E3
   DUP
   PLOG/1.0E-2 9.91E11 -6.6E-1 -6.0E-1/
   PLOG/1.0E-1 6.94E14 -1.16E0 4.542E3/
   PLOG/3.16E-1 2.79E13 -7.2E-1 3.479E3/
   PLOG/1.0E0 4.99E11 -1.4E-1 1.995E3/
   PLOG/3.16E0 2.35E10 2.3E-1 1.573E3/
   PLOG/1.0E1 1.7E14 -8.2E-1 4.45E3/
   PLOG/3.16E1 1.42E11 5.0E-2 3.774E3/
   PLOG/1.0E2 3.17E11 -2.0E-2 5.338E3/
C2H3+O2=CH2CHO+O    1.76E12 0.15 4.205E3
   DUP
   PLOG/1.0E-2 7.88E20 -2.67E0 6.742E3/
   PLOG/1.0E-1 7.72E20 -2.67E0 6.713E3/
   PLOG/3.16E-1 9.87E20 -2.7E0 6.724E3/
   PLOG/1.0E0 7.1E20 -2.65E0 6.489E3/
   PLOG/3.16E0 4.5E20 -2.53E0 6.406E3/
   PLOG/1.0E1 1.76E23 -3.22E0 8.697E3/
   PLOG/3.16E1 3.14E25 -3.77E0 1.153E4/
   PLOG/1.0E2 1.02E26 -3.8E0 1.391E4/
C2H3+O2=CH2CHO+O    1.76E12 0.15 4.205E3
   DUP
   PLOG/1.0E-2 1.36E10 6.2E-1 -2.776E2/
   PLOG/1.0E-1 1.42E10 6.2E-1 -2.477E2/
   PLOG/3.16E-1 1.66E10 6.0E-1 -1.625E2/
   PLOG/1.0E0 2.02E10 5.8E-1 3.84E1/
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   PLOG/3.16E0 9.75E9 6.7E-1 2.48E2/
   PLOG/1.0E1 7.34E9 7.2E-1 7.781E2/
   PLOG/3.16E1 1.57E9 9.2E-1 1.219E3/
   PLOG/1.0E2 7.85E7 1.28E0 1.401E3/
C2H3+O2=C2H2+HO2    6.49E6 1.5 5.218E3
   DUP
   PLOG/1.0E-2 1.08E7 1.28E0 3.322E3/
   PLOG/1.0E-1 7.75E6 1.33E0 3.216E3/
   PLOG/3.16E-1 1.21E7 1.27E0 3.311E3/
   PLOG/1.0E0 2.15E7 1.19E0 3.367E3/
   PLOG/3.16E0 1.13E8 1.0E0 3.695E3/
   PLOG/1.0E1 1.31E11 1.2E-1 5.872E3/
   PLOG/3.16E1 1.19E9 8.2E-1 5.617E3/
   PLOG/1.0E2 1.06E17 -1.45E0 1.223E4/
C2H3+O2=C2H2+HO2    6.49E6 1.5 5.218E3
   DUP
   PLOG/1.0E-2 4.76E1 2.75E0 -7.964E2/
   PLOG/1.0E-1 5.16E1 2.73E0 -7.683E2/
   PLOG/3.16E-1 5.55E1 2.73E0 -6.585E2/
   PLOG/1.0E0 4.6E1 2.76E0 -4.928E2/
   PLOG/3.16E0 3.75E0 3.07E0 -6.01E2/
   PLOG/1.0E1 5.48E0 3.07E0 8.57E1/
   PLOG/3.16E1 4.47E8 0.0E0 9.55E2/
   PLOG/1.0E2 2.02E1 2.94E0 1.847E3/
C2H3+O2=CH2CO+OH    1.17E3 2.43 7.074E3
   DUP
   PLOG/1.0E-2 8.66E2 2.41E0 6.061E3/
   PLOG/1.0E-1 8.91E2 2.41E0 6.078E3/
   PLOG/3.16E-1 9.43E2 2.4E0 6.112E3/
   PLOG/1.0E0 1.06E3 2.39E0 6.18E3/
   PLOG/3.16E0 1.09E3 2.38E0 6.179E3/
   PLOG/1.0E1 1.39E3 2.36E0 6.074E3/
   PLOG/3.16E1 2.49E6 1.42E0 8.48E3/
   PLOG/1.0E2 1.66E10 3.6E-1 1.201E4/
C2H3+O2=CH2CO+OH    1.17E3 2.43 7.074E3
   DUP
   PLOG/1.0E-2 1.82E-1 3.12E0 1.331E3/
   PLOG/1.0E-1 2.07E-1 3.11E0 1.383E3/
   PLOG/3.16E-1 2.71E-1 3.08E0 1.496E3/
   PLOG/1.0E0 5.26E-1 3.01E0 1.777E3/
   PLOG/3.16E0 1.37E0 2.9E0 2.225E3/
   PLOG/1.0E1 4.19E-1 2.93E0 2.052E3/
   PLOG/3.16E1 1.19E-4 4.21E0 2.043E3/
   PLOG/1.0E2 1.3E-3 3.97E0 3.414E3/
C2H3+O2=CH2O+HCO    1.16E16 -1.13 3.791E3
   DUP
   PLOG/1.0E-2 2.49E36 -7.6E0 1.264E4/
   PLOG/1.0E-1 2.43E36 -7.6E0 1.261E4/
   PLOG/3.16E-1 1.95E36 -7.57E0 1.249E4/
   PLOG/1.0E0 2.73E35 -7.32E0 1.182E4/
   PLOG/3.16E0 1.43E36 -7.47E0 1.246E4/
   PLOG/1.0E1 5.18E35 -7.2E0 1.343E4/
   PLOG/3.16E1 3.19E20 -2.57E0 5.578E3/
   PLOG/1.0E2 2.73E33 -6.28E0 1.6E4/
C2H3+O2=CH2O+HCO    1.16E16 -1.13 3.791E3
   DUP
   PLOG/1.0E-2 4.54E15 -1.28E0 5.153E2/
   PLOG/1.0E-1 4.59E15 -1.28E0 5.13E2/
   PLOG/3.16E-1 4.81E15 -1.29E0 5.206E2/
   PLOG/1.0E0 6.08E15 -1.31E0 6.457E2/
   PLOG/3.16E0 9.45E15 -1.36E0 1.066E3/
   PLOG/1.0E1 2.56E15 -1.18E0 1.429E3/
   PLOG/3.16E1 1.03E69 -1.923E1 1.476E4/
   PLOG/1.0E2 4.21E10 1.9E-1 8.306E2/
C2H3+O2=>CH2O+H+CO    1.16E16 -1.13 3.791E3
   DUP
   PLOG/1.0E-2 5.82E36 -7.6E0 1.264E4/
   PLOG/1.0E-1 5.66E36 -7.6E0 1.261E4/
   PLOG/3.16E-1 4.55E36 -7.57E0 1.249E4/
   PLOG/1.0E0 6.36E35 -7.32E0 1.182E4/
   PLOG/3.16E0 3.35E36 -7.47E0 1.246E4/
   PLOG/1.0E1 1.21E36 -7.2E0 1.343E4/
   PLOG/3.16E1 7.43E20 -2.57E0 5.578E3/
   PLOG/1.0E2 6.36E33 -6.28E0 1.6E4/
C2H3+O2=>CH2O+H+CO    1.16E16 -1.13 3.791E3
   DUP
   PLOG/1.0E-2 1.06E16 -1.28E0 5.153E2/
   PLOG/1.0E-1 1.07E16 -1.28E0 5.13E2/
   PLOG/3.16E-1 1.13E16 -1.29E0 5.206E2/
   PLOG/1.0E0 1.42E16 -1.31E0 6.457E2/
   PLOG/3.16E0 2.2E16 -1.36E0 1.066E3/
   PLOG/1.0E1 5.98E15 -1.18E0 1.429E3/
   PLOG/3.16E1 2.39E69 -1.923E1 1.476E4/
   PLOG/1.0E2 9.81E10 1.9E-1 8.306E2/
C2H3+O2=CO+CH3O    3.09E13 -0.89 3.682E3
   DUP
   PLOG/1.0E-2 8.19E18 -2.66E0 3.201E3/
   PLOG/1.0E-1 4.06E14 -1.32E0 8.858E2/
   PLOG/3.16E-1 4.34E14 -1.33E0 9.006E2/
   PLOG/1.0E0 1.03E11 -3.3E-1 -7.478E2/
   PLOG/3.16E0 1.89E12 -3.0E0 -8.995E3/
   PLOG/1.0E1 1.93E24 -5.63E0 1.8E0/
   PLOG/3.16E1 1.1E18 -2.22E0 5.178E3/
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   PLOG/1.0E2 5.79E32 -6.45E0 1.681E4/
C2H3+O2=CO+CH3O    3.09E13 -0.89 3.682E3
   DUP
   PLOG/1.0E-2 1.29E9 1.8E-1 -1.717E3/
   PLOG/1.0E-1 5.99E11 -2.93E0 -9.564E3/
   PLOG/3.16E-1 2.91E11 -2.93E0 -1.012E4/
   PLOG/1.0E0 5.77E21 -3.54E0 4.772E3/
   PLOG/3.16E0 4.99E15 -1.62E0 1.849E3/
   PLOG/1.0E1 9.33E16 -1.96E0 3.324E3/
   PLOG/3.16E1 1.02E72 -2.069E1 1.586E4/
   PLOG/1.0E2 1.1E9 3.1E-1 1.024E3/
C2H3+O2=CO2+CH3    6.16E13 -1.05 3.743E3
   DUP
   PLOG/1.0E-2 2.37E35 -7.76E0 1.263E4/
   PLOG/1.0E-1 1.73E35 -7.72E0 1.252E4/
   PLOG/3.16E-1 4.47E34 -7.55E0 1.214E4/
   PLOG/1.0E0 7.25E31 -6.7E0 1.044E4/
   PLOG/3.16E0 3.63E35 -7.75E0 1.283E4/
   PLOG/1.0E1 2.09E35 -7.53E0 1.405E4/
   PLOG/3.16E1 3.84E18 -2.44E0 5.408E3/
   PLOG/1.0E2 1.21E32 -6.32E0 1.619E4/
C2H3+O2=CO2+CH3    6.16E13 -1.05 3.743E3
   DUP
   PLOG/1.0E-2 6.27E13 -1.16E0 4.063E2/
   PLOG/1.0E-1 6.24E13 -1.16E0 4.014E2/
   PLOG/3.16E-1 6.12E13 -1.16E0 3.97E2/
   PLOG/1.0E0 5.32E13 -1.14E0 4.467E2/
   PLOG/3.16E0 1.45E14 -1.26E0 9.877E2/
   PLOG/1.0E1 5.02E13 -1.11E0 1.409E3/
   PLOG/3.16E1 1.4E70 -2.011E1 1.543E4/
   PLOG/1.0E2 9.21E8 2.5E-1 8.553E2/
C2H3+H=C2H2+H2    1.7E14 0.0 0.0E0
C2H3+OH=C2H2+H2O    3.011E13 0.0 0.0E0
C2H3+CH3=C2H2+CH4    3.92E11 0.0 0.0E0
2C2H3=C2H2+C2H4    9.6E11 0.0 0.0E0
C2H2+O=CH2+CO    7.395E8 1.28 2.472E3
C2H2+O=HCCO+H    2.958E9 1.28 2.472E3
C2H2+HO2=CH2CO+OH    6.03E9 0.0 7.949E3
C2H2+HCO=C2H3+CO    1.0E7 2.0 6.0E3
C2H2+OH=CH2CO+H    1.578E3 2.56 -8.445E2
   PLOG/1.0E-2 1.578E3 2.56E0 -8.445E2/
   PLOG/2.5E-2 1.518E4 2.28E0 -2.921E2/
   PLOG/1.0E-1 3.017E5 1.92E0 5.981E2/
   PLOG/1.0E0 7.528E6 1.55E0 2.106E3/
   PLOG/1.0E1 5.101E6 1.65E0 3.4E3/
   PLOG/1.0E2 1.457E4 2.45E0 4.477E3/
C2H2+OH=CH3+CO    4.757E5 1.68 -3.298E2
   PLOG/1.0E-2 4.757E5 1.68E0 -3.298E2/
   PLOG/2.5E-2 4.372E6 1.4E0 2.265E2/
   PLOG/1.0E-1 7.648E7 1.05E0 1.115E3/
   PLOG/1.0E0 1.277E9 7.3E-1 2.579E3/
   PLOG/1.0E1 4.312E8 9.2E-1 3.736E3/
   PLOG/1.0E2 8.25E5 1.77E0 4.697E3/
CH3CHO(+M)=CH3+HCO(+M)    2.45E22 -1.74 8.6355E4
   LOW/1.03E59 -1.13E1 9.59125E4/
   TROE/2.49E-3 7.181E2 6.089E0 3.78E3/
CH3CHO(+M)=CH4+CO(+M)    2.72E21 -1.74 8.6355E4
   LOW/1.144E58 -1.13E1 9.59125E4/
   TROE/2.49E-3 7.181E2 6.089E0 3.78E3/
CH3CHO+H=CH2CHO+H2    2.72E3 3.1 5.21E3
CH3CHO+OH=CH2CHO+H2O    1.72E5 2.4 8.15E2
CH3CHO+OH=CH3+HOCHO    3.0E15 -1.076 0.0E0
CH2CHO(+M)=CH2CO+H(+M)    1.43E15 -0.15 4.56E4
   LOW/6.0E29 -3.8E0 4.34239E4/
   TROE/9.85E-1 3.93E2 9.8E9 5.0E9/
CH2CHO(+M)=CH3+CO(+M)    2.93E12 0.29 4.03E4
   LOW/9.52E33 -5.07E0 4.13E4/
   TROE/7.13E-17 1.15E3 4.99E9 1.79E9/
CH2CHO+O2=CH2CO+HO2    1.88E5 2.37 2.373E4
   PLOG/1.0E-2 1.88E5 2.37E0 2.373E4/
   PLOG/1.0E-1 1.88E5 2.37E0 2.737E4/
   PLOG/1.0E0 2.51E5 2.33E0 2.38E4/
   PLOG/1.0E1 7.05E7 1.63E0 2.529E4/
CH2CHO+O2=>CH2O+CO+OH    2.68E17 -1.84 6.53E3
   PLOG/1.0E-2 2.68E17 -1.84E0 6.53E3/
   PLOG/1.0E-1 1.52E20 -2.58E0 8.98E3/
   PLOG/1.0E0 1.65E19 -2.22E0 1.034E4/
   PLOG/1.0E1 8.953E13 -6.0E-1 1.012E4/
CH2+CO(+M)=CH2CO(+M)    8.1E11 0.0 0.0E0
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/2.69E33 -5.11E0 7.095E3/
   TROE/5.907E-1 2.75E2 1.226E3 5.185E3/
CH2CO+H=HCCO+H2    1.401E15 -0.171 8.7832E3
CH2CO+O=HCCO+OH    1.0E13 0.0 8.0E3
CH2CO+OH=HCCO+H2O    1.0E13 0.0 2.0E3
CH2CO+H=CH3+CO    7.704E13 -0.171 4.1832E3
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CH+CH2O=H+CH2CO    9.46E13 0.0 -5.15E2
CH2CO+O=CH2+CO2    1.75E12 0.0 1.35E3
CH2CO+OH=CH2OH+CO    2.0E12 0.0 -1.01E3
CH2CO+CH2(S)=C2H4+CO    1.6E14 0.0 0.0E0
CH2CO+CH3=C2H5+CO    4.769E4 2.312 9.468E3
CH+CO+M=HCCO+M    7.57E22 -1.9 0.0E0
HCCO+OH=>H2+2CO    1.0E14 0.0 0.0E0
HCCO+O=>H+2CO    8.0E13 0.0 0.0E0
HCCO+CH=CO+C2H2    5.0E13 0.0 0.0E0
HCCO+H=CH2(S)+CO    1.0E14 0.0 0.0E0
HCCO+O2=>OH+2CO    1.91E11 -0.02 1.02E3
HCCO+O2=>CO2+CO+H    4.78E12 -0.142 1.15E3
C3H8(+M)=CH3+C2H5(+M)    1.29E37 -5.84 9.738E4
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/5.64E74 -1.574E1 9.8714E4/
   TROE/3.1E-1 5.0E1 3.0E3 9.0E3/
NC3H7+H=C3H8    1.0E14 0.0 0.0E0
IC3H7+H=C3H8    1.0E14 0.0 0.0E0
C3H8+IC3H7=NC3H7+C3H8    3.0E10 0.0 1.29E4
C3H8+O2=NC3H7+HO2    6.0E13 0.0 5.229E4
C3H8+H=NC3H7+H2    3.49E5 2.69 6.45E3
C3H8+O=NC3H7+OH    3.71E6 2.4 5.505E3
C3H8+OH=NC3H7+H2O    2.732E7 1.811 8.684E2
C3H8+HO2=NC3H7+H2O2    4.08E1 3.59 1.716E4
C3H8+CH3=NC3H7+CH4    9.04E-1 3.65 7.154E3
C3H8+C2H3=NC3H7+C2H4    1.0E11 0.0 1.04E4
C3H8+C2H5=NC3H7+C2H6    1.0E11 0.0 1.04E4
C3H8+C3H5-A=NC3H7+C3H6    7.94E11 0.0 2.05E4
C3H8+CH3O2=NC3H7+CH3O2H    1.386E0 3.97 1.828E4
C3H8+O2CHO=NC3H7+HO2CHO    5.52E4 2.55 1.648E4
C3H8+O2=IC3H7+HO2    2.0E13 0.0 4.964E4
C3H8+H=IC3H7+H2    1.3E6 2.4 4.471E3
C3H8+O=IC3H7+OH    5.49E5 2.5 3.14E3
C3H8+OH=IC3H7+H2O    9.1715E9 0.935 5.047E2
C3H8+HO2=IC3H7+H2O2    6.32E1 3.37 1.372E4
C3H8+CH3=IC3H7+CH4    6.4E4 2.17 7.52E3
C3H8+C2H3=IC3H7+C2H4    1.0E11 0.0 1.04E4
C3H8+C2H5=IC3H7+C2H6    1.0E11 0.0 1.04E4
C3H8+C3H5-A=IC3H7+C3H6    7.94E11 0.0 1.62E4
C3H8+CH3O2=IC3H7+CH3O2H    1.019E1 3.58 1.481E4
C3H8+O2CHO=IC3H7+HO2CHO    1.475E4 2.6 1.391E4
IC3H7+H=C2H5+CH3    2.0E13 0.0 0.0E0
IC3H7+OH=C3H6+H2O    2.41E13 0.0 0.0E0
IC3H7+O=CH3COCH3+H    4.818E13 0.0 0.0E0
IC3H7+O=CH3CHO+CH3    4.818E13 0.0 0.0E0
O2+NC3H7=HO2+C3H6    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 5.05E10 2.06E-2 5.01905E2/
   PLOG/1.0E-1 7.47E15 -1.45E0 4.1129E3/
   PLOG/1.0E0 1.18E19 -2.35E0 7.29953E3/
   PLOG/1.0E1 2.63E0 3.46E0 2.48117E3/
   PLOG/1.0E2 7.37E2 2.71E0 5.49647E3/
O2+IC3H7=HO2+C3H6    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 5.91E9 4.28E-1 -1.43857E3/
   PLOG/1.0E-1 1.6E14 -8.45E-1 1.42377E3/
   PLOG/1.0E0 4.05E18 -2.07E0 4.97147E3/
   PLOG/1.0E1 4.91E17 -1.66E0 6.96404E3/
   PLOG/1.0E2 9.84E7 1.34E0 5.37912E3/
O2+NC3H7=NC3H7O2    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 9.2E8 4.05E-1 -4.39865E3/
   PLOG/1.0E-1 1.45001E14 -9.84E-1 -1.7108E3/
   PLOG/1.0E0 2.09001E13 -4.99E-1 -9.38423E2/
   PLOG/1.0E1 1.15001E20 -2.42E0 2.45126E3/
   PLOG/1.0E2 2.07001E16 -1.3E0 8.03419E2/
O2+IC3H7=IC3H7O2    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 7.33E5 1.33E0 -6.34564E3/
   PLOG/1.0E-1 2.24E11 -1.05E-1 -3.69787E3/
   PLOG/1.0E0 1.54E18 -2.02E0 -4.98567E2/
   PLOG/1.0E1 6.74E27 -4.85E0 3.77982E3/
   PLOG/1.0E2 1.67E29 -5.15E0 5.03645E3/
NC3H7O2=HO2+C3H6    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 4.3E53 -1.4E1 3.9526E4/
   PLOG/1.0E-1 9.52E57 -1.5E1 4.26843E4/
   PLOG/1.0E0 6.9E33 -7.03E0 3.65435E4/
   PLOG/1.0E1 2.55E16 -1.22E0 3.24803E4/
   PLOG/1.0E2 2.26E32 -6.22E0 3.79482E4/
IC3H7O2=C3H6+HO2    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 1.61E75 -2.06E1 4.6203E4/
   PLOG/1.0E-1 1.72E66 -1.73E1 4.54589E4/
   PLOG/1.0E0 4.03E56 -1.4E1 4.40102E4/
   PLOG/1.0E1 1.29E40 -8.58E0 3.94186E4/
   PLOG/1.0E2 6.4E25 -4.02E0 3.49139E4/
CH2(S)+C2H4=C3H6    4.82E57 -14.3 1.71E4
   DUP
   PLOG/1.0E-2 4.82E57 -1.43E1 1.71E4/
   PLOG/1.0E-1 3.84E59 -1.44E1 1.84E4/
   PLOG/1.0E0 2.13E58 -1.35E1 2.04E4/
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   PLOG/1.0E1 8.48E52 -1.16E1 2.07E4/
   PLOG/1.0E2 6.07E47 -9.85E0 2.21E4/
CH2(S)+C2H4=C3H6    4.82E57 -14.3 1.71E4
   DUP
   PLOG/1.0E-2 1.15E45 -1.11E1 6.1452E3/
   PLOG/1.0E-1 1.83E45 -1.07E1 6.6385E3/
   PLOG/1.0E0 1.3E40 -8.77E0 5.8638E3/
   PLOG/1.0E1 2.27E32 -6.14E0 4.3179E3/
   PLOG/1.0E2 1.28E24 -3.49E0 2.5299E3/
CH2(S)+C2H4=C3H5-A+H    8.2E19 -2.06 1.15E3
   DUP
   PLOG/1.0E-2 8.2E19 -2.06E0 1.15E3/
   PLOG/1.0E-1 2.27E21 -2.44E0 2.65E3/
   PLOG/1.0E0 4.44E35 -6.55E0 1.39E4/
   PLOG/1.0E1 1.18E28 -4.09E0 1.4E4/
   PLOG/1.0E2 6.51E26 -3.58E0 1.89E4/
CH2(S)+C2H4=C3H5-A+H    8.2E19 -2.06 1.15E3
   DUP
   PLOG/1.0E-2 1.08E7 1.62E0 -3.1746E3/
   PLOG/1.0E-1 1.37E5 2.15E0 -3.7992E3/
   PLOG/1.0E0 3.89E14 -4.2E-1 1.2376E3/
   PLOG/1.0E1 2.45E10 6.7E-1 7.5093E2/
   PLOG/1.0E2 1.81E2 2.97E0 -7.4603E2/
CH2(S)+C2H4=C2H3+CH3    1.77E19 -1.94 6.79E3
   DUP
   PLOG/1.0E-2 1.77E19 -1.94E0 6.79E3/
   PLOG/1.0E-1 1.68E19 -1.8E0 4.31E3/
   PLOG/1.0E0 4.16E24 -3.19E0 9.76E3/
   PLOG/1.0E1 7.89E24 -3.07E0 1.39E4/
   PLOG/1.0E2 7.36E29 -4.28E0 2.38E4/
CH2(S)+C2H4=C2H3+CH3    1.77E19 -1.94 6.79E3
   DUP
   PLOG/1.0E-2 4.3E12 1.9E-1 -1.1041E2/
   PLOG/1.0E-1 2.26E11 5.4E-1 4.781E1/
   PLOG/1.0E0 4.92E9 1.02E0 5.9977E2/
   PLOG/1.0E1 1.47E8 1.33E0 1.2284E3/
   PLOG/1.0E2 8.11E10 5.5E-1 5.5065E3/
C2H3+CH3=C3H5-A+H    4.12E29 -4.95 8.0E3
   DUP
   PLOG/1.0E-2 4.12E29 -4.95E0 8.0E3/
   PLOG/1.0E-1 4.86E30 -5.03E0 1.13E4/
   PLOG/1.0E0 5.3E29 -4.57E0 1.44E4/
   PLOG/1.0E1 1.32E30 -4.54E0 1.93E4/
   PLOG/1.0E2 5.16E28 -4.03E0 2.38E4/
C2H3+CH3=C3H5-A+H    4.12E29 -4.95 8.0E3
   DUP
   PLOG/1.0E-2 5.73E15 -7.7E-1 1.1959E3/
   PLOG/1.0E-1 2.06E13 -7.4E-2 1.4287E3/
   PLOG/1.0E0 4.48E10 6.0E-1 1.4216E3/
   PLOG/1.0E1 4.1E6 1.71E0 1.0569E3/
   PLOG/1.0E2 1.37E-1 3.91E0 -3.5355E2/
C3H6=C2H3+CH3    1.88E78 -18.7 1.3E5
   DUP
   PLOG/1.0E-2 1.88E78 -1.87E1 1.3E5/
   PLOG/1.0E-1 8.73E76 -1.79E1 1.32E5/
   PLOG/1.0E0 5.8E75 -1.72E1 1.34E5/
   PLOG/1.0E1 8.12E71 -1.58E1 1.36E5/
   PLOG/1.0E2 2.15E64 -1.34E1 1.35E5/
C3H6=C2H3+CH3    1.88E78 -18.7 1.3E5
   DUP
   PLOG/1.0E-2 1.69E59 -1.36E1 1.1329E5/
   PLOG/1.0E-1 2.0E60 -1.37E1 1.1489E5/
   PLOG/1.0E0 6.7E54 -1.18E1 1.1384E5/
   PLOG/1.0E1 1.06E47 -9.27E0 1.1151E5/
   PLOG/1.0E2 7.29E38 -6.7E0 1.0874E5/
C3H6=C3H5-A+H    9.16E74 -17.6 1.2E5
   DUP
   PLOG/1.0E-2 9.16E74 -1.76E1 1.2E5/
   PLOG/1.0E-1 1.73E70 -1.6E1 1.2E5/
   PLOG/1.0E0 1.08E71 -1.59E1 1.2486E5/
   PLOG/1.0E1 6.4E65 -1.42E1 1.25E5/
   PLOG/1.0E2 8.05E56 -1.15E1 1.22E5/
C3H6=C3H5-A+H    9.16E74 -17.6 1.2E5
   DUP
   PLOG/1.0E-2 2.98E54 -1.23E1 1.012E5/
   PLOG/1.0E-1 1.37E43 -8.87E0 9.6365E4/
   PLOG/1.0E0 6.28E42 -8.51E0 9.8004E4/
   PLOG/1.0E1 4.73E35 -6.26E0 9.5644E4/
   PLOG/1.0E2 4.34E28 -4.06E0 9.3114E4/
C3H6+H=C3H5-A+H2    3.644E5 2.455 4.3612E3
C3H6+O2=C3H5-A+HO2    5.96E19 -1.67 4.61921E4
C3H6+O=C3H5-A+OH    5.24E11 0.7 5.884E3
C3H6+OH=C3H5-A+H2O    4.46E6 2.072 1.0508E3
C3H6+HO2=C3H5-A+H2O2    3.07E-2 4.403 1.35472E4
C3H6+CH3=C3H5-A+CH4    2.21E0 3.5 5.675E3
C3H6+CH3O2=C3H5-A+CH3O2H    7.68E-2 4.403 1.35472E4
C3H6+C2H5=C3H5-A+C2H6    1.0E11 0.0 9.8E3
C3H6+O=C2H4+CH2O    2.11E12 0.36357832 3.6251147E3
   PLOG/1.0E-1 3.239515E10 8.6277366E-1 2.1012156E3/
   PLOG/1.0E0 3.7102143E10 8.4675413E-1 2.152084E3/
   PLOG/1.0E1 6.4621495E10 7.7988106E-1 2.3372114E3/
   PLOG/3.0E1 1.79581E11 6.5836787E-1 2.7279312E3/
   PLOG/1.0E2 2.11E12 3.6357832E-1 3.6251147E3/
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C3H6+O=C2H5+HCO    4.5392427E9 0.46990082 3.3909714E3
   PLOG/1.0E-1 3.81938E20 -2.8445151E0 2.2008093E3/
   PLOG/1.0E0 6.782E23 -3.7431204E0 5.0411938E3/
   PLOG/1.0E1 5.78554E21 -3.0582581E0 6.6882314E3/
   PLOG/3.0E1 4.41563E16 -1.5513902E0 5.3826196E3/
   PLOG/1.0E2 4.5392427E9 4.6990082E-1 3.3909714E3/
C3H6+O=CH3+CH2CHO    6.118106E10 0.72471172 1.7372183E3
   PLOG/1.0E-1 7.1169661E8 1.2452729E0 -2.2913843E2/
   PLOG/1.0E0 2.7972334E9 1.0825886E0 2.8259222E2/
   PLOG/1.0E1 1.8003295E10 8.6375535E-1 1.0689554E3/
   PLOG/3.0E1 3.3952128E10 7.9012293E-1 1.3842371E3/
   PLOG/1.0E2 6.118106E10 7.2471172E-1 1.7372183E3/
C3H6+O=H2+CH3CHCO    2.92162E11 -0.46592912 -7.2082123E2
   PLOG/1.0E-1 4.34829E14 -1.3823626E0 3.2638251E2/
   PLOG/1.0E0 5.03596E17 -2.2524612E0 2.2980547E3/
   PLOG/1.0E1 1.88555E14 -1.2406751E0 9.8652802E2/
   PLOG/3.0E1 1.45046E14 -1.2325199E0 8.0590204E2/
   PLOG/1.0E2 2.92162E11 -4.6592912E-1 -7.2082123E2/
C3H6+O=CO+C2H6    2.8063963E10 -0.15197791 8.5133477E3
   PLOG/1.0E-1 3.30559E19 -3.0550032E0 4.0607322E3/
   PLOG/1.0E0 4.47648E13 -1.2992022E0 2.5097214E3/
   PLOG/1.0E1 7.29311E16 -2.0833492E0 7.7710391E3/
   PLOG/3.0E1 2.2306699E1 2.136199E0 -3.9348716E3/
   PLOG/1.0E2 2.8063963E10 -1.5197791E-1 8.5133477E3/
C3H6+O=H2+C2H4+CO    1.9064245E5 1.4148871 1.8470398E3
   PLOG/1.0E-1 1.40605E19 -2.7684405E0 1.5882145E3/
   PLOG/1.0E0 1.42188E22 -3.5758173E0 4.455772E3/
   PLOG/1.0E1 4.5976E19 -2.7595153E0 6.0180806E3/
   PLOG/3.0E1 5.57149E13 -1.0280579E0 4.2239531E3/
   PLOG/1.0E2 1.9064245E5 1.4148871E0 1.8470398E3/
C3H6+H=NC3H7    1.0E0 1.0 0.0E0
   DUP
   PLOG/1.3E-3 7.99E81 -2.3161E1 2.2239E4/
   PLOG/4.0E-2 4.24E68 -1.8427E1 1.9665E4/
   PLOG/1.0E0 1.04E49 -1.15E1 1.5359E4/
   PLOG/1.0E1 6.2E41 -8.892E0 1.4637E4/
   PLOG/1.0E2 4.22E27 -4.39E0 9.3458E3/
C3H6+H=NC3H7    1.0E0 1.0 0.0E0
   DUP
   PLOG/1.3E-3 1.85E26 -5.83E0 3.8658E3/
   PLOG/4.0E-2 2.82E30 -6.49E0 5.4708E3/
   PLOG/1.0E0 3.78E28 -5.57E0 5.6251E3/
   PLOG/1.0E1 1.46E25 -4.28E0 5.2478E3/
   PLOG/1.0E2 1.0E-10 0.0E0 0.0E0/
C3H6+H=C2H4+CH3    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.3E-3 1.54E9 1.35E0 2.542E3/
   PLOG/4.0E-2 7.88E10 8.7E-1 3.5996E3/
   PLOG/1.0E0 2.67E12 4.7E-1 5.4311E3/
   PLOG/1.0E1 9.25E22 -2.6E0 1.2898E4/
   PLOG/1.0E2 1.32E23 -2.42E0 1.65E4/
C3H6+H=C2H4+CH3    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.3E-3 1.0E-10 0.0E0 0.0E0/
   PLOG/4.0E-2 1.0E-10 0.0E0 0.0E0/
   PLOG/1.0E0 1.0E-10 0.0E0 0.0E0/
   PLOG/1.0E1 1.24E5 2.52E0 3.6791E3/
   PLOG/1.0E2 2.51E3 2.91E0 3.9809E3/
C3H6+H=IC3H7    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.3E-3 1.35E44 -1.068E1 8.1964E3/
   PLOG/4.0E-2 2.11E57 -1.423E1 1.5147E4/
   PLOG/1.0E0 3.26E61 -1.494E1 2.0161E4/
   PLOG/1.0E1 5.3E56 -1.312E1 2.0667E4/
   PLOG/1.0E2 1.11E50 -1.08E1 2.0202E4/
C3H6+H=IC3H7    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.3E-3 2.17E130 -3.258E1 1.3614E5/
   PLOG/4.0E-2 2.25E29 -5.84E0 4.2419E3/
   PLOG/1.0E0 1.06E30 -5.63E0 5.6134E3/
   PLOG/1.0E1 6.11E26 -4.44E0 5.1823E3/
   PLOG/1.0E2 2.73E23 -3.26E0 4.597E3/
C2H4+CH3=NC3H7    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.3E-3 8.67E48 -1.254E1 1.8206E4/
   PLOG/4.0E-2 1.06E49 -1.204E1 2.0001E4/
   PLOG/1.0E0 7.67E47 -1.117E1 2.2366E4/
   PLOG/1.0E1 1.81E45 -1.003E1 2.3769E4/
   PLOG/1.0E2 2.04E40 -8.25E0 2.4214E4/
C2H4+CH3=NC3H7    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.3E-3 1.12E43 -1.13E1 1.308E4/
   PLOG/4.0E-2 7.28E39 -9.88E0 1.3164E4/
   PLOG/1.0E0 2.6E33 -7.46E0 1.2416E4/
   PLOG/1.0E1 3.85E27 -5.38E0 1.1455E4/
   PLOG/1.0E2 1.66E21 -3.17E0 1.0241E4/
C3H5-A+C2H5=C2H4+C3H6    4.0E11 0.0 0.0E0
C3H5-A+HCO=C3H6+CO    6.0E13 0.0 0.0E0
C2H3+CH2O=C2H4+HCO    1.0E11 0.0 0.0E0
   PLOG/1.0E-3 1.11E7 1.09E0 1.8072E3/
   PLOG/1.0E-2 2.47E7 9.93E-1 1.9949E3/
   PLOG/1.0E-1 2.47E8 7.04E-1 2.5962E3/
   PLOG/1.0E0 1.42E10 2.09E-1 3.9342E3/
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   PLOG/1.0E1 3.45E13 -7.26E-1 6.9443E3/
   PLOG/1.0E2 3.31E14 -8.66E-1 1.09657E4/
   PLOG/1.0E3 1.65E1 3.17E0 9.3998E3/
C3H6+OH=CH3CHO+CH3    6.93E5 1.49 -5.36E2
   PLOG/1.3E-3 6.93E5 1.49E0 -5.36E2/
   PLOG/1.0E-2 5.94E3 2.01E0 -5.6E2/
   PLOG/1.3E-2 1.1E3 2.22E0 -6.8E2/
   PLOG/2.5E-2 1.07E2 2.5E0 -7.59E2/
   PLOG/1.0E-1 7.83E-1 3.1E0 -9.19E2/
   PLOG/1.315E-1 3.07E-1 3.22E0 -9.46E2/
   PLOG/1.0E0 3.16E-4 4.05E0 -1.144E3/
   PLOG/1.0E1 7.59E-6 4.49E0 -6.8E2/
   PLOG/1.0E2 5.45E-5 4.22E0 1.141E3/
C3H6+OH=C3H6OH2-1    5.1E54 -20.7 3.2402E4
   DUP
   PLOG/1.3E-3 2.14E59 -1.584E1 1.1594E4/
   PLOG/1.0E-2 2.43E59 -1.551E1 1.2898E4/
   PLOG/1.3E-2 9.3E58 -1.534E1 1.2913E4/
   PLOG/2.5E-2 8.83E57 -1.493E1 1.2936E4/
   PLOG/1.0E-1 4.5E55 -1.404E1 1.2945E4/
   PLOG/1.315E-1 1.33E55 -1.385E1 1.2887E4/
   PLOG/1.0E0 5.18E49 -1.204E1 1.1493E4/
   PLOG/1.0E1 2.14E41 -9.35E0 8.921E3/
   PLOG/1.0E2 7.65E31 -6.31E0 6.088E3/
C3H6+OH=C3H6OH2-1    5.1E54 -20.7 3.2402E4
   DUP
   PLOG/1.3E-3 7.68E77 -2.07E1 3.2402E4/
   PLOG/1.0E-2 9.13E76 -2.0E1 3.3874E4/
   PLOG/1.3E-2 3.55E75 -1.958E1 3.2874E4/
   PLOG/2.5E-2 1.23E73 -1.879E1 3.1361E4/
   PLOG/1.0E-1 3.45E67 -1.701E1 2.7909E4/
   PLOG/1.315E-1 2.41E66 -1.664E1 2.7162E4/
   PLOG/1.0E0 6.5E58 -1.417E1 2.3079E4/
   PLOG/1.0E1 2.53E53 -1.223E1 2.2976E4/
   PLOG/1.0E2 4.78E47 -1.023E1 2.3772E4/
C2H2+CH3=C3H5-A    8.2E53 -13.32 3.32E4
   PLOG/1.0E-1 8.2E53 -1.332E1 3.32E4/
   PLOG/1.0E0 2.68E53 -1.282E1 3.573E4/
   PLOG/2.0E0 3.64E52 -1.246E1 3.6127E4/
   PLOG/5.0E0 1.04E51 -1.189E1 3.6476E4/
   PLOG/1.0E1 4.4E49 -1.14E1 3.67E4/
   PLOG/1.0E2 3.8E44 -9.63E0 3.76E4/
CH3CHCO+OH=C2H5+CO2    1.73E12 0.0 -1.01E3
CH3CHCO+H=C2H5+CO    4.4E12 0.0 1.459E3
CH3CHCO+O=CH3CHO+CO    3.2E12 0.0 -4.37E2
CH3COCH3+H=C3H6OH2-1    8.0E12 0.0 9.5E3
C3H6OH2-1+O2=CH3COCH3+HO2    1.5E12 0.0 5.0E3
END
```

APPENDIX E

ARIES 67 Mechanism

```
ELEMENTS
C H N O AR
HE
END
SPECIES
AR N2 HE H2 H
O2 O H2O OH OHV
H2O2 HO2 CO CO2 CH4
CH3 CH2 CH2(S) CH CHV
CH3O2H CH3O2 CH3O CH2OH CH2O
HCO HCOH HO2CHO O2CHO HOCHO
OCHO C2H6 C2H5 C2H5O2 C2H4
C2H3 CHCHO C2H2 C2H CH3CHO
CH3CO CH2CHO O2CH2CHO HO2CH2CO CH2CO
HCCO C3H8 IC3H7 NC3H7 NC3H7O2
IC3H7O2H IC3H7O2 C3H6OOH1-2 C3H6OOH1-3 C3H6OOH1-3O2
C3KET13 C3H6 C3H5-A C3H5-T CH3CHCO
C3H4-A C3H3 C3H6OH2-1 CH3COCH3 C2H3CHO
IC3H6CO C5H81-3
END

THERMO ALL
   300.000  1000.000  5000.000
AR               G-5-97AR  1               G     200.0    6000.0  1000.0      1
        2.5E0         0.0E0         0.0E0         0.0E0         0.0E0    2
    -7.45375E2   4.37967491E0         2.5E0         0.0E0         0.0E0    3
        0.0E0         0.0E0    -7.45375E2   4.37967491E0                   4
N2               G-8-02N   2               G     200.0    6000.0  1000.0      1
   2.95257637E0   1.3969004E-3 -4.92631603E-7 7.86010195E-11-4.60755204E-15    2
  -9.23948688E2   5.87188762E0   3.53100528E0 -1.23660988E-4 -5.02999433E-7    3
   2.43530612E-9-1.40881235E-12  -1.04697628E3   2.96747038E0                   4
HE               G-5-97HE  1               G     200.0    6000.0  1000.0      1
        2.5E0         0.0E0         0.0E0         0.0E0         0.0E0    2
    -7.45375E2   9.28723974E-1         2.5E0         0.0E0         0.0E0    3
        0.0E0         0.0E0    -7.45375E2   9.28723974E-1                   4
H2               TPIS78H   2               G     200.0    6000.0  1000.0      1
   2.93286575E0  8.26608026E-4 -1.46402364E-7 1.54100414E-11  -6.888048E-16    2
  -8.13065581E2  -1.02432865E0   2.34433112E0  7.98052075E-3  -1.9478151E-5    3
   2.01572094E-8-7.37611761E-12  -9.17935173E2  6.83010238E-1                   4
H                L-6-94H   1               G     200.0    6000.0  1000.0      1
        2.5E0         0.0E0         0.0E0         0.0E0         0.0E0    2
     2.547366E4  -4.4668285E-1         2.5E0         0.0E0         0.0E0    3
        0.0E0         0.0E0    2.547366E4  -4.4668285E-1                   4
O2               RUS-89O   2               G     200.0    6000.0  1000.0      1
   3.66096065E0  6.56365811E-4 -1.41149627E-7 2.05797935E-11-1.29913436E-15    2
  -1.21597718E3   3.41536279E0   3.78245636E0 -2.99673416E-3  9.84730201E-6    3
  -9.68129509E-9 3.24372837E-12  -1.06394356E3   3.65767573E0                   4
O                L-1-90O   1               G     200.0    6000.0  1000.0      1
   2.54363697E0 -2.73162486E-5  -4.1902952E-9 4.95481845E-12-4.79553694E-16    2
    2.9226012E4   4.92229457E0   3.1682671E0 -3.27931884E-3  6.64306396E-6    3
  -6.12806624E-9 2.11265971E-12   2.91222592E4   2.05193346E0                   4
H2O              L-5-89H   2O  1               G     200.0    6000.0  1000.0      1
    2.6770389E0   2.9731816E-3  -7.7376889E-7  9.4433514E-11 -4.2689991E-15    2
   -2.9885894E4      6.88255E0   4.1986352E0  -2.0364017E-3   6.5203416E-6    3
   -5.4879269E-9   1.771968E-12   -3.0293726E4  -8.4900901E-1                   4
OH               IU3-03H   1O  1               G     200.0    6000.0  1000.0      1
   2.83853033E0  1.10741289E-3 -2.94000209E-7 4.20698729E-11 -2.4228989E-15    2
   3.69780808E3   5.84494652E0   3.99198424E0 -2.40106655E-3  4.61664033E-6    3
  -3.87916306E-9 1.36319502E-12   3.36889836E3 -1.03998477E-1                   4
!UB REFIT 13-11-2018
OHV              -THERMH   1O  1               G     300.0    5000.0  1710.0      1
    2.8537604E0  1.02994334E-3 -2.32666477E-7 1.93750704E-11-3.15759847E-16    2
   5.03225473E4   5.76240468E0   3.41896226E0  3.19255801E-4 -3.08292717E-7    3
 3.64407494E-10-1.00195479E-13   5.00756946E4   2.51917016E0                   4
H2O2             T-8-03H   2O  2               G     200.0    6000.0  1000.0      1
   4.57977305E0  4.05326003E-3  -1.2984473E-6   1.982114E-10-1.13968792E-14    2
  -1.80071775E4  6.64970694E-1   4.31515149E0 -8.47390622E-4  1.76404323E-5    3
  -2.26762944E-8 9.08950158E-12  -1.77067437E4   3.27373319E0                   4
HO2              T-1-09H   1O  2               G     200.0    5000.0  1000.0      1
   4.17228741E0  1.88117627E-3 -3.46277286E-7 1.94657549E-11 1.76256905E-16    2
   3.10206839E1   2.95767672E0   4.30179807E0 -4.74912097E-3  2.11582905E-5    3
  -2.42763914E-8 9.29225225E-12   2.64018485E2   3.7166622E0                   4
CO               RUS-79O   1C  1               G     200.0    6000.0  1000.0      1
    3.0484859E0   1.3517281E-3  -4.8579405E-7  7.8853644E-11 -4.6980746E-15    2
   -1.4266117E4   6.0170977E0   3.5795335E0  -6.1035369E-4   1.0168143E-6    3
  9.0700586E-10 -9.0442449E-13   -1.4344086E4   3.5084093E0                   4
CO2              L-7-88O   2C  1               G     200.0    6000.0  1000.0      1
    4.6365111E0   2.7414569E-3  -9.9589759E-7  1.6038666E-10 -9.1619857E-15    2
   -4.9024904E4   -1.9348955E0   2.356813E0   8.9841299E-3  -7.1220632E-6    3
   2.4573008E-9 -1.4288548E-13   -4.8371971E4   9.9009035E0                   4
CH4              G-8-99H   4C  1               G     200.0    6000.0  1000.0      1
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  1.65326226E0  1.00263099E-2 -3.31661238E-6 5.36483138E-10-3.14696758E-14    2
 -1.00095936E4  9.90506283E0   5.14911468E0 -1.36622009E-2  4.91453921E-5    3
 -4.84246767E-8 1.66603441E-11  -1.02465983E4  -4.63848842E0                  4
CH3             IU0702H   3C   1         G     200.0    6000.0  1000.0      1
   2.9781206E0    5.797852E-3    -1.97558E-6   3.072979E-10 -1.7917416E-14    2
   1.6509513E4    4.7224799E0    3.6571797E0   2.1265979E-3   5.4583883E-6    3
 -6.6181003E-9  2.4657074E-12    1.6422716E4   1.6735354E0                    4
CH2             IU3-03H   2C   1         G     200.0    6000.0  1000.0      1
  3.14631886E0  3.03671259E-3 -9.96474439E-7  1.5048358E-10-8.57335515E-15    2
  4.60412605E4  4.72341711E0   3.71757846E0   1.2739126E-3  2.17347251E-6    3
 -3.488585E-9  1.65208866E-12   4.58723866E4   1.75297945E0                  4
CH2(S)          IU6-03H   2C   1         G     200.0    6000.0  1000.0      1
  3.13501686E0  2.89593926E-3  -8.1666809E-7 1.13572697E-10-6.36262835E-15    2
  5.05040504E4  4.06030621E0   4.19331325E0 -2.33105184E-3  8.15676451E-6    3
 -6.62985981E-9 1.93233199E-12   5.03662246E4  -7.4673431E-1                  4
CH              IU3-03H   1C   1         G     200.0    6000.0  1000.0      1
   2.5209369E0   1.7653639E-3   -4.614766E-7  5.9289675E-11 -3.3474501E-15    2
   7.0946769E4   7.4051829E0    3.4897583E0   3.243216E-4  -1.6899751E-6    3
   3.162842E-9 -1.4061803E-12    7.0612646E4   2.0842841E0                  4
!UB REFIT 13-11-2018
CHV             -THERMH   1C   1         G     300.0    5000.0  1365.0      1
  2.21703785E0  2.15314038E-3 -5.71569209E-7 6.54441183E-11-2.66374894E-15    2
  1.04414085E5  9.18247549E0   3.50775836E0 -4.57470019E-4  1.32602633E-6    3
 -5.1421376E-10 5.82219975E-14   1.03920991E5   2.09911232E0                  4
CH3O2H          A-7-05H   4O   2C   1    G     200.0    6000.0  1000.0      1
  7.76538058E0  8.61499712E-3 -2.98006935E-6 4.68638071E-10-2.75339255E-14    2
 -1.82979984E4  -1.43992663E1   2.90540897E0  1.74994735E-2   5.2824363E-6    3
 -2.52827275E-8 1.34368212E-11  -1.68894632E4   1.13741987E1                  4
CH3O2             H   3O   2C   1    G     300.0    5000.0  1374.0      1
  6.47970487E0   7.4440108E-3 -2.52348555E-6 3.89577296E-10-2.25182399E-14    2
 -1.56285441E3  -8.19477074E0   1.97339205E0  1.5354234E-2 -6.37314891E-6    3
 3.19930565E-10 2.82193915E-13   2.54278835E2   1.69194215E1                  4
CH3O            IU1-03H   3O   1C   1    G     200.0    6000.0  1000.0      1
  4.75779238E0  7.44142474E-3 -2.69705176E-6 4.38090504E-10-2.63537098E-14    2
   3.7811194E2  -1.96680028E0   3.71180502E0 -2.80463306E-3  3.76550971E-5    3
 -4.73072089E-8  1.8658842E-11    1.2956976E3   6.57240864E0                  4
CH2OH           IU2-03H   3O   1C   1    G     200.0    6000.0  1000.0      1
   5.0931437E0   5.9476126E-3  -2.0649746E-6 3.23008173E-10-1.88125902E-14    2
  -4.0340964E3  -1.84691493E0   4.47834367E0  -1.3507031E-3   2.7848498E-5    3
  -3.6486906E-8  1.4790745E-11   -3.5007289E3    3.309135E0                  4
CH2O            T-5-11H   2O   1C   1    G     200.0    6000.0  1000.0      1
  3.16952665E0   6.1932056E-3 -2.25056366E-6  3.6597566E-10-2.20149458E-14    2
 -1.45486831E4   6.04207898E0   4.79372312E0 -9.90833322E-3   3.7321999E-5    3
 -3.79285237E-8 1.31772641E-11  -1.43791953E4  6.02798058E-1                  4
HCO             T-5-03H   1O   1C   1    G     200.0    6000.0  1000.0      1
  3.92001542E0  2.52279324E-3 -6.71004164E-7 1.05615948E-10-7.43798261E-15    2
  3.65342928E3   3.58077056E0    4.2375461E0 -3.32075257E-3  1.40030264E-5    3
 -1.34239995E-8 4.37416208E-12   3.87241185E3   3.30834869E0                  4
HCOH            -MAR94H   2O   1C   1    G     300.0    5000.0  1398.0      1
  9.18749272E0  1.52011152E-3 -6.27603516E-7 1.09727989E-10-6.89655128E-15    2
  7.81364593E3  -2.73434214E1  -2.82157421E0  3.57331702E-2  -3.8086158E-5    3
 1.86205951E-8-3.45957838E-12   1.12956672E4   3.48487757E1                  4
HO2CHO          -THERMH   2O   3C   1    G     300.0    5000.0  1378.0      1
  9.87503878E0  4.64663708E-3 -1.67230522E-6 2.68624413E-10-1.59595232E-14    2
 -3.80502496E4  -2.24939155E1   2.42464726E0  2.1970638E-2 -1.68705546E-5    3
 6.25612194E-9-9.11645843E-13  -3.54828006E4   1.75027796E1                  4
O2CHO           -THERMH   1O   3C   1    G     300.0    5000.0  1368.0      1
  7.24075139E0  4.63312951E-3 -1.63693995E-6 2.59706693E-10-1.52964699E-14    2
 -1.87027618E4  -6.49547212E0   3.96059309E0  1.06002279E-2 -5.25713351E-6    3
  1.01716726E-9-2.87487602E-14  -1.73599383E4   1.17807483E1                  4
HOCHO           L-8-88H   2O   2C   1    G     200.0    6000.0  1000.0      1
   4.6138316E0   6.4496364E-3  -2.2908251E-6  3.6716047E-10 -2.1873675E-14    2
   -4.751485E4   8.4788383E-1    3.8983616E0  -3.5587795E-3   3.5520538E-5    3
  -4.3849959E-8  1.7107769E-11   -4.6770609E4   7.3495397E0                  4
OCHO            ATCT-AH   1O   2C   1    G     200.0    6000.0  1000.0      1
  4.14394211E0  5.59738818E-3 -1.99794019E-6 3.16179193E-10-1.85614483E-14    2
 -1.72459887E4  5.07778617E0   4.68825921E0 -4.14871834E-3   2.5506601E-5    3
  -2.844739E-8  1.04422559E-11  -1.69867041E4   4.2842648E0                  4
C2H6            G-8-88H   6C   2         G     200.0    6000.0  1000.0      1
  4.04666411E0  1.53538802E-2 -5.47039485E-6 8.77826544E-10-5.23167531E-14    2
 -1.24473499E4 -9.68698313E-1   4.29142572E0 -5.50154901E-3  5.99438458E-5    3
 -7.08466469E-8 2.68685836E-11  -1.15222056E4   2.66678994E0                  4
C2H5            -THERMH   5C   2         G     300.0    5000.0  1387.0      1
   5.8878439E0  1.03076793E-2 -3.46844396E-6 5.32499257E-10-3.06512651E-14    2
  1.15065499E4  -8.49651771E0   1.32730217E0  1.76656753E-2 -6.14926558E-6    3
-3.01143466E-10 4.38617775E-13   1.34284028E4   1.71789216E1                  4
C2H5O2            H   5O   2C   2    G     300.0    5000.0  1389.0      1
  9.5028257E0  1.20429839E-2 -4.09491581E-6 6.33049241E-10-3.66133788E-14    2
 -7.37069391E3  -2.2171713E1   3.90351912E0  2.22599212E-2 -1.01610079E-5    3
  1.71709751E-9  1.88166738E-14  -5.09654081E3   8.9872275E0                  4
C2H4              H   4C   2         G     300.0    5000.0  1392.0      1
  5.07061289E0  9.11140768E-3 -3.10506692E-6 4.80733851E-10-2.78321396E-14    2
  3.66391217E3  -6.64501414E0   4.81118223E-1   1.8377806E-2 -9.99633565E-6    3
  2.73211039E-9-3.01837289E-13   5.44386648E3   1.85867157E1                  4
C2H3              H   3C   2         G     300.0    5000.0  1400.0      1
  4.99675415E0  6.55838271E-3 -2.20921909E-6 3.39300272E-10-1.95316926E-14    2
  3.34604382E4  -3.01451097E0   1.25545094E0  1.57481597E-2 -1.12218328E-5    3
 4.50915682E-9-7.74861577E-13   3.47435574E4   1.69664043E1                  4
CHCHO             H   2O   1C   2    G   298.15    2000.0  1000.0      1
  4.9263291E0  9.71712147E-3  -5.5485598E-6  1.53068537E-9-1.64742462E-13    2
  2.89499494E4  5.27874677E-1   2.33256751E0  1.62952986E-2 -9.72052177E-6    3
 5.15124155E-10 1.03836514E-12   2.96585452E4   1.39904923E1                  4
C2H2            G-1-91H   2C   2         G     200.0    6000.0  1000.0      1
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   4.65878489E0  4.88396667E-3 -1.60828888E-6 2.46974544E-10-1.38605959E-14    2
   2.57594042E4  -3.99838194E0  8.08679682E-1  2.33615762E-2 -3.55172234E-5    3
   2.80152958E-8-8.50075165E-12   2.64289808E4   1.39396761E1                  4
C2H              T-5-10H   1C   2        G     200.0    6000.0  1000.0      1
   3.66270248E0  3.82492252E-3   -1.366325E-6  2.1345504E-10-1.23216848E-14    2
    6.7168379E4   3.92205792E0   2.89867676E0  1.32988489E-2 -2.80733327E-5    3
   2.89484755E-8-1.07502351E-11    6.7061605E4   6.18547632E0                  4
CH3CHO           L-8-88H   4O   1C   2    G     200.0    6000.0  1000.0      1
    5.4041108E0   1.1723059E-2  -4.2263137E-6  6.8372451E-10 -4.0984863E-14    2
   -2.2593122E4   -3.4807917E0    4.7294595E0  -3.1932858E-3   4.7534921E-5    3
   -5.7458611E-8  2.1931112E-11   -2.1572878E4   4.1030159E0                  4
CH3CO            IU2-03H   3O   1C   2    G     200.0    6000.0  1000.0      1
    5.3137165E0   9.1737793E-3  -3.3220386E-6  5.3947456E-10 -3.2452368E-14    2
   -3.6450414E3   -1.6757558E0    4.0358705E0   8.7729487E-4   3.071001E-5    3
   -3.9247565E-8  1.5296869E-11   -2.6820738E3   7.8617682E0                  4
CH2CHO           T03-10H   3O   1C   2    G     200.0    6000.0  1000.0      1
   6.53928338E0  7.80238629E-3 -2.76413612E-6 4.42098906E-10 -2.6295429E-14    2
  -1.18858659E3  -8.72091393E0    2.795026E0  1.01099472E-2  1.61750645E-5    3
  -3.10303145E-8 1.39436139E-11   1.62944975E2   1.23646657E1                  4
O2CH2CHO         BOZ-03H   3O   3C   2    G     300.0    5000.0  1393.0      1
   1.11807543E1  9.14479256E-3 -3.15089833E-6 4.91944238E-10 -2.8663918E-14    2
  -1.55790331E4   -2.8789274E1  -1.29465843E0  4.44936393E-2 -4.26577074E-5    3
   2.0739195E-8-3.96828771E-12  -1.18275628E4   3.60778797E1                  4
HO2CH2CO         BOZ-03H   3O   3C   2    G     300.0    5000.0  1386.0      1
   1.04146322E1  1.12680116E-2 -5.17494839E-6  1.00333285E-9-6.68165911E-14    2
  -1.40955672E4   -2.278944E1   2.22681686E0   3.5678138E-2 -3.26401909E-5    3
   1.47651988E-8 -2.6479438E-12  -1.18735095E4   1.91581197E1                  4
!UB REFIT 13-11-2018
CH2CO            -THERMH   2O   1C   2    G     300.0    5000.0  1400.0      1
   6.32896692E0  5.44012978E-3 -1.82687969E-6 2.80010787E-10 -1.6096416E-14    2
  -8.36526176E3  -9.53528539E0   2.35724171E0  1.62213064E-2 -1.34812364E-5    3
   6.11939897E-9-1.13613089E-12  -7.11393356E3   1.12990053E1                  4
HCCO             T-4-09H   1O   1C   2    G     200.0    6000.0  1000.0      1
   5.91479333E0  3.7140873E-3  -1.3013701E-6 2.06473345E-10-1.21476759E-14    2
   1.93596301E4  -5.50567269E0   1.87607969E0  2.21205418E-2 -3.58869325E-5    3
   3.05402541E-8-1.01281069E-11    2.0163384E4   1.3696829E1                  4
C3H8               H   8C   3        G     300.0    5000.0  1390.0      1
    9.1554131E0  1.72574139E-2 -5.85614868E-6 9.04190155E-10-5.22523772E-14    2
  -1.75762439E4   -2.7741851E1   2.4087847E-1  3.39548599E-2 -1.60930874E-5    3
   2.83480628E-9 2.78195172E-14  -1.40362853E4    2.165008E1                  4
IC3H7              H   7C   3        G     298.0    6000.0  1000.0      1
   6.70775549E0  1.74048076E-2 -6.07615926E-6 9.60084351E-10 -5.6565649E-14    2
   7.55377821E3  -1.03686516E1 -8.97467137E-1  4.15744022E-2 -4.94778349E-5    3
   4.56493655E-8-1.79085437E-11   9.93950407E3   2.92641758E1                  4
NC3H7              H   7C   3        G     298.0    6000.0  1000.0      1
   7.48614243E0  1.65769478E-2 -5.74876481E-6 9.04103694E-10-5.30867231E-14    2
   8.93710008E3  -1.42595379E1  -2.20120865E0  5.29641653E-2 -7.23640506E-5    3
   6.3699694E-8-2.29332581E-11   1.15130744E4   3.43669174E1                  4
NC3H7O2            H   7O   2C   3    G     300.0    5000.0  1390.0      1
   1.32753283E1  1.61303126E-2 -5.52348308E-6 8.58197168E-10-4.98172586E-14    2
  -1.16032968E4  -4.15091215E1   2.13311681E0  3.96692045E-2 -2.37570127E-5    3
   6.96020417E-9-7.82576856E-13  -7.46687112E3   1.92444565E1                  4
IC3H7O2H           H   8O   2C   3    G     300.0    5000.0  1405.0      1
   1.44896107E1  1.68268026E-2 -5.67601391E-6 8.72850837E-10-5.02993991E-14    2
  -3.06478491E4  -5.01352281E1   1.77384705E0  4.75813498E-2 -3.43745304E-5    3
   1.31405381E-8-2.06922904E-12  -2.63458844E4   1.77669753E1                  4
IC3H7O2            H   7O   2C   3    G     300.0    5000.0  1407.0      1
    1.3526812E1  1.54306581E-2 -5.17464218E-6 7.92548669E-10-4.55415379E-14    2
  -1.33946348E4  -4.40461451E1   2.58517502E0  4.16107259E-2 -2.92193877E-5    3
   1.08614807E-8-1.66312005E-12  -9.67013161E3    1.447313E1                  4
C3H6OOH1-2         H   7O   2C   3    G     300.0    5000.0  1387.0      1
   1.38088686E1  1.4384565E-2 -4.74440961E-6  7.1930828E-10-4.10654123E-14    2
  -5.14352831E3  -4.20210765E1   2.83631132E0  3.88229894E-2 -2.47944364E-5    3
   7.85644898E-9  -9.586343E-13  -1.26002528E3   1.72549973E1                  4
C3H6OOH1-3         H   7O   2C   3    G     300.0    5000.0  1401.0      1
   1.39130757E1  1.40218463E-2 -4.55921149E-6 6.84182417E-10-3.87696213E-14    2
  -3.65650518E3  -4.21532559E1   1.74271107E0  4.53733504E-2 -3.57580373E-5    3
   1.48540053E-8-2.49981756E-12   2.32580844E2   2.20973041E1                  4
C3H6OOH1-3O2       ----12H   7O   4C   3    G     300.0    5000.0  1416.0      1
   1.81661664E1  1.47644887E-2 -4.74842743E-6 7.06972467E-10-3.98305587E-14    2
  -2.26256376E4  -5.93719393E1   5.5693335E0  4.68523421E-2 -3.58917784E-5    3
   1.43314525E-8-2.29776083E-12  -1.86065694E4   7.18655005E0                  4
C3KET13            H   6O   3C   3    G     300.0    5000.0  1508.0      1
   1.73612692E1  1.32330813E-2  -4.7533211E-6 7.62529227E-10-4.52613717E-14    2
  -4.0624806E4  -6.17768199E1   4.74956819E0  3.14080991E-2 -6.83838427E-6    3
  -5.67123901E-9 2.27686972E-12   -3.5192457E4   9.83753744E0                  4
C3H6               H   6C   3        G     298.0    6000.0  1000.0      1
   6.59032304E0  1.52592866E-2 -5.30369441E-6 8.35510888E-10-4.91215549E-14    2
  -2.47481113E2  -1.15748238E1  -1.54606737E0  4.36553128E-2 -5.61392417E-5    3
   4.98421927E-8-1.84798923E-11   2.07056233E3   2.99232495E1                  4
C3H5-A             H   5C   3        G     298.0    6000.0  1000.0      1
   7.37604097E0  1.23449782E-2 -4.26463882E-6 6.69045835E-10-3.92202554E-14    2
    1.7733296E4  -1.61758204E1  -3.32899442E0  5.38423469E-2 -7.65500752E-5    3
   6.35512285E-8-2.14283003E-11   2.03420628E4   3.68038362E1                  4
C3H5-T             H   5C   3        G     300.0    5000.0  1376.0      1
   7.69949212E0  1.17803985E-2 -4.07791749E-6 6.38119222E-10-3.72229675E-14    2
   2.61747145E4  -1.6830589E1   2.29256998E0  1.98527646E-2 -6.42635654E-6    3
-5.90016395E-10 5.05491095E-13   2.85773377E4   1.39407124E1                  4
CH3CHCO          -THERMH   4O   1C   3    G     300.0    5000.0  1400.0      1
   1.00219123E1   9.569663E-3 -3.26221644E-6 5.05231706E-10-2.92593257E-14    2
  -1.42482738E4  -2.77829973E1   1.48380119E0  3.22203013E-2 -2.70250033E-5    3
   1.20499164E-8-2.18365931E-12  -1.1527654E4   1.71552068E1                  4
C3H4-A           L-8-89H   4C   3        G     200.0    6000.0  1000.0      1
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   6.3168722E0   1.1133728E-2  -3.9629378E-6  6.3564238E-10  -3.787554E-14    2
   2.0117495E4   -1.0995766E1    2.6130445E0   1.2122575E-2    1.853988E-5    3
  -3.4525149E-8  1.5335079E-11    2.1541567E4    1.0226139E1                   4
C3H3             T-7-11H   3C   3          G     200.0    6000.0  1000.0      1
   7.14221719E0  7.61902211E-3  -2.6746003E-6 4.24914904E-10-2.51475443E-14    2
   3.95709594E4   -1.2584869E1   1.35110873E0  3.27411291E-2 -4.73827407E-5    3
   3.7631022E-8-1.18541128E-11   4.07679941E4   1.52058598E1                   4
C3H6OH2-1        -THERMH   7O   1C   3     G     300.0    5000.0  1392.0      1
   1.12222277E1  1.36444398E-2 -4.51406709E-6 7.10523275E-10-4.22690392E-14    2
  -1.75350136E4  -3.18911926E1    1.0967036E0  3.80727565E-2 -2.75022497E-5    3
   1.07477493E-8-1.74895773E-12  -1.40764487E4   2.22475799E1                   4
CH3COCH3               H   6O   1C   3     G     300.0    5000.0  1394.0      1
   8.87619308E0  1.45700263E-2  -4.8482328E-6 7.38614777E-10-4.22831194E-14    2
  -3.06046242E4  -2.12730484E1   2.20008426E0  2.74019559E-2 -1.31342003E-5    3
   2.57150371E-9-6.21509091E-14  -2.79933966E4   1.55883508E1                   4
C2H3CHO          -KPS12H   4O   1C   3     G     300.0    5000.0  1398.0      1
   9.99155394E0  9.82348001E-3 -3.31203088E-6 5.09524422E-10 -2.9382189E-14    2
  -1.25303509E4  -2.85168883E1  7.33844455E-1  3.17482671E-2 -2.29599468E-5    3
   8.42104232E-9-1.23613478E-12  -9.38473548E3   2.10308851E1                   4
IC3H6CO          -THERMH   6O   1C   4     G     300.0    5000.0  1397.0      1
   1.32548232E1  1.40142787E-2 -4.78910215E-6 7.42924342E-10-4.30737566E-14    2
  -2.00529779E4  -4.44810221E1   2.28039055E0  4.17016989E-2 -3.25089661E-5    3
   1.37243419E-8-2.40573132E-12  -1.63939712E4   1.38187714E1                   4
C5H81-3                H   8C   5          G     300.0    5000.0  1385.0      1
   1.29945372E1  1.92678312E-2 -6.58966712E-6  1.02295969E-9-5.93441369E-14    2
   4.59040047E3  -4.35689825E1   1.54882436E0  4.15042709E-2  -2.1435989E-5    3
   4.71145517E-9-2.42142508E-13   9.05636062E3    1.9566591E1                   4
END

TRANSPORT
AR 0 136.5 3.33 0.0 0.0 0.0
N2 1 97.53 3.621 0.0 1.76 4.0
HE 0 10.2 2.576 0.0 0.0 0.0
H2 1 38.0 2.92 0.0 0.79 280.0
H 0 145.0 2.05 0.0 0.0 0.0
O2 1 107.4 3.458 0.0 1.6 3.8
O 0 80.0 2.75 0.0 0.0 0.0
H2O 2 572.4 2.605 1.844 0.0 4.0
OH 1 80.0 2.75 0.0 0.0 0.0
OHV 1 80.0 2.75 0.0 0.0 0.0
H2O2 2 107.4 3.458 0.0 0.0 3.8
HO2 2 107.4 3.458 0.0 0.0 1.0
CO 1 98.1 3.65 0.0 1.95 1.8
CO2 1 244.0 3.763 0.0 2.65 2.1
CH4 2 141.4 3.746 0.0 2.6 13.0
CH3 1 144.0 3.8 0.0 0.0 0.0
CH2 1 144.0 3.8 0.0 0.0 0.0
CH2(S) 1 144.0 3.8 0.0 0.0 0.0
CH 1 80.0 2.75 0.0 0.0 0.0
CHV 1 80.0 2.75 0.0 0.0 0.0
CH3O2H 2 481.8 3.626 0.0 0.0 1.0
CH3O2 2 481.8 3.626 0.0 0.0 1.0
CH3O 2 417.0 3.69 1.7 0.0 2.0
CH2OH 2 417.0 3.69 1.7 0.0 2.0
CH2O 2 498.0 3.59 0.0 0.0 2.0
HCO 2 498.0 3.59 0.0 0.0 0.0
HCOH 2 498.0 3.59 0.0 0.0 1.0
HO2CHO 2 436.0 3.97 0.0 0.0 2.0
O2CHO 2 436.0 3.97 0.0 0.0 2.0
HOCHO 2 436.0 3.97 0.0 0.0 2.0
OCHO 2 498.0 3.59 0.0 0.0 2.0
C2H6 2 247.5 4.35 0.0 0.0 1.5
C2H5 2 247.5 4.35 0.0 0.0 1.5
C2H5O2 2 470.6 4.41 0.0 0.0 1.5
C2H4 2 238.4 3.496 0.0 0.0 1.5
C2H3 2 265.3 3.721 0.0 0.0 1.0
CHCHO 2 436.0 3.97 0.0 0.0 2.0
C2H2 1 265.3 3.721 0.0 0.0 2.5
C2H 1 265.3 3.721 0.0 0.0 2.5
CH3CHO 2 436.0 3.97 0.0 0.0 2.0
CH3CO 2 436.0 3.97 0.0 0.0 2.0
CH2CHO 2 436.0 3.97 0.0 0.0 2.0
O2CH2CHO 2 275.049 5.428 0.0 0.0 1.0
HO2CH2CO 2 279.007 5.505 1.3 0.0 1.0
CH2CO 2 436.0 3.97 0.0 0.0 2.0
HCCO 2 150.0 2.5 0.0 0.0 1.0
C3H8 2 303.4 4.81 0.0 0.0 1.0
IC3H7 2 303.4 4.81 0.0 0.0 1.0
NC3H7 2 303.4 4.81 0.0 0.0 1.0
NC3H7O2 2 481.5 4.997 1.7 0.0 1.0
IC3H7O2H 2 459.5 5.036 1.7 0.0 1.0
IC3H7O2 2 459.5 5.036 1.7 0.0 1.0
C3H6OOH1-2 2 435.2 4.662 2.7 0.0 1.0
C3H6OOH1-3 2 435.2 4.662 2.7 0.0 1.0
C3H6OOH1-3O2 2 435.2 4.662 2.7 0.0 1.0
C3KET13 2 464.2 5.009 2.6 0.0 1.0
C3H6 2 307.8 4.14 0.0 0.0 1.0
C3H5-A 2 316.0 4.22 0.0 0.0 1.0
C3H5-T 2 316.0 4.22 0.0 0.0 1.0
CH3CHCO 2 443.2 4.12 0.0 0.0 1.0
C3H4-A 1 324.8 4.29 0.0 0.0 1.0
C3H3 1 324.8 4.29 0.0 0.0 1.0
C3H6OH2-1 2 487.9 4.82 0.0 0.0 1.0
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CH3COCH3 2 435.5 4.86 0.0 0.0 1.0
C2H3CHO 2 428.8 4.958 2.9 0.0 1.0
IC3H6CO 2 436.4 5.352 0.0 0.0 1.0
C5H81-3 2 408.0 5.2 0.0 0.0 1.0
END

REACTIONS MOLES CAL/MOLE
H2+M=2H+M    4.577E19 -1.4 1.044E5
   H2/2.5/
   H2O/12.0/
   CO/1.9/
   CO2/3.8/
   HE/0.83/
   CH4/2.0/
   C2H6/3.0/
H2+O=H+OH    5.08E4 2.67 6.292E3
H2+OH=H+H2O    4.38E13 0.0 6.99E3
2O+M=O2+M    6.165E15 -0.5 0.0E0
   H2/2.5/
   H2O/12.0/
   AR/0.83/
   CO/1.9/
   CO2/3.8/
   HE/0.83/
   CH4/2.0/
   C2H6/3.0/
O2+H=O+OH    1.04E14 0.0 1.5286E4
H+OH+M=H2O+M    3.5E22 -2.0 0.0E0
   H2/0.73/
   H2O/3.65/
   CH4/2.0/
   C2H6/3.0/
   AR/0.38/
O+H2O=2OH    6.7E7 1.704 1.49868E4
O+H+M=OH+M    4.714E18 -1.0 0.0E0
   H2/2.5/
   H2O/12.0/
   AR/0.75/
   CO/1.5/
   CO2/2.0/
   HE/0.75/
   CH4/2.0/
   C2H6/3.0/
H+O+M=OHV+M    1.5E13 0.0 5.975E3
   H2/1.0/
   H2O/6.5/
   O2/0.4/
   N2/0.4/
   AR/0.35/
OHV+H2O=OH+H2O    5.93E12 0.5 -8.6E2
OHV+H2=OH+H2    2.95E12 0.5 -4.44E2
OHV+N2=OH+N2    1.08E11 0.5 -1.242E3
OHV+OH=2OH    6.01E12 0.5 -7.64E2
OHV+H=OH+H    1.31E12 0.5 -1.67E2
OHV+AR=OH+AR    1.69E12 0.0 4.135E3
OHV=OH    1.45E6 0.0 0.0E0
OHV+O2=OH+O2    2.1E12 0.5 -4.78E2
OHV+CO2=OH+CO2    2.75E12 0.5 -9.68E2
OHV+CO=OH+CO    3.23E12 0.5 -7.87E2
OHV+CH4=OH+CH4    3.36E12 0.5 -6.35E2
H2O2(+M)=2OH(+M)    2.0E12 0.9 4.8749E4
   H2O/7.65/
   CO2/1.6/
   N2/1.5/
   O2/1.2/
   HE/0.65/
   H2O2/7.7/
   H2/3.7/
   CO/2.8/
   LOW/2.49E24 -2.3E0 4.8749E4/
   TROE/4.3E-1 1.0E-30 1.0E30/
H2O2+H=H2O+OH    2.41E13 0.0 3.97E3
H2O2+H=H2+HO2    2.15E10 1.0 6.0E3
H2O2+O=OH+HO2    9.55E6 2.0 3.97E3
H2O2+OH=H2O+HO2    1.74E12 0.0 3.18E2
   DUP
H2O2+OH=H2O+HO2    7.59E13 0.0 7.269E3
   DUP
HO2+H=2OH    7.079E13 0.0 2.95E2
HO2+H=H2+O2    1.1402E10 1.0827 5.5378E2
HO2+O=OH+O2    3.25E13 0.0 0.0E0
HO2+OH=H2O+O2    2.456E13 0.0 -4.97E2
2HO2=H2O2+O2    1.0E14 0.0 1.1040883E4
   DUP
2HO2=H2O2+O2    1.9E11 0.0 -1.4089248E3
   DUP
H+O2(+M)=HO2(+M)    4.65E12 0.44 0.0E0
   H2/1.3/
   CO/1.9/
   CO2/3.8/
   HE/0.64/
   H2O/10.0/
   AR/0.5/
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   CH4/2.0/
   C2H6/3.0/
   LOW/1.737E19 -1.23E0 0.0E0/
   TROE/6.7E-1 1.0E-30 1.0E30 1.0E30/
CO+O(+M)=CO2(+M)    1.362E10 0.0 2.384E3
   H2/2.0/
   H2O/12.0/
   CO/1.75/
   CO2/3.6/
   AR/0.7/
   HE/0.7/
   LOW/1.173E24 -2.79E0 4.191E3/
CO+OH=CO2+H    7.015E4 2.053 -3.557E2
   DUP
CO+OH=CO2+H    5.757E12 -0.664 3.318E2
   DUP
CO+HO2=CO2+OH    1.57E5 2.18 1.794E4
CO+O2=CO2+O    1.119E12 0.0 4.77E4
H+CO2=OCHO    7.5E13 0.0 2.9E4
CH3+H(+M)=CH4(+M)    1.27E16 -0.63 3.83E2
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/2.477E33 -4.76E0 2.44E3/
   TROE/7.83E-1 7.4E1 2.941E3 6.964E3/
CH4+H=CH3+H2    6.14E5 2.5 9.587E3
CH4+O=CH3+OH    1.02E9 1.5 8.6E3
CH4+OH=CH3+H2O    5.83E4 2.6 2.19E3
CH4+HO2=CH3+H2O2    1.13E1 3.74 2.101E4
CH4+CH3O2=CH3+CH3O2H    9.6E-1 3.77 1.781E4
CH3+HO2=CH4+O2    1.16E5 2.23 -3.022E3
CH4+CH2=2CH3    2.46E6 2.0 8.27E3
CH2(S)+N2=CH2+N2    1.5E13 0.0 6.0E2
CH2(S)+AR=CH2+AR    9.0E12 0.0 6.0E2
CH2(S)+H2O=CH2+H2O    3.0E13 0.0 0.0E0
CH2(S)+CO=CH2+CO    9.0E12 0.0 0.0E0
CH2(S)+CO2=CH2+CO2    7.0E12 0.0 0.0E0
CH2(S)+O2=>H+OH+CO    2.8E13 0.0 0.0E0
CH2(S)+O2=CO+H2O    1.2E13 0.0 0.0E0
CH2(S)+O=CO+H2    1.5E13 0.0 0.0E0
CH2(S)+O=HCO+H    1.5E13 0.0 0.0E0
CH2(S)+H2=CH3+H    7.0E13 0.0 0.0E0
CH2(S)+H=CH+H2    3.0E13 0.0 0.0E0
CH2(S)+OH=CH2O+H    3.0E13 0.0 0.0E0
CH2(S)+CO2=CH2O+CO    1.4E13 0.0 0.0E0
CH2+H(+M)=CH3(+M)    2.5E16 -0.8 0.0E0
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/3.2E27 -3.14E0 1.23E3/
   TROE/6.8E-1 7.8E1 1.995E3 5.59E3/
CH2+O2=HCO+OH    1.06E13 0.0 1.5E3
CH2+O2=>CO2+2H    2.64E12 0.0 1.5E3
CH2+O=>CO+2H    5.0E13 0.0 0.0E0
CH2+H=CH+H2    3.0E13 0.0 0.0E0
CH2+OH=CH+H2O    1.13E7 2.0 3.0E3
CHV+AR=CH+AR    4.0E11 0.5 0.0E0
CHV+H2O=CH+H2O    5.3E13 0.0 0.0E0
CHV+CO=CH+CO    2.44E12 0.5 0.0E0
CHV+CO2=CH+CO2    2.41E-1 4.3 -1.694E3
CHV+O2=CH+O2    2.48E6 2.14 -1.72E3
CHV+H2=CH+H2    1.47E14 0.0 1.361E3
CHV+CH4=CH+CH4    1.73E13 0.0 1.67E2
CHV=CH    1.86E6 0.0 0.0E0
CHV+N2=CH+N2    3.03E2 3.4 -3.81E2
CH+O2=CO+OHV    4.04E13 0.0 0.0E0
CH+O2=HCO+O    3.3E13 0.0 0.0E0
CH+O=CO+H    5.7E13 0.0 0.0E0
CH+OH=HCO+H    3.0E13 0.0 0.0E0
CH+H2O=H+CH2O    1.774E16 -1.22 2.38E1
CH+CO2=HCO+CO    1.7E12 0.0 6.85E2
CH3+O2(+M)=CH3O2(+M)    7.812E9 0.9 0.0E0
   LOW/6.85E24 -3.0E0 0.0E0/
   TROE/6.0E-1 1.0E3 7.0E1 1.7E3/
CH3+O2=CH3O+O    7.546E12 0.0 2.832E4
CH3+O2=CH2O+OH    2.641E0 3.283 8.105E3
CH3+O=CH2O+H    5.54E13 0.05 -1.36E2
CH3+OH=CH2(S)+H2O    4.936E14 -0.669 -4.458E2
   PLOG/1.0E-2 4.936E14 -6.69E-1 -4.458E2/
   PLOG/1.0E-1 1.207E15 -7.78E-1 -1.756E2/
   PLOG/1.0E0 5.282E17 -1.518E0 1.772E3/
   PLOG/1.0E1 4.788E23 -3.155E0 7.003E3/
   PLOG/1.0E2 8.433E19 -1.962E0 8.244E3/
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CH3+OH=CH2O+H2    3.502E5 1.441 -3.244E3
   PLOG/1.0E-2 3.502E5 1.441E0 -3.244E3/
   PLOG/1.0E-1 8.854E5 1.327E0 -2.975E3/
   PLOG/1.0E0 1.65E7 9.73E-1 -2.01E3/
   PLOG/1.0E1 5.374E9 2.87E-1 2.8E2/
   PLOG/1.0E2 9.494E18 -2.199E0 9.769E3/
CH3+OH=CH2OH+H    1.621E10 0.965 3.21E3
   PLOG/1.0E-2 1.621E10 9.65E-1 3.214E3/
   PLOG/1.0E-1 1.807E10 9.5E-1 3.247E3/
   PLOG/1.0E0 4.686E10 8.33E-1 3.566E3/
   PLOG/1.0E1 1.525E13 1.34E-1 5.641E3/
   PLOG/1.0E2 3.59E14 -1.86E-1 8.601E3/
CH3+OH=H+CH3O    1.186E9 1.016 1.194E4
   PLOG/1.0E-2 1.186E9 1.016E0 1.194E4/
   PLOG/1.0E-1 1.188E9 1.016E0 1.194E4/
   PLOG/1.0E0 1.23E9 1.011E0 1.195E4/
   PLOG/1.0E1 1.798E9 9.65E-1 1.206E4/
   PLOG/1.0E2 5.242E10 5.51E-1 1.307E4/
CH3+OH=HCOH+H2    8.674E8 0.787 -3.046E3
   PLOG/1.0E-2 8.674E8 7.87E-1 -3.046E3/
   PLOG/1.0E-1 3.115E9 6.3E-1 -2.669E3/
   PLOG/1.0E0 1.557E11 1.56E-1 -1.368E3/
   PLOG/1.0E1 1.704E21 -2.641E0 6.412E3/
   PLOG/1.0E2 7.25E20 -2.402E0 9.639E3/
CH3+OH=CH2+H2O    4.293E4 2.568 3.9978E3
CH3+HO2=CH3O+OH    1.0E12 0.269 -6.875E2
CH3O2+O=CH3O+O2    3.6E13 0.0 0.0E0
CH3O2+H=CH3O+OH    9.6E13 0.0 0.0E0
CH3O2+HO2=CH3O2H+O2    2.47E11 0.0 -1.57E3
CH3O2+H2O2=CH3O2H+HO2    2.41E12 0.0 9.936E3
CH3O2+CH3=2CH3O    5.08E12 0.0 -1.411E3
2CH3O2=>O2+2CH3O    1.4E16 -1.61 1.86E3
H2+CH3O2=H+CH3O2H    1.5E14 0.0 2.603E4
CH3O2H=CH3O+OH    6.31E14 0.0 4.23E4
CH2OH+O2=CH2O+HO2    1.51E15 -1.0 0.0E0
   DUP
CH2OH+O2=CH2O+HO2    2.41E14 0.0 5.017E3
   DUP
CH2OH+H=CH2O+H2    6.0E12 0.0 0.0E0
CH2OH+HO2=CH2O+H2O2    1.2E13 0.0 0.0E0
CH2OH+HCO=2CH2O    1.8E14 0.0 0.0E0
CH2OH+OH=H2O+CH2O    2.4E13 0.0 0.0E0
CH2OH+O=OH+CH2O    4.2E13 0.0 0.0E0
CH3O+O2=CH2O+HO2    4.38E-19 9.5 -5.501E3
CH3O+H=CH2O+H2    2.0E13 0.0 0.0E0
CH3O+HO2=CH2O+H2O2    3.01E11 0.0 0.0E0
CH3O+CH3=CH2O+CH4    1.2E13 0.0 0.0E0
HCOH+O2=>CO2+H+OH    5.0E12 0.0 0.0E0
HCOH+O2=CO2+H2O    3.0E13 0.0 0.0E0
HCOH+O=>CO2+2H    5.0E13 0.0 0.0E0
HCOH+O=>CO+OH+H    3.0E13 0.0 0.0E0
HCOH+H=CH2O+H    2.0E14 0.0 0.0E0
HCOH+OH=HCO+H2O    2.0E13 0.0 0.0E0
HCO+H(+M)=CH2O(+M)    1.09E12 0.48 -2.6E2
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/1.35E24 -2.57E0 1.425E3/
   TROE/7.824E-1 2.71E2 2.755E3 6.57E3/
CO+H2(+M)=CH2O(+M)    4.3E7 1.5 7.96E4
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/5.07E27 -3.42E0 8.4348E4/
   TROE/9.32E-1 1.97E2 1.54E3 1.03E4/
CH2O+O2=HCO+HO2    8.07E15 0.0 5.342E4
CH2O+O=HCO+OH    6.26E9 1.15 2.26E3
CH2O+H=HCO+H2    5.74E7 1.9 2.74E3
CH2O+OH=HCO+H2O    7.82E7 1.63 -1.055E3
CH2O+HO2=HCO+H2O2    1.88E4 2.7 1.152E4
CH2O+CH3=HCO+CH4    3.83E1 3.36 4.312E3
CH2O+O2CHO=HCO+HO2CHO    1.99E12 0.0 1.166E4
CH2O+OCHO=HCO+HOCHO    5.6E12 0.0 1.36E4
CH2O+CH3O2=HCO+CH3O2H    1.99E12 0.0 1.166E4
HCO+M=H+CO+M    5.7E11 0.66 1.487E4
   H2/2.0/
   H2O/6.0/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
HCO+O2=CO+HO2    7.58E12 0.0 4.1E2
HCO+O=CO+OH    3.02E13 0.0 0.0E0
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HCO+H=CO+H2    7.34E13 0.0 0.0E0
HCO+OH=CO+H2O    3.011E13 0.0 0.0E0
HCO+CH3=CO+CH4    2.65E13 0.0 0.0E0
2HCO=CO+CH2O    1.8E13 0.0 0.0E0
HCO+O=CO2+H    3.0E13 0.0 0.0E0
HCO+HO2=>CO2+H+OH    3.0E13 0.0 0.0E0
2HCO=>H2+2CO    3.0E12 0.0 0.0E0
CH2O+H(+M)=CH2OH(+M)    5.4E11 0.454 3.6E3
   H2/2.0/
   H2O/6.0/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   LOW/1.27E32 -4.82E0 6.53E3/
   TROE/7.187E-1 1.03E2 1.291E3 4.16E3/
CH3O(+M)=CH2O+H(+M)    6.8E13 0.0 2.617E4
   H2/2.0/
   H2O/6.0/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   LOW/1.867E25 -3.0E0 2.4307E4/
   TROE/9.0E-1 2.5E3 1.3E3 1.0E99/
HCO+O2=O2CHO    1.2E11 0.0 -1.1E3
HOCHO=CO+H2O    2.45E12 0.0 6.047E4
HOCHO=CO2+H2    2.95E9 0.0 4.852E4
OCHO+HO2=HOCHO+O2    3.5E10 0.0 -3.275E3
OCHO+H2O2=HOCHO+HO2    2.4E12 0.0 1.0E4
HOCHO+H=>H2+CO2+H    4.24E6 2.1 4.868E3
HOCHO+H=>H2+CO+OH    6.03E13 -0.35 2.988E3
HOCHO+O=>CO+2OH    1.77E18 -1.9 2.975E3
HOCHO+OH=>H2O+CO2+H    2.62E6 2.06 9.16E2
HOCHO+OH=>H2O+CO+OH    1.85E7 1.51 -9.62E2
HOCHO+CH3=>CH4+CO+OH    3.9E-7 5.8 2.2E3
HOCHO+HO2=>H2O2+CO+OH    1.0E12 0.0 1.192E4
OCHO+OH=HO2CHO    2.0E13 0.0 0.0E0
2CH3(+M)=C2H6(+M)    2.277E15 -0.69 1.749E2
   H2O/5.0/
   CO/2.0/
   CO2/3.0/
   LOW/8.054E31 -3.75E0 9.816E2/
   TROE/0.0E0 5.7E2 1.0E30 1.0E30/
C2H5+H(+M)=C2H6(+M)    5.21E17 -0.99 1.58E3
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/1.99E41 -7.08E0 6.685E3/
   TROE/8.42E-1 1.25E2 2.219E3 6.882E3/
2CH3=H+C2H5    4.74E12 0.105 1.06643E4
   PLOG/1.0E-2 4.74E12 1.05E-1 1.06643E4/
   PLOG/1.0E-1 2.57E13 -9.6E-2 1.14061E4/
   PLOG/1.0E0 3.1E14 -3.62E-1 1.33725E4/
   PLOG/1.0E1 2.15E10 8.85E-1 1.35325E4/
   PLOG/1.0E2 1.032E2 3.23E0 1.12361E4/
C2H6+O2=C2H5+HO2    6.03E13 0.0 5.187E4
C2H6+O=C2H5+OH    3.55E6 2.4 5.83E3
C2H6+H=C2H5+H2    1.15E8 1.9 7.53E3
C2H6+OH=C2H5+H2O    1.48E7 1.9 9.5E2
C2H6+HO2=C2H5+H2O2    3.46E1 3.61 1.692E4
C2H6+CH=C2H5+CH2    1.1E14 0.0 -2.6E2
C2H6+CH2(S)=C2H5+CH3    1.2E14 0.0 0.0E0
C2H6+CH3=C2H5+CH4    5.55E-4 4.72 3.231E3
C2H6+CH3O2=C2H5+CH3O2H    1.94E1 3.64 1.71E4
C2H4+H(+M)=C2H5(+M)    9.569E8 1.463 1.355E3
   H2/2.0/
   H2O/6.0/
   CH4/2.0/
   CO/1.5/
   CO2/2.0/
   C2H6/3.0/
   AR/0.7/
   LOW/1.419E39 -6.642E0 5.769E3/
   TROE/-5.69E-1 2.99E2 -9.147E3 1.524E2/
C2H5+H=C2H4+H2    2.0E12 0.0 0.0E0
2C2H4=C2H5+C2H3    4.82E14 0.0 7.153E4
C2H5+CH3=CH4+C2H4    1.18E4 2.45 -2.921E3
C2H5+O=CH3CHO+H    1.1E14 0.0 0.0E0
C2H5+O2=C2H5O2    3.398E53 -13.9 9.279E3
   PLOG/4.0E-2 3.398E53 -1.39E1 9.279E3/
   PLOG/1.0E0 9.362E59 -1.528E1 1.424E4/
   PLOG/1.0E1 1.262E60 -1.491E1 1.624E4/
C2H5+O2=C2H4+HO2    2.094E9 0.49 -3.914E2
   PLOG/4.0E-2 2.094E9 4.9E-1 -3.914E2/
   PLOG/1.0E0 1.843E7 1.13E0 -7.206E2/
   PLOG/1.0E1 7.561E14 -1.01E0 4.749E3/
C2H5+O2=CH3CHO+OH    4.908E-6 4.76 2.543E2
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    PLOG/4.0E-2 4.908E-6 4.76E0 2.543E2/
    PLOG/1.0E0 6.803E-2 3.57E0 2.643E3/
    PLOG/1.0E1 8.265E2 2.41E0 5.285E3/
C2H5O2=CH3CHO+OH    1.237E35 -9.42 3.636E4
    PLOG/4.0E-2 1.237E35 -9.42E0 3.636E4/
    PLOG/1.0E0 1.687E36 -9.22E0 3.87E4/
    PLOG/1.0E1 2.52E41 -1.02E1 4.371E4/
C2H5O2=C2H4+HO2    1.782E32 -7.1 3.284E4
    PLOG/4.0E-2 1.782E32 -7.1E0 3.284E4/
    PLOG/1.0E0 2.701E37 -8.47E0 3.584E4/
    PLOG/1.0E1 1.98E38 -8.46E0 3.79E4/
C2H3+H(+M)=C2H4(+M)    6.08E12 0.27 2.8E2
    H2/2.0/
    H2O/6.0/
    AR/0.7/
    CO/1.5/
    CO2/2.0/
    CH4/2.0/
    C2H6/3.0/
    HE/0.7/
    LOW/1.4E30 -3.86E0 3.32E3/
    TROE/7.82E-1 2.075E2 2.663E3 6.095E3/
C2H4+O2=C2H3+HO2    4.22E13 0.0 5.76231E4
C2H4+H=C2H3+H2    5.07E7 1.93 1.295E4
C2H4+OH=C2H3+H2O    2.23E4 2.745 2.2155E3
C2H4+CH3O2=C2H3+CH3O2H    8.59E0 3.754 2.7132E4
C2H4+CH3=C2H3+CH4    9.76E2 2.947 1.5148E4
    DUP
C2H4+CH3=C2H3+CH4    8.13E-5 4.417 8.8358E3
    DUP
C2H4+O=CH3+HCO    7.453E6 1.88 1.83E2
C2H4+O=CH2CHO+H    6.098E6 1.88 1.83E2
CH+CH4=C2H4+H    6.0E13 0.0 0.0E0
CH2(S)+CH3=C2H4+H    2.0E13 0.0 0.0E0
C2H4+OH=CH3+CH2O    5.35E0 2.92 -1.7327E3
    PLOG/1.0E-2 5.35E0 2.92E0 -1.7327E3/
    PLOG/2.5E-2 3.19E1 2.71E0 -1.1723E3/
    PLOG/1.0E-1 5.55E2 2.36E0 -1.808E2/
    PLOG/1.0E0 1.78E5 1.68E0 2.0605E3/
    PLOG/1.0E1 2.37E9 5.6E-1 6.0067E3/
    PLOG/1.0E2 2.76E13 -5.0E-1 1.14551E4/
C2H4+OH=CH3CHO+H    2.37E-7 5.3 -2.0506E3
    PLOG/1.0E-2 2.37E-7 5.3E0 -2.0506E3/
    PLOG/2.5E-2 8.73E-5 4.57E0 -6.18E2/
    PLOG/1.0E-1 4.03E-1 3.54E0 1.8817E3/
    PLOG/1.0E0 2.38E-2 3.91E0 1.7227E3/
    PLOG/1.0E1 8.25E8 1.01E0 1.05073E4/
    PLOG/1.0E2 6.8E9 8.1E-1 1.38673E4/
C2H2+H(+M)=C2H3(+M)    1.71E10 1.266 2.709E3
    H2/2.0/
    H2O/6.0/
    AR/0.7/
    CO/1.5/
    CO2/2.0/
    CH4/2.0/
    C2H6/3.0/
    HE/0.7/
    LOW/6.346E31 -4.664E0 3.78E3/
    TROE/7.88E-1 -1.02E4 1.0E-30/
C2H3+O2=CHCHO+OH    2.84E14 -0.8 7.232E3
    DUP
    PLOG/1.0E-2 3.91E11 -1.1E-1 2.131E3/
    PLOG/1.0E-1 1.13E9 5.5E-1 4.6E1/
    PLOG/3.16E-1 8.46E8 5.6E-1 7.0E-1/
    PLOG/1.0E0 2.75E14 -1.83E0 4.6E0/
    PLOG/3.16E0 2.58E20 -2.84E0 7.53E3/
    PLOG/1.0E1 9.18E14 -2.26E0 -4.0E-1/
    PLOG/3.16E1 6.11E25 -4.21E0 1.305E4/
    PLOG/1.0E2 1.65E30 -5.35E0 1.843E4/
C2H3+O2=CHCHO+OH    2.84E14 -0.8 7.232E3
    DUP
    PLOG/1.0E-2 9.91E11 -6.6E-1 -6.0E-1/
    PLOG/1.0E-1 6.94E14 -1.16E0 4.542E3/
    PLOG/3.16E-1 2.79E13 -7.2E-1 3.479E3/
    PLOG/1.0E0 4.99E11 -1.4E-1 1.995E3/
    PLOG/3.16E0 2.35E10 2.3E-1 1.573E3/
    PLOG/1.0E1 1.7E14 -8.2E-1 4.45E3/
    PLOG/3.16E1 1.42E11 5.0E-2 3.774E3/
    PLOG/1.0E2 3.17E11 -2.0E-2 5.338E3/
C2H3+O2=CH2CHO+O    1.76E12 0.15 4.205E3
    DUP
    PLOG/1.0E-2 7.88E20 -2.67E0 6.742E3/
    PLOG/1.0E-1 7.72E20 -2.67E0 6.713E3/
    PLOG/3.16E-1 9.87E20 -2.7E0 6.724E3/
    PLOG/1.0E0 7.1E20 -2.65E0 6.489E3/
    PLOG/3.16E0 4.5E20 -2.53E0 6.406E3/
    PLOG/1.0E1 1.76E23 -3.22E0 8.697E3/
    PLOG/3.16E1 3.14E25 -3.77E0 1.153E4/
    PLOG/1.0E2 1.02E26 -3.8E0 1.391E4/
C2H3+O2=CH2CHO+O    1.76E12 0.15 4.205E3
    DUP
    PLOG/1.0E-2 1.36E10 6.2E-1 -2.776E2/
    PLOG/1.0E-1 1.42E10 6.2E-1 -2.477E2/
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    PLOG/3.16E-1 1.66E10 6.0E-1 -1.625E2/
    PLOG/1.0E0 2.02E10 5.8E-1 3.84E1/
    PLOG/3.16E0 9.75E9 6.7E-1 2.48E2/
    PLOG/1.0E1 7.34E9 7.2E-1 7.781E2/
    PLOG/3.16E1 1.57E9 9.2E-1 1.219E3/
    PLOG/1.0E2 7.85E7 1.28E0 1.401E3/
C2H3+O2=C2H2+HO2    6.49E6 1.5 5.218E3
    DUP
    PLOG/1.0E-2 1.08E7 1.28E0 3.322E3/
    PLOG/1.0E-1 7.75E6 1.33E0 3.216E3/
    PLOG/3.16E-1 1.21E7 1.27E0 3.311E3/
    PLOG/1.0E0 2.15E7 1.19E0 3.367E3/
    PLOG/3.16E0 1.13E8 1.0E0 3.695E3/
    PLOG/1.0E1 1.31E11 1.2E-1 5.872E3/
    PLOG/3.16E1 1.19E9 8.2E-1 5.617E3/
    PLOG/1.0E2 1.06E17 -1.45E0 1.223E4/
C2H3+O2=C2H2+HO2    6.49E6 1.5 5.218E3
    DUP
    PLOG/1.0E-2 4.76E1 2.75E0 -7.964E2/
    PLOG/1.0E-1 5.16E1 2.73E0 -7.683E2/
    PLOG/3.16E-1 5.55E1 2.73E0 -6.585E2/
    PLOG/1.0E0 4.6E1 2.76E0 -4.928E2/
    PLOG/3.16E0 3.75E0 3.07E0 -6.01E2/
    PLOG/1.0E1 5.48E0 3.07E0 8.57E1/
    PLOG/3.16E1 4.47E8 0.0E0 9.55E2/
    PLOG/1.0E2 2.02E1 2.94E0 1.847E3/
C2H3+O2=CH2CO+OH    1.17E3 2.43 7.074E3
    DUP
    PLOG/1.0E-2 8.66E2 2.41E0 6.061E3/
    PLOG/1.0E-1 8.91E2 2.41E0 6.078E3/
    PLOG/3.16E-1 9.43E2 2.4E0 6.112E3/
    PLOG/1.0E0 1.06E3 2.39E0 6.18E3/
    PLOG/3.16E0 1.09E3 2.38E0 6.179E3/
    PLOG/1.0E1 1.39E3 2.36E0 6.074E3/
    PLOG/3.16E1 2.49E6 1.42E0 8.48E3/
    PLOG/1.0E2 1.66E10 3.6E-1 1.201E4/
C2H3+O2=CH2CO+OH    1.17E3 2.43 7.074E3
    DUP
    PLOG/1.0E-2 1.82E-1 3.12E0 1.331E3/
    PLOG/1.0E-1 2.07E-1 3.11E0 1.383E3/
    PLOG/3.16E-1 2.71E-1 3.08E0 1.496E3/
    PLOG/1.0E0 5.26E-1 3.01E0 1.777E3/
    PLOG/3.16E0 1.37E0 2.9E0 2.225E3/
    PLOG/1.0E1 4.19E-1 2.93E0 2.052E3/
    PLOG/3.16E1 1.19E-4 4.21E0 2.043E3/
    PLOG/1.0E2 1.3E-3 3.97E0 3.414E3/
C2H3+O2=CH2O+HCO    1.16E16 -1.13 3.791E3
    DUP
    PLOG/1.0E-2 2.49E36 -7.6E0 1.264E4/
    PLOG/1.0E-1 2.43E36 -7.6E0 1.261E4/
    PLOG/3.16E-1 1.95E36 -7.57E0 1.249E4/
    PLOG/1.0E0 2.73E35 -7.32E0 1.182E4/
    PLOG/3.16E0 1.43E36 -7.47E0 1.246E4/
    PLOG/1.0E1 5.18E35 -7.2E0 1.343E4/
    PLOG/3.16E1 3.19E20 -2.57E0 5.578E3/
    PLOG/1.0E2 2.73E33 -6.28E0 1.6E4/
C2H3+O2=CH2O+HCO    1.16E16 -1.13 3.791E3
    DUP
    PLOG/1.0E-2 4.54E15 -1.28E0 5.153E2/
    PLOG/1.0E-1 4.59E15 -1.28E0 5.13E2/
    PLOG/3.16E-1 4.81E15 -1.29E0 5.206E2/
    PLOG/1.0E0 6.08E15 -1.31E0 6.457E2/
    PLOG/3.16E0 9.45E15 -1.36E0 1.066E3/
    PLOG/1.0E1 2.56E15 -1.18E0 1.429E3/
    PLOG/3.16E1 1.03E69 -1.923E1 1.476E4/
    PLOG/1.0E2 4.21E10 1.9E-1 8.306E2/
C2H3+O2=>CH2O+H+CO    1.16E16 -1.13 3.791E3
    DUP
    PLOG/1.0E-2 5.82E36 -7.6E0 1.264E4/
    PLOG/1.0E-1 5.66E36 -7.6E0 1.261E4/
    PLOG/3.16E-1 4.55E36 -7.57E0 1.249E4/
    PLOG/1.0E0 6.36E35 -7.32E0 1.182E4/
    PLOG/3.16E0 3.35E36 -7.47E0 1.246E4/
    PLOG/1.0E1 1.21E36 -7.2E0 1.343E4/
    PLOG/3.16E1 7.43E20 -2.57E0 5.578E3/
    PLOG/1.0E2 6.36E33 -6.28E0 1.6E4/
C2H3+O2=>CH2O+H+CO    1.16E16 -1.13 3.791E3
    DUP
    PLOG/1.0E-2 1.06E16 -1.28E0 5.153E2/
    PLOG/1.0E-1 1.07E16 -1.28E0 5.13E2/
    PLOG/3.16E-1 1.13E16 -1.29E0 5.206E2/
    PLOG/1.0E0 1.42E16 -1.31E0 6.457E2/
    PLOG/3.16E0 2.2E16 -1.36E0 1.066E3/
    PLOG/1.0E1 5.98E15 -1.18E0 1.429E3/
    PLOG/3.16E1 2.39E69 -1.923E1 1.476E4/
    PLOG/1.0E2 9.81E10 1.9E-1 8.306E2/
C2H3+O2=CO+CH3O    3.09E13 -0.89 3.682E3
    DUP
    PLOG/1.0E-2 8.19E18 -2.66E0 3.201E3/
    PLOG/1.0E-1 4.06E14 -1.32E0 8.858E2/
    PLOG/3.16E-1 4.34E14 -1.33E0 9.006E2/
    PLOG/1.0E0 1.03E11 -3.3E-1 -7.478E2/
    PLOG/3.16E0 1.89E12 -3.0E0 -8.995E3/
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   PLOG/1.0E1 1.93E24 -5.63E0 1.8E0/
   PLOG/3.16E1 1.1E18 -2.22E0 5.178E3/
   PLOG/1.0E2 5.79E32 -6.45E0 1.681E4/
C2H3+O2=CO+CH3O    3.09E13 -0.89 3.682E3
   DUP
   PLOG/1.0E-2 1.29E9 1.8E-1 -1.717E3/
   PLOG/1.0E-1 5.99E11 -2.93E0 -9.564E3/
   PLOG/3.16E-1 2.91E11 -2.93E0 -1.012E4/
   PLOG/1.0E0 5.77E21 -3.54E0 4.772E3/
   PLOG/3.16E0 4.99E15 -1.62E0 1.849E3/
   PLOG/1.0E1 9.33E16 -1.96E0 3.324E3/
   PLOG/3.16E1 1.02E72 -2.069E1 1.586E4/
   PLOG/1.0E2 1.1E9 3.1E-1 1.024E3/
C2H3+O2=CO2+CH3    6.16E13 -1.05 3.743E3
   DUP
   PLOG/1.0E-2 2.37E35 -7.76E0 1.263E4/
   PLOG/1.0E-1 1.73E35 -7.72E0 1.252E4/
   PLOG/3.16E-1 4.47E34 -7.55E0 1.214E4/
   PLOG/1.0E0 7.25E31 -6.7E0 1.044E4/
   PLOG/3.16E0 3.63E35 -7.75E0 1.283E4/
   PLOG/1.0E1 2.09E35 -7.53E0 1.405E4/
   PLOG/3.16E1 3.84E18 -2.44E0 5.408E3/
   PLOG/1.0E2 1.21E32 -6.32E0 1.619E4/
C2H3+O2=CO2+CH3    6.16E13 -1.05 3.743E3
   DUP
   PLOG/1.0E-2 6.27E13 -1.16E0 4.063E2/
   PLOG/1.0E-1 6.24E13 -1.16E0 4.014E2/
   PLOG/3.16E-1 6.12E13 -1.16E0 3.97E2/
   PLOG/1.0E0 5.32E13 -1.14E0 4.467E2/
   PLOG/3.16E0 1.45E14 -1.26E0 9.877E2/
   PLOG/1.0E1 5.02E13 -1.11E0 1.409E3/
   PLOG/3.16E1 1.4E70 -2.011E1 1.543E4/
   PLOG/1.0E2 9.21E8 2.5E-1 8.553E2/
C2H3+H=C2H2+H2    1.7E14 0.0 0.0E0
C2H3+OH=C2H2+H2O    3.011E13 0.0 0.0E0
C2H3+CH3=C2H2+CH4    3.92E11 0.0 0.0E0
2C2H3=C2H2+C2H4    9.6E11 0.0 0.0E0
C2H+H(+M)=C2H2(+M)    1.0E17 0.0 0.0E0
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/3.75E33 -4.8E0 1.9E3/
   TROE/6.46E-1 1.32E2 1.315E3 5.566E3/
C2H+H2=H+C2H2    4.9E5 2.5 5.6E2
C2H+O2=CO2+CHV    2.17E10 0.0 0.0E0
C2H+O2=HCO+CO    5.0E13 0.0 1.5E3
C2H+O=CO+CHV    6.2E12 0.0 0.0E0
C2H+O=CO+CH    5.0E13 0.0 0.0E0
C2H+OH=H+HCCO    2.0E13 0.0 0.0E0
C2H2+O=CH2+CO    7.395E8 1.28 2.472E3
C2H2+O=HCCO+H    2.958E9 1.28 2.472E3
C2H2+HO2=CH2CO+OH    6.03E9 0.0 7.949E3
C2H2+CH2=C3H3+H    1.2E13 0.0 6.62E3
C2H2+CH2(S)=C3H3+H    2.0E13 0.0 0.0E0
C2H2+HCO=C2H3+CO    1.0E7 2.0 6.0E3
C2H2+HCCO=C3H3+CO    1.0E11 0.0 3.0E3
C2H2+OH=C2H+H2O    2.632E6 2.14 1.706E4
C2H2+OH=CH2CO+H    1.578E3 2.56 -8.445E2
   PLOG/1.0E-2 1.578E3 2.56E0 -8.445E2/
   PLOG/2.5E-2 1.518E4 2.28E0 -2.921E2/
   PLOG/1.0E-1 3.017E5 1.92E0 5.981E2/
   PLOG/1.0E0 7.528E6 1.55E0 2.106E3/
   PLOG/1.0E1 5.101E6 1.65E0 3.4E3/
   PLOG/1.0E2 1.457E4 2.45E0 4.477E3/
C2H2+OH=CH3+CO    4.757E5 1.68 -3.298E2
   PLOG/1.0E-2 4.757E5 1.68E0 -3.298E2/
   PLOG/2.5E-2 4.372E6 1.4E0 2.265E2/
   PLOG/1.0E-1 7.648E7 1.05E0 1.115E3/
   PLOG/1.0E0 1.277E9 7.3E-1 2.579E3/
   PLOG/1.0E1 4.312E8 9.2E-1 3.736E3/
   PLOG/1.0E2 8.25E5 1.77E0 4.697E3/
CH3CHO(+M)=CH3+HCO(+M)    2.45E22 -1.74 8.6355E4
   LOW/1.03E59 -1.13E1 9.59125E4/
   TROE/2.49E-3 7.181E2 6.089E0 3.78E3/
CH3CHO(+M)=CH4+CO(+M)    2.72E21 -1.74 8.6355E4
   LOW/1.144E58 -1.13E1 9.59125E4/
   TROE/2.49E-3 7.181E2 6.089E0 3.78E3/
CH3CHO+O2=CH3CO+HO2    3.01E13 0.0 3.915E4
CH3CHO+O=CH3CO+OH    5.94E12 0.0 1.868E3
CH3CHO+H=CH3CO+H2    1.31E5 2.58 1.22E3
CH3CHO+OH=CH3CO+H2O    3.37E12 0.0 -6.19E2
CH3CHO+HO2=CH3CO+H2O2    3.01E12 0.0 1.192E4
CH3CHO+CH3=CH3CO+CH4    7.08E-4 4.58 1.966E3
CH3CHO+C2H3=CH3CO+C2H4    1.65E1 3.17 9.3998E3
CH3CHO+CH3O2=CH3CO+CH3O2H    3.01E12 0.0 1.192E4
CH3CHO+H=CH2CHO+H2    2.72E3 3.1 5.21E3
CH3CHO+OH=CH2CHO+H2O    1.72E5 2.4 8.15E2
CH3CHO+OH=CH3+HOCHO    3.0E15 -1.076 0.0E0
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CH3CO(+M)=CH3+CO(+M)    1.07E12 0.63 1.69E4
   LOW/5.65E18 -9.7E-1 1.46E4/
   TROE/6.29E-1 8.73E9 5.52E0 7.6E7/
CH3CO(+M)=CH2CO+H(+M)    9.413E7 1.917 4.49872E4
   LOW/1.516E51 -1.027E1 5.539E4/
   TROE/6.009E-1 8.103E9 6.677E2 5.0E9/
CH3CO+H=CH2CO+H2    2.0E13 0.0 0.0E0
CH3CO+O=CH2CO+OH    2.0E13 0.0 0.0E0
CH3CO+CH3=CH2CO+CH4    5.0E13 0.0 0.0E0
CH2CHO(+M)=CH2CO+H(+M)    1.43E15 -0.15 4.56E4
   LOW/6.0E29 -3.8E0 4.34239E4/
   TROE/9.85E-1 3.93E2 9.8E9 5.0E9/
CH2CHO(+M)=CH3+CO(+M)    2.93E12 0.29 4.03E4
   LOW/9.52E33 -5.07E0 4.13E4/
   TROE/7.13E-17 1.15E3 4.99E9 1.79E9/
CH2CHO+O2=O2CH2CHO    1.58E77 -21.9 1.935E4
   PLOG/1.0E-2 1.58E77 -2.19E1 1.935E4/
   PLOG/1.0E-1 3.88E69 -1.884E1 1.924E4/
   PLOG/1.0E0 7.8E59 -1.54E1 1.765E4/
   PLOG/1.0E1 3.05E50 -1.22E1 1.563E4/
CH2CHO+O2=CH2CO+HO2    1.88E5 2.37 2.373E4
   PLOG/1.0E-2 1.88E5 2.37E0 2.373E4/
   PLOG/1.0E-1 1.88E5 2.37E0 2.737E4/
   PLOG/1.0E0 2.51E5 2.33E0 2.38E4/
   PLOG/1.0E1 7.05E7 1.63E0 2.529E4/
CH2CHO+O2=>CH2O+CO+OH    2.68E17 -1.84 6.53E3
   PLOG/1.0E-2 2.68E17 -1.84E0 6.53E3/
   PLOG/1.0E-1 1.52E20 -2.58E0 8.98E3/
   PLOG/1.0E0 1.65E19 -2.22E0 1.034E4/
   PLOG/1.0E1 8.953E13 -6.0E-1 1.012E4/
CH2CHO+O2=HO2CH2CO    3.64E65 -21.87 1.902E4
   PLOG/1.0E-2 3.64E65 -2.187E1 1.902E4/
   PLOG/1.0E-1 3.64E58 -1.9E1 1.909E4/
   PLOG/1.0E0 6.65E48 -1.555E1 1.746E4/
   PLOG/1.0E1 4.8E38 -1.214E1 1.496E4/
O2CH2CHO=HO2CH2CO    8.27E30 -6.65 2.45E4
   PLOG/1.0E-2 8.27E30 -6.65E0 2.45E4/
   PLOG/1.0E-1 1.73E26 -4.99E0 2.376E4/
   PLOG/1.0E0 9.03E19 -2.92E0 2.217E4/
   PLOG/1.0E1 1.43E16 -1.67E0 2.121E4/
O2CH2CHO=CH2CO+HO2    2.05E40 -13.31 5.215E4
   PLOG/1.0E-2 2.05E40 -1.331E1 5.215E4/
   PLOG/1.0E-1 5.72E45 -1.4E1 5.22E4/
   PLOG/1.0E0 4.16E55 -1.576E1 5.508E4/
   PLOG/1.0E1 1.12E61 -1.604E1 6.001E4/
HO2CH2CO=>CO+CH2O+OH    2.36E17 -2.95 8.1E3
   PLOG/1.0E-2 2.36E17 -2.95E0 8.1E3/
   PLOG/1.0E-1 2.38E18 -2.95E0 8.1E3/
   PLOG/1.0E0 2.51E19 -2.95E0 8.11E3/
   PLOG/1.0E1 4.16E20 -3.02E0 8.24E3/
HO2CH2CO=CH2CO+HO2    1.12E7 -3.76 2.168E4
   PLOG/1.0E-2 1.12E7 -3.76E0 2.168E4/
   PLOG/1.0E-1 1.1E8 -3.76E0 2.168E4/
   PLOG/1.0E0 9.2E8 -3.73E0 2.163E4/
   PLOG/1.0E1 2.09E9 -3.55E0 2.122E4/
CH2+CO(+M)=CH2CO(+M)    8.1E11 0.0 0.0E0
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/2.69E33 -5.11E0 7.095E3/
   TROE/5.907E-1 2.75E2 1.226E3 5.185E3/
CH2CO+H=HCCO+H2    1.401E15 -0.171 8.7832E3
CH2CO+O=HCCO+OH    1.0E13 0.0 8.0E3
CH2CO+OH=HCCO+H2O    1.0E13 0.0 2.0E3
CH2CO+H=CH3+CO    7.704E13 -0.171 4.1832E3
CH+CH2O=H+CH2CO    9.46E13 0.0 -5.15E2
CH2CO+O=CH2+CO2    1.75E12 0.0 1.35E3
CH2CO+OH=CH2OH+CO    2.0E12 0.0 -1.01E3
CH2CO+CH2(S)=C2H4+CO    1.6E14 0.0 0.0E0
CH2CO+CH3=C2H5+CO    4.769E4 2.312 9.468E3
CH+CO+M=HCCO+M    7.57E22 -1.9 0.0E0
HCCO+OH=>H2+2CO    1.0E14 0.0 0.0E0
HCCO+O=>H+2CO    8.0E13 0.0 0.0E0
HCCO+CH=CO+C2H2    5.0E13 0.0 0.0E0
HCCO+H=CH2(S)+CO    1.0E14 0.0 0.0E0
HCCO+O2=>OH+2CO    1.91E11 -0.02 1.02E3
HCCO+O2=>CO2+CO+H    4.78E12 -0.142 1.15E3
C3H8(+M)=CH3+C2H5(+M)    1.29E37 -5.84 9.738E4
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/5.64E74 -1.574E1 9.8714E4/
   TROE/3.1E-1 5.0E1 3.0E3 9.0E3/
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NC3H7+H=C3H8    1.0E14 0.0 0.0E0
IC3H7+H=C3H8    1.0E14 0.0 0.0E0
C3H8+IC3H7=NC3H7+C3H8    3.0E10 0.0 1.29E4
C3H8+O2=NC3H7+HO2    6.0E13 0.0 5.229E4
C3H8+H=NC3H7+H2    3.49E5 2.69 6.45E3
C3H8+O=NC3H7+OH    3.71E6 2.4 5.505E3
C3H8+OH=NC3H7+H2O    2.732E7 1.811 8.684E2
C3H8+HO2=NC3H7+H2O2    4.08E1 3.59 1.716E4
C3H8+CH3=NC3H7+CH4    9.04E-1 3.65 7.154E3
C3H8+C2H3=NC3H7+C2H4    1.0E11 0.0 1.04E4
C3H8+C2H5=NC3H7+C2H6    1.0E11 0.0 1.04E4
C3H8+C3H5-A=NC3H7+C3H6    7.94E11 0.0 2.05E4
C3H8+CH3O2=NC3H7+CH3O2H    1.386E0 3.97 1.828E4
C3H8+IC3H7O2=NC3H7+IC3H7O2H    1.7E13 0.0 2.046E4
C3H8+O2CHO=NC3H7+HO2CHO    5.52E4 2.55 1.648E4
C3H8+O2=IC3H7+HO2    2.0E13 0.0 4.964E4
C3H8+H=IC3H7+H2    1.3E6 2.4 4.471E3
C3H8+O=IC3H7+OH    5.49E5 2.5 3.14E3
C3H8+OH=IC3H7+H2O    9.1715E9 0.935 5.047E2
C3H8+HO2=IC3H7+H2O2    6.32E1 3.37 1.372E4
C3H8+CH3=IC3H7+CH4    6.4E4 2.17 7.52E3
C3H8+C2H3=IC3H7+C2H4    1.0E11 0.0 1.04E4
C3H8+C2H5=IC3H7+C2H6    1.0E11 0.0 1.04E4
C3H8+C3H5-A=IC3H7+C3H6    7.94E11 0.0 1.62E4
C3H8+CH3O2=IC3H7+CH3O2H    1.019E1 3.58 1.481E4
C3H8+O2CHO=IC3H7+HO2CHO    1.475E4 2.6 1.391E4
C3H8+IC3H7O2=IC3H7+IC3H7O2H    2.0E12 0.0 1.7E4
IC3H7+H=C2H5+CH3    2.0E13 0.0 0.0E0
IC3H7+OH=C3H6+H2O    2.41E13 0.0 0.0E0
IC3H7+O=CH3COCH3+H    4.818E13 0.0 0.0E0
IC3H7+O=CH3CHO+CH3    4.818E13 0.0 0.0E0
O2+NC3H7=HO2+C3H6    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 5.05E10 2.06E-2 5.01905E2/
   PLOG/1.0E-1 7.47E15 -1.45E0 4.1129E3/
   PLOG/1.0E0 1.18E19 -2.35E0 7.29953E3/
   PLOG/1.0E1 2.63E0 3.46E0 2.48117E3/
   PLOG/1.0E2 7.37E2 2.71E0 5.49647E3/
O2+IC3H7=HO2+C3H6    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 5.91E9 4.28E-1 -1.43857E3/
   PLOG/1.0E-1 1.6E14 -8.45E-1 1.42377E3/
   PLOG/1.0E0 4.05E18 -2.07E0 4.97147E3/
   PLOG/1.0E1 4.91E17 -1.66E0 6.96404E3/
   PLOG/1.0E2 9.84E7 1.34E0 5.37912E3/
O2+NC3H7=C3H6OOH1-2    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 2.97E15 -2.84E0 3.56751E3/
   PLOG/1.0E-1 2.64E12 -1.58E0 3.36232E3/
   PLOG/1.0E0 2.78E2 1.63E0 -4.92364E2/
   PLOG/1.0E1 1.3E14 -1.73E0 5.16366E3/
   PLOG/1.0E2 7.63E16 -2.3E0 9.03614E3/
O2+NC3H7=C3H6OOH1-3    1.0E11 0.0 0.0E0
   DUP
   PLOG/1.0E-2 3.09E146 -4.59E1 3.12822E4/
   PLOG/1.0E-1 1.26E47 -1.24E1 8.20313E3/
   PLOG/1.0E0 1.3E23 -4.03E0 5.08867E3/
   PLOG/1.0E1 3.94E-18 8.88E0 -6.1997E3/
   PLOG/1.0E2 6.58E-15 7.8E0 -3.43101E3/
O2+NC3H7=C3H6OOH1-3    1.0E11 0.0 0.0E0
   DUP
   PLOG/1.0E-2 6.19E8 8.78E-1 1.11866E4/
   PLOG/1.0E-1 1.12E14 -5.31E-1 1.38975E4/
   PLOG/1.0E0 2.07E14 -4.0E-1 1.51581E4/
   PLOG/1.0E1 1.02E21 -2.26E0 1.8554E4/
   PLOG/1.0E2 1.05E15 -4.86E-1 1.58767E4/
O2+NC3H7=NC3H7O2    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 9.2E8 4.05E-1 -4.39865E3/
   PLOG/1.0E-1 1.45001E14 -9.84E-1 -1.7108E3/
   PLOG/1.0E0 2.09001E13 -4.99E-1 -9.38423E2/
   PLOG/1.0E1 1.15001E20 -2.42E0 2.45126E3/
   PLOG/1.0E2 2.07001E16 -1.3E0 8.03419E2/
O2+IC3H7=IC3H7O2    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 7.33E5 1.33E0 -6.34564E3/
   PLOG/1.0E-1 2.24E11 -1.05E-1 -3.69787E3/
   PLOG/1.0E0 1.54E18 -2.02E0 -4.98567E2/
   PLOG/1.0E1 6.74E27 -4.85E0 3.77982E3/
   PLOG/1.0E2 1.67E29 -5.15E0 5.03645E3/
NC3H7O2=HO2+C3H6    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 4.3E53 -1.4E1 3.9526E4/
   PLOG/1.0E-1 9.52E57 -1.5E1 4.26843E4/
   PLOG/1.0E0 6.9E33 -7.03E0 3.65435E4/
   PLOG/1.0E1 2.55E16 -1.22E0 3.24803E4/
   PLOG/1.0E2 2.26E32 -6.22E0 3.79482E4/
IC3H7O2=C3H6+HO2    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 1.61E75 -2.06E1 4.6203E4/
   PLOG/1.0E-1 1.72E66 -1.73E1 4.54589E4/
   PLOG/1.0E0 4.03E56 -1.4E1 4.40102E4/
   PLOG/1.0E1 1.29E40 -8.58E0 3.94186E4/
   PLOG/1.0E2 6.4E25 -4.02E0 3.49139E4/
NC3H7O2=C3H6OOH1-2    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 9.48E20 -5.14E0 2.37097E4/
   PLOG/1.0E-1 1.24E22 -4.93E0 2.64778E4/
   PLOG/1.0E0 1.99E20 -3.92E0 2.76341E4/
   PLOG/1.0E1 2.58E42 -1.03E1 3.76702E4/
   PLOG/1.0E2 2.79E42 -1.01E1 3.91082E4/
```

```
NC3H7O2=C3H6OOH1-3    1.0E11 0.0 0.0E0
   DUP
   PLOG/1.0E-2 1.69E4 1.56E0 1.85703E4/
   PLOG/1.0E-1 5.85E4 1.66E0 1.9612E4/
   PLOG/1.0E0 1.5E3 2.32E0 1.97537E4/
   PLOG/1.0E1 1.01E0 3.38E0 1.89948E4/
   PLOG/1.0E2 3.39E0 3.23E0 1.92093E4/
NC3H7O2=C3H6OOH1-3    1.0E11 0.0 0.0E0
   DUP
   PLOG/1.0E-2 7.72E17 5.57E-4 4.03931E4/
   PLOG/1.0E-1 7.02E18 -1.18E-3 4.69318E4/
   PLOG/1.0E0 1.19E20 -7.68E-3 5.52238E4/
   PLOG/1.0E1 1.26E23 -3.15E-2 7.54407E4/
   PLOG/1.0E2 4.06E26 -3.66E-2 9.94007E4/
C3H6OOH1-2=C3H6OOH1-3    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 6.24E-135 4.57E1 -1.94619E4/
   PLOG/1.0E-1 3.0E-176 5.79E1 -4.04217E4/
   PLOG/1.0E0 1.0E-15 1.02E1 2.85937E4/
   PLOG/1.0E1 5.36E-85 3.1E1 5.35821E2/
   PLOG/1.0E2 1.58E-133 4.51E1 -2.11265E4/
C3H6OOH1-2=HO2+C3H6    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 1.49E-15 9.24E0 1.89606E4/
   PLOG/1.0E-1 2.9E-44 1.76E1 1.8887E3/
   PLOG/1.0E0 1.08E31 -4.56E0 3.21226E4/
   PLOG/1.0E1 1.16E-9 7.46E0 1.47457E4/
   PLOG/1.0E2 1.27E-15 8.78E0 9.26654E3/
C3H6OOH1-3=HO2+C3H6    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 3.55E-90 2.75E1 -3.5057E4/
   PLOG/1.0E-1 3.21E4 -3.42E-1 4.33923E3/
   PLOG/1.0E0 1.97E26 -5.97E0 1.87428E4/
   PLOG/1.0E1 1.6E10 -4.44E-1 1.75318E4/
   PLOG/1.0E2 3.45E17 -2.82E0 2.15791E4/
O2+C3H6OOH1-3=C3H6OOH1-3O2    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 2.95E42 -1.02E1 5.86236E3/
   PLOG/1.0E-1 4.3E42 -9.88E0 7.52686E3/
   PLOG/1.0E0 7.47E36 -7.85E0 6.72435E3/
   PLOG/1.0E1 2.18E27 -4.75E0 4.02617E3/
   PLOG/1.0E2 1.46E18 -1.85E0 1.00584E3/
O2+C3H6OOH1-3=OH+C3KET13    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 6.2E30 -6.23E0 5.24155E3/
   PLOG/1.0E-1 2.42E32 -6.58E0 8.14472E3/
   PLOG/1.0E0 3.7E27 -5.03E0 8.65443E3/
   PLOG/1.0E1 3.58E15 -1.36E0 5.98573E3/
   PLOG/1.0E2 6.32E0 3.02E0 1.62507E3/
C3H6OOH1-3O2=C3KET13+OH    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 4.08E29 -6.39E0 2.34402E4/
   PLOG/1.0E-1 2.49E25 -4.95E0 2.26125E4/
   PLOG/1.0E0 1.01E19 -2.88E0 2.08036E4/
   PLOG/1.0E1 4.46E11 -5.38E-1 1.84411E4/
   PLOG/1.0E2 1.67E5 1.48E0 1.62379E4/
C3KET13=>CH2O+CH2CHO+OH    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 3.41E64 -1.59E1 5.57614E4/
   PLOG/1.0E-1 1.97E61 -1.46E1 5.60115E4/
   PLOG/1.0E0 1.07E54 -1.21E1 5.45628E4/
   PLOG/1.0E1 5.29E43 -8.74E0 5.15685E4/
   PLOG/1.0E2 4.06E33 -5.54E0 4.82254E4/
IC3H7O2+H2=IC3H7O2H+H    3.01E13 0.0 2.603E4
IC3H7O2+HO2=IC3H7O2H+O2    1.75E10 0.0 -3.275E3
IC3H7O2+CH2O=IC3H7O2H+HCO    5.6E12 0.0 1.36E4
IC3H7O2+CH4=IC3H7O2H+CH3    1.12E13 0.0 2.464E4
IC3H7O2+CH3CHO=IC3H7O2H+CH3CO    2.8E12 0.0 1.36E4
IC3H7O2+C2H4=IC3H7O2H+C2H3    1.13E13 0.0 3.043E4
IC3H7O2+C2H6=IC3H7O2H+C2H5    1.7E13 0.0 2.046E4
CH2(S)+C2H4=C3H6    4.82E57 -14.3 1.71E4
   DUP
   PLOG/1.0E-2 4.82E57 -1.43E1 1.71E4/
   PLOG/1.0E-1 3.84E59 -1.44E1 1.84E4/
   PLOG/1.0E0 2.13E58 -1.35E1 2.04E4/
   PLOG/1.0E1 8.48E52 -1.16E1 2.07E4/
   PLOG/1.0E2 6.07E47 -9.85E0 2.21E4/
CH2(S)+C2H4=C3H6    4.82E57 -14.3 1.71E4
   DUP
   PLOG/1.0E-2 1.15E45 -1.11E1 6.1452E3/
   PLOG/1.0E-1 1.83E45 -1.07E1 6.6385E3/
   PLOG/1.0E0 1.3E40 -8.77E0 5.8638E3/
   PLOG/1.0E1 2.27E32 -6.14E0 4.3179E3/
   PLOG/1.0E2 1.28E24 -3.49E0 2.5299E3/
CH2(S)+C2H4=C3H5-A+H    8.2E19 -2.06 1.15E3
   DUP
   PLOG/1.0E-2 8.2E19 -2.06E0 1.15E3/
   PLOG/1.0E-1 2.27E21 -2.44E0 2.65E3/
   PLOG/1.0E0 4.44E35 -6.55E0 1.39E4/
   PLOG/1.0E1 1.18E28 -4.09E0 1.4E4/
   PLOG/1.0E2 6.51E26 -3.58E0 1.89E4/
CH2(S)+C2H4=C3H5-A+H    8.2E19 -2.06 1.15E3
   DUP
   PLOG/1.0E-2 1.08E7 1.62E0 -3.1746E3/
   PLOG/1.0E-1 1.37E5 2.15E0 -3.7992E3/
   PLOG/1.0E0 3.89E14 -4.2E-1 1.2376E3/
   PLOG/1.0E1 2.45E10 6.7E-1 7.5093E2/
   PLOG/1.0E2 1.81E2 2.97E0 -7.4603E2/
CH2(S)+C2H4=C2H3+CH3    1.77E19 -1.94 6.79E3
   DUP
```

PLOG/1.0E-2 1.77E19 -1.94E0 6.79E3/
PLOG/1.0E-1 1.68E19 -1.8E0 4.31E3/
PLOG/1.0E0 4.16E24 -3.19E0 9.76E3/
PLOG/1.0E1 7.89E24 -3.07E0 1.39E4/
PLOG/1.0E2 7.36E29 -4.28E0 2.38E4/
CH2(S)+C2H4=C2H3+CH3 1.77E19 -1.94 6.79E3
DUP
PLOG/1.0E-2 4.3E12 1.9E-1 -1.1041E2/
PLOG/1.0E-1 2.26E11 5.4E-1 4.781E1/
PLOG/1.0E0 4.92E9 1.02E0 5.9977E2/
PLOG/1.0E1 1.47E8 1.33E0 1.2284E3/
PLOG/1.0E2 8.11E10 5.5E-1 5.5065E3/
C2H3+CH3=C3H5-A+H 4.12E29 -4.95 8.0E3
DUP
PLOG/1.0E-2 4.12E29 -4.95E0 8.0E3/
PLOG/1.0E-1 4.86E30 -5.03E0 1.13E4/
PLOG/1.0E0 5.3E29 -4.57E0 1.44E4/
PLOG/1.0E1 1.32E30 -4.54E0 1.93E4/
PLOG/1.0E2 5.16E28 -4.03E0 2.38E4/
C2H3+CH3=C3H5-A+H 4.12E29 -4.95 8.0E3
DUP
PLOG/1.0E-2 5.73E15 -7.7E-1 1.1959E3/
PLOG/1.0E-1 2.06E13 -7.4E-2 1.4287E3/
PLOG/1.0E0 4.48E10 6.0E-1 1.4216E3/
PLOG/1.0E1 4.1E6 1.71E0 1.0569E3/
PLOG/1.0E2 1.37E-1 3.91E0 -3.5355E2/
C3H6=C2H3+CH3 1.88E78 -18.7 1.3E5
DUP
PLOG/1.0E-2 1.88E78 -1.87E1 1.3E5/
PLOG/1.0E-1 8.73E76 -1.79E1 1.32E5/
PLOG/1.0E0 5.8E75 -1.72E1 1.34E5/
PLOG/1.0E1 8.12E71 -1.58E1 1.36E5/
PLOG/1.0E2 2.15E64 -1.34E1 1.35E5/
C3H6=C2H3+CH3 1.88E78 -18.7 1.3E5
DUP
PLOG/1.0E-2 1.69E59 -1.36E1 1.1329E5/
PLOG/1.0E-1 2.0E60 -1.37E1 1.1489E5/
PLOG/1.0E0 6.7E54 -1.18E1 1.1384E5/
PLOG/1.0E1 1.06E47 -9.27E0 1.1151E5/
PLOG/1.0E2 7.29E38 -6.7E0 1.0874E5/
C3H6=C3H5-A+H 9.16E74 -17.6 1.2E5
DUP
PLOG/1.0E-2 9.16E74 -1.76E1 1.2E5/
PLOG/1.0E-1 1.73E70 -1.6E1 1.2E5/
PLOG/1.0E0 1.08E71 -1.59E1 1.2486E5/
PLOG/1.0E1 6.4E65 -1.42E1 1.25E5/
PLOG/1.0E2 8.05E56 -1.15E1 1.22E5/
C3H6=C3H5-A+H 9.16E74 -17.6 1.2E5
DUP
PLOG/1.0E-2 2.98E54 -1.23E1 1.012E5/
PLOG/1.0E-1 1.37E43 -8.87E0 9.6365E4/
PLOG/1.0E0 6.28E42 -8.51E0 9.8004E4/
PLOG/1.0E1 4.73E35 -6.26E0 9.5644E4/
PLOG/1.0E2 4.34E28 -4.06E0 9.3114E4/
C3H5-T+H=C3H6 4.96E60 -15.2 1.8E4
DUP
PLOG/1.0E-2 4.96E60 -1.52E1 1.8E4/
PLOG/1.0E-1 3.2E62 -1.51E1 2.01E4/
PLOG/1.0E0 2.31E60 -1.4E1 2.19E4/
PLOG/1.0E1 3.69E54 -1.2E1 2.21E4/
PLOG/1.0E2 1.15E50 -1.04E1 2.33E4/
C3H5-T+H=C3H6 4.96E60 -15.2 1.8E4
DUP
PLOG/1.0E-2 1.49E48 -1.2E1 7.2033E3/
PLOG/1.0E-1 6.76E46 -1.11E1 7.6299E3/
PLOG/1.0E0 1.09E40 -8.66E0 6.4478E3/
PLOG/1.0E1 2.38E31 -5.73E0 4.506E3/
PLOG/1.0E2 5.69E25 -3.83E0 3.2504E3/
C3H5-T+H=C3H5-A+H 2.11E17 -1.08 1.29E3
DUP
PLOG/1.0E-2 2.11E17 -1.08E0 1.29E3/
PLOG/1.0E-1 9.05E29 -4.91E0 8.54E3/
PLOG/1.0E0 2.98E30 -4.79E0 1.2E4/
PLOG/1.0E1 8.22E28 -4.14E0 1.54E4/
PLOG/1.0E2 2.28E29 -4.12E0 2.09E4/
C3H5-T+H=C3H5-A+H 2.11E17 -1.08 1.29E3
DUP
PLOG/1.0E-2 6.41E3 2.61E0 -3.7784E3/
PLOG/1.0E-1 5.19E14 -3.0E-1 1.0904E3/
PLOG/1.0E0 8.17E11 4.9E-1 1.1846E3/
PLOG/1.0E1 2.79E9 1.09E0 1.1875E3/
PLOG/1.0E2 6.75E3 2.7E0 3.738E2/
C3H5-T+H=C2H3+CH3 3.31E16 -0.69 5.2E3
DUP
PLOG/1.0E-2 3.31E16 -6.9E-1 5.2E3/
PLOG/1.0E-1 9.04E16 -8.1E-1 4.8E3/
PLOG/1.0E0 2.01E24 -2.86E0 1.09E4/
PLOG/1.0E1 2.75E26 -3.31E0 1.58E4/
PLOG/1.0E2 3.15E32 -4.83E0 2.6E4/
C3H5-T+H=C2H3+CH3 3.31E16 -0.69 5.2E3
DUP
PLOG/1.0E-2 8.04E13 -1.4E-1 1.15E3/
PLOG/1.0E-1 7.17E10 6.7E-1 6.738E2/

PLOG/1.0E0 9.97E8 1.36E0 1.5964E3/
PLOG/1.0E1 7.41E7 1.57E0 2.1088E3/
PLOG/1.0E2 2.7E12 3.2E-1 6.7918E3/
C3H6+H=C3H5-A+H2 3.644E5 2.455 4.3612E3
C3H6+O2=C3H5-A+HO2 5.96E19 -1.67 4.61921E4
C3H6+O=C3H5-A+OH 5.24E11 0.7 5.884E3
C3H6+OH=C3H5-A+H2O 4.46E6 2.072 1.0508E3
C3H6+HO2=C3H5-A+H2O2 3.07E-2 4.403 1.35472E4
C3H6+CH3=C3H5-A+CH4 2.21E0 3.5 5.675E3
C3H6+CH3O2=C3H5-A+CH3O2H 7.68E-2 4.403 1.35472E4
C3H6+C2H5=C3H5-A+C2H6 1.0E11 0.0 9.8E3
C3H6+IC3H7O2=C3H5-A+IC3H7O2H 7.68E-2 4.403 1.35472E4
C3H6+H=C3H5-T+H2 1.498E2 3.381 8.9095E3
C3H6+O=C3H5-T+OH 6.03E10 0.7 7.632E3
C3H6+OH=C3H5-T+H2O 1.8E6 1.979 2.2352E3
C3H6+HO2=C3H5-T+H2O2 1.56E4 2.82 2.44279E4
C3H6+O2=C3H5-T+HO2 1.0E13 0.0 5.877E4
C3H6+CH3=C3H5-T+CH4 8.4E-1 3.5 1.166E4
C3H6+O=C2H4+CH2O 2.11E12 0.36357832 3.6251147E3
PLOG/1.0E-1 3.239515E10 8.6277366E-1 2.1012156E3/
PLOG/1.0E0 3.7102143E10 8.4675413E-1 2.152084E3/
PLOG/1.0E1 6.4621495E10 7.7988106E-1 2.3372114E3/
PLOG/3.0E1 1.79581E11 6.5836787E-1 2.7279312E3/
PLOG/1.0E2 2.11E12 3.6357832E-1 3.6251147E3/
C3H6+O=C2H5+HCO 4.5392427E9 0.46990082 3.3909714E3
PLOG/1.0E-1 3.81938E20 -2.8445151E0 2.2008093E3/
PLOG/1.0E0 6.782E23 -3.7431204E0 5.0411938E3/
PLOG/1.0E1 5.78554E21 -3.0582581E0 6.6882314E3/
PLOG/3.0E1 4.41563E16 -1.5513902E0 5.3826196E3/
PLOG/1.0E2 4.5392427E9 4.6990082E-1 3.3909714E3/
C3H6+O=CH3+CH2CHO 6.118106E10 0.72471172 1.7372183E3
PLOG/1.0E-1 7.1169661E8 1.2452729E0 -2.2913843E2/
PLOG/1.0E0 2.7972334E9 1.0825886E0 2.8259222E2/
PLOG/1.0E1 1.8003295E10 8.6375535E-1 1.0689554E3/
PLOG/3.0E1 3.3952128E10 7.9012293E-1 1.3842371E3/
PLOG/1.0E2 6.118106E10 7.2471172E-1 1.7372183E3/
C3H6+O=H2+CH3CHCO 2.92162E11 -0.46592912 -7.2082123E2
PLOG/1.0E-1 4.34829E14 -1.3823626E0 3.2638251E2/
PLOG/1.0E0 5.03596E17 -2.2524612E0 2.2980547E3/
PLOG/1.0E1 1.88555E14 -1.2406751E0 9.8652802E2/
PLOG/3.0E1 1.45046E14 -1.2325199E0 8.0590204E2/
PLOG/1.0E2 2.92162E11 -4.6592912E-1 -7.2082123E2/
C3H6+O=CO+C2H6 2.8063963E10 -0.15197791 8.5133477E3
PLOG/1.0E-1 3.30559E19 -3.0550032E0 4.0607322E3/
PLOG/1.0E0 4.47648E13 -1.2992022E0 2.5097214E3/
PLOG/1.0E1 7.29311E16 -2.0833492E0 7.7710391E3/
PLOG/3.0E1 2.2306699E1 2.136199E0 -3.9348716E3/
PLOG/1.0E2 2.8063963E10 -1.5197791E-1 8.5133477E3/
C3H6+O=H2+C2H4+CO 1.9064245E5 1.4148871 1.8470398E3
PLOG/1.0E-1 1.40605E19 -2.7684405E0 1.5882145E3/
PLOG/1.0E0 1.42188E22 -3.5758173E0 4.455772E3/
PLOG/1.0E1 4.5976E19 -2.7595153E0 6.0180806E3/
PLOG/3.0E1 5.57149E13 -1.0280579E0 4.2239531E3/
PLOG/1.0E2 1.9064245E5 1.4148871E0 1.8470398E3/
C3H6+H=NC3H7 1.0E0 1.0 0.0E0
DUP
PLOG/1.3E-3 7.99E81 -2.3161E1 2.2239E4/
PLOG/4.0E-2 4.24E68 -1.8427E1 1.9665E4/
PLOG/1.0E0 1.04E49 -1.15E1 1.5359E4/
PLOG/1.0E1 6.2E41 -8.892E0 1.4637E4/
PLOG/1.0E2 4.22E27 -4.39E0 9.3458E3/
C3H6+H=NC3H7 1.0E0 1.0 0.0E0
DUP
PLOG/1.3E-3 1.85E26 -5.83E0 3.8658E3/
PLOG/4.0E-2 2.82E30 -6.49E0 5.4708E3/
PLOG/1.0E0 3.78E28 -5.57E0 5.6251E3/
PLOG/1.0E1 1.46E25 -4.28E0 5.2478E3/
PLOG/1.0E2 1.0E-10 0.0E0 0.0E0/
C3H6+H=C2H4+CH3 1.0E0 1.0 1.0E0
DUP
PLOG/1.3E-3 1.54E9 1.35E0 2.542E3/
PLOG/4.0E-2 7.88E10 8.7E-1 3.5996E3/
PLOG/1.0E0 2.67E12 4.7E-1 5.4311E3/
PLOG/1.0E1 9.25E22 -2.6E0 1.2898E4/
PLOG/1.0E2 1.32E23 -2.42E0 1.65E4/
C3H6+H=C2H4+CH3 1.0E0 1.0 1.0E0
DUP
PLOG/1.3E-3 1.0E-10 0.0E0 0.0E0/
PLOG/4.0E-2 1.0E-10 0.0E0 0.0E0/
PLOG/1.0E0 1.0E-10 0.0E0 0.0E0/
PLOG/1.0E1 1.24E5 2.52E0 3.6791E3/
PLOG/1.0E2 2.51E3 2.91E0 3.9809E3/
C3H6+H=IC3H7 1.0E0 1.0 1.0E0
DUP
PLOG/1.3E-3 1.35E44 -1.068E1 8.1964E3/
PLOG/4.0E-2 2.11E57 -1.423E1 1.5147E4/
PLOG/1.0E0 3.26E61 -1.494E1 2.0161E4/
PLOG/1.0E1 5.3E56 -1.312E1 2.0667E4/
PLOG/1.0E2 1.11E50 -1.08E1 2.0202E4/
C3H6+H=IC3H7 1.0E0 1.0 1.0E0
DUP
PLOG/1.3E-3 2.17E130 -3.258E1 1.3614E5/
PLOG/4.0E-2 2.25E29 -5.84E0 4.2419E3/

```
   PLOG/1.0E0 1.06E30 -5.63E0 5.6134E3/
   PLOG/1.0E1 6.11E26 -4.44E0 5.1823E3/
   PLOG/1.0E2 2.73E23 -3.26E0 4.597E3/
C2H4+CH3=NC3H7    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.3E-3 8.67E48 -1.254E1 1.8206E4/
   PLOG/4.0E-2 1.06E49 -1.204E1 2.0001E4/
   PLOG/1.0E0 7.67E47 -1.117E1 2.2366E4/
   PLOG/1.0E1 1.81E45 -1.003E1 2.3769E4/
   PLOG/1.0E2 2.04E40 -8.25E0 2.4214E4/
C2H4+CH3=NC3H7    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.3E-3 1.12E43 -1.13E1 1.308E4/
   PLOG/4.0E-2 7.28E39 -9.88E0 1.3164E4/
   PLOG/1.0E0 2.6E33 -7.46E0 1.2416E4/
   PLOG/1.0E1 3.85E27 -5.38E0 1.1455E4/
   PLOG/1.0E2 1.66E21 -3.17E0 1.0241E4/
C3H5-A+H=C3H4-A+H2    1.232E3 3.035 2.582E3
C3H5-A+OH=C3H4-A+H2O    6.0E12 0.0 0.0E0
C3H5-A+CH3=C3H4-A+CH4    3.0E12 -0.32 -1.31E2
C3H5-A+C2H5=C3H4-A+C2H6    4.0E11 0.0 0.0E0
C3H5-A+C2H3=C3H4-A+C2H4    1.0E12 0.0 0.0E0
2C3H4-A=C3H5-A+C3H3    5.0E14 0.0 6.47467E4
2C3H5-A=C3H4-A+C3H6    9.55E40 -9.3 1.247E4
   PLOG/1.0E0 4.77E40 -9.3E0 1.247E4/
   PLOG/4.0E0 3.97E32 -6.8E0 9.18E3/
   PLOG/1.0E1 1.46E28 -5.5E0 7.41E3/
C3H5-A+C2H5=C2H4+C3H6    4.0E11 0.0 0.0E0
C3H5-A+HCO=C3H6+CO    6.0E13 0.0 0.0E0
C3H5-T+O=CH3+CH2CO    6.0E13 0.0 0.0E0
C3H5-T+OH=>CH3+CH2CO+H    5.0E12 0.0 0.0E0
C3H5-T+HO2=>CH3+CH2CO+OH    2.0E13 0.0 0.0E0
C3H5-T+HCO=C3H6+CO    9.0E13 0.0 0.0E0
C3H5-A+O=C2H3CHO+H    6.0E13 0.0 0.0E0
C3H5-A+OH=>C2H3CHO+2H    5.3E37 -6.71 2.9306E4
   PLOG/1.0E-1 5.3E37 -6.71E0 2.9306E4/
   PLOG/1.0E0 4.2E32 -5.16E0 3.0126E4/
   PLOG/1.0E1 1.6E20 -1.56E0 2.633E4/
C3H5-A+O2=C3H4-A+HO2    4.99E15 -1.4 2.2428E4
   PLOG/1.0E0 4.99E15 -1.4E0 2.2428E4/
   PLOG/1.0E1 2.18E21 -2.85E0 3.0755E4/
C3H5-A+O2=CH3CO+CH2O    1.19E15 -1.01 2.0128E4
   PLOG/1.0E0 1.19E15 -1.01E0 2.0128E4/
   PLOG/1.0E1 7.14E15 -1.21E0 2.1046E4/
C3H5-A+O2=C2H3CHO+OH    1.82E13 -0.41 2.2859E4
   PLOG/1.0E0 1.82E13 -4.1E-1 2.2859E4/
   PLOG/1.0E1 2.47E13 -4.5E-1 2.3017E4/
C3H5-T+O2=CH3CO+CH2O    2.55E20 -2.608 1.5657E3
C3H5-T+O2=C3H4-A+HO2    3.59E10 -0.27 -4.136E2
C3H5-A+HO2=C2H3CHO+H2O    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 1.09E0 3.01E0 -3.4211E3/
   PLOG/1.0E-1 6.35E1 2.5E0 -2.3414E3/
   PLOG/1.0E0 6.05E5 1.39E0 5.951E2/
   PLOG/1.0E1 3.1E5 1.59E0 2.6776E3/
   PLOG/1.0E2 5.07E-5 4.59E0 9.275E2/
C2H3+CH2O=C2H3CHO+H    1.0E11 0.0 0.0E0
   PLOG/1.0E-3 2.6E4 2.26E0 1.5103E3/
   PLOG/1.0E-2 5.13E4 2.17E0 1.6755E3/
   PLOG/1.0E-1 3.99E5 1.91E0 2.2183E3/
   PLOG/1.0E0 1.75E7 1.45E0 3.428E3/
   PLOG/1.0E1 1.35E9 9.33E-1 5.173E3/
   PLOG/1.0E2 2.24E11 3.57E-1 8.0013E3/
   PLOG/1.0E3 6.01E5 2.09E0 7.8956E3/
C2H3+CH2O=C2H4+HCO    1.0E11 0.0 0.0E0
   PLOG/1.0E-3 1.11E7 1.09E0 1.8072E3/
   PLOG/1.0E-2 2.47E7 9.93E-1 1.9949E3/
   PLOG/1.0E-1 2.47E8 7.04E-1 2.5962E3/
   PLOG/1.0E0 1.42E10 2.09E-1 3.9342E3/
   PLOG/1.0E1 3.45E13 -7.26E-1 6.9443E3/
   PLOG/1.0E2 3.31E14 -8.66E-1 1.09657E4/
   PLOG/1.0E3 1.65E1 3.17E0 9.3998E3/
C3H6+OH=CH3CHO+CH3    6.93E5 1.49 -5.36E2
   PLOG/1.3E-3 6.93E5 1.49E0 -5.36E2/
   PLOG/1.0E-2 5.94E3 2.01E0 -5.6E2/
   PLOG/1.3E-2 1.1E3 2.22E0 -6.8E2/
   PLOG/2.5E-2 1.07E2 2.5E0 -7.59E2/
   PLOG/1.0E-1 7.83E-1 3.1E0 -9.19E2/
   PLOG/1.315E-1 3.07E-1 3.22E0 -9.46E2/
   PLOG/1.0E0 3.16E-4 4.05E0 -1.144E3/
   PLOG/1.0E1 7.59E-6 4.49E0 -6.8E2/
   PLOG/1.0E2 5.45E-5 4.22E0 1.141E3/
C3H6+OH=C3H6OH2-1    5.1E54 -20.7 3.2402E4
   DUP
   PLOG/1.3E-3 2.14E59 -1.584E1 1.1594E4/
   PLOG/1.0E-2 2.43E59 -1.551E1 1.2898E4/
   PLOG/1.3E-2 9.3E58 -1.534E1 1.2913E4/
   PLOG/2.5E-2 8.83E57 -1.493E1 1.2936E4/
   PLOG/1.0E-1 4.5E55 -1.404E1 1.2945E4/
   PLOG/1.315E-1 1.33E55 -1.385E1 1.2887E4/
   PLOG/1.0E0 5.18E49 -1.204E1 1.1493E4/
   PLOG/1.0E1 2.14E41 -9.35E0 8.921E3/
   PLOG/1.0E2 7.65E31 -6.31E0 6.088E3/
C3H6+OH=C3H6OH2-1    5.1E54 -20.7 3.2402E4
```

DUP
PLOG/1.3E-3 7.68E77 -2.07E1 3.2402E4/
PLOG/1.0E-2 9.13E76 -2.0E1 3.3874E4/
PLOG/1.3E-2 3.55E75 -1.958E1 3.2874E4/
PLOG/2.5E-2 1.23E73 -1.879E1 3.1361E4/
PLOG/1.0E-1 3.45E67 -1.701E1 2.7909E4/
PLOG/1.315E-1 2.41E66 -1.664E1 2.7162E4/
PLOG/1.0E0 6.5E58 -1.417E1 2.3079E4/
PLOG/1.0E1 2.53E53 -1.223E1 2.2976E4/
PLOG/1.0E2 4.78E47 -1.023E1 2.3772E4/
C3H4-A=C3H3+H 1.32E31 -4.749 9.20795E4
PLOG/1.0E0 1.32E31 -4.749E0 9.20795E4/
PLOG/1.0E1 3.65E25 -2.95E0 9.06249E4/
C3H4-A+H=C3H3+H2 6.625E3 3.095 5.522E3
C3H4-A+O2=C3H3+HO2 4.0E13 0.0 4.132E4
C3H4-A+OH=C3H3+H2O 1.482E5 2.492 1.8072E3
C3H4-A+CH3=C3H3+CH4 1.3E12 0.0 7.7E3
C3H4-A+HO2=C3H3+H2O2 3.58E-2 4.17 9.6328E3
C3H4-A+CH3O2=C3H3+CH3O2H 7.161E-2 4.17 9.6328E3
C3H4-A+C3H5-A=C3H3+C3H6 2.0E11 0.0 7.7E3
C3H4-A+H=C3H5-A 2.21E61 -15.25 2.0076E4
DUP
PLOG/1.0E-3 2.21E61 -1.525E1 2.0076E4/
PLOG/3.9E-2 1.24E52 -1.202E1 1.7839E4/
PLOG/1.0E0 4.67E51 -1.145E1 2.134E4/
PLOG/1.0E1 3.75E48 -1.027E1 2.2511E4/
PLOG/1.0E2 4.23E43 -8.61E0 2.2522E4/
C3H4-A+H=C3H5-A 2.21E61 -15.25 2.0076E4
DUP
PLOG/1.0E-3 2.8E38 -8.67E0 8.035E3/
PLOG/3.9E-2 9.33E36 -8.19E0 7.462E3/
PLOG/1.0E0 3.32E30 -5.78E0 6.913E3/
PLOG/1.0E1 2.29E26 -4.32E0 6.163E3/
PLOG/1.0E2 4.38E21 -2.71E0 5.187E3/
C3H4-A+H=C3H5-T 6.44E102 -27.51 5.1768E4
DUP
PLOG/1.0E-3 6.44E102 -2.751E1 5.1768E4/
PLOG/3.9E-2 1.55E53 -1.31E1 1.4472E4/
PLOG/1.0E0 1.9E53 -1.259E1 1.6726E4/
PLOG/1.0E1 7.95E51 -1.182E1 1.8286E4/
PLOG/1.0E2 4.21E52 -1.164E1 2.2262E4/
C3H4-A+H=C3H5-T 6.44E102 -27.51 5.1768E4
DUP
PLOG/1.0E-3 1.1E54 -1.429E1 1.0809E4/
PLOG/3.9E-2 9.88E44 -1.121E1 8.212E3/
PLOG/1.0E0 2.81E40 -9.42E0 7.85E3/
PLOG/1.0E1 2.6E35 -7.57E0 7.147E3/
PLOG/1.0E2 9.88E29 -5.53E0 6.581E3/
C3H4-A+H=CH3+C2H2 3.74E1 3.35 5.78E1
DUP
PLOG/1.0E-3 1.23E8 1.53E0 4.737E3/
PLOG/3.9E-2 2.72E9 1.2E0 6.834E3/
PLOG/1.0E0 1.26E20 -1.83E0 1.5003E4/
PLOG/1.0E1 1.68E16 -6.0E-1 1.4754E4/
PLOG/1.0E2 1.37E17 -7.9E-1 1.7603E4/
C3H4-A+H=CH3+C2H2 3.74E1 3.35 5.78E1
DUP
PLOG/1.0E-3 1.0E-10 0.0E0 0.0E0/
PLOG/3.9E-2 1.0E-10 0.0E0 0.0E0/
PLOG/1.0E0 1.23E4 2.68E0 6.335E3/
PLOG/1.0E1 3.31E8 1.14E0 8.886E3/
PLOG/1.0E2 1.28E6 1.71E0 9.774E3/
C3H5-A=C3H5-T 3.9E59 -15.42 7.54E4
PLOG/1.0E-1 3.9E59 -1.542E1 7.54E4/
PLOG/1.0E0 7.06E56 -1.408E1 7.5868E4/
PLOG/2.0E0 4.8E55 -1.359E1 7.5949E4/
PLOG/5.0E0 4.86E53 -1.281E1 7.5883E4/
PLOG/1.0E1 6.4E51 -1.212E1 7.57E4/
PLOG/1.0E2 2.8E43 -9.27E0 7.4E4/
C2H2+CH3=C3H5-T 6.8E20 -4.16 1.8E4
PLOG/1.0E-1 6.8E20 -4.16E0 1.8E4/
PLOG/1.0E0 4.99E22 -4.39E0 1.885E4/
PLOG/2.0E0 6.0E23 -4.6E0 1.9571E4/
PLOG/5.0E0 7.31E25 -5.06E0 2.115E4/
PLOG/1.0E1 9.3E27 -5.55E0 2.29E4/
PLOG/1.0E2 3.8E36 -7.58E0 3.13E4/
C2H2+CH3=C3H5-A 8.2E53 -13.32 3.32E4
PLOG/1.0E-1 8.2E53 -1.332E1 3.32E4/
PLOG/1.0E0 2.68E53 -1.282E1 3.573E4/
PLOG/2.0E0 3.64E52 -1.246E1 3.6127E4/
PLOG/5.0E0 1.04E51 -1.189E1 3.6476E4/
PLOG/1.0E1 4.4E49 -1.14E1 3.67E4/
PLOG/1.0E2 3.8E44 -9.63E0 3.76E4/
C3H4-A+O=C2H4+CO 2.0E7 1.8 1.0E3
C3H4-A+O=C2H2+CH2O 3.0E-3 4.61 -4.243E3
C3H4-A+HO2=>C2H4+CO+OH 1.0E11 0.0 1.4E4
C3H4-A+HO2=>CH2CO+CH2+OH 4.0E12 0.0 1.9E4
C3H4-A+C2H=C2H2+C3H3 1.0E13 0.0 0.0E0
C3H3+O=CH2O+C2H 2.0E13 0.0 0.0E0
C3H3+HO2=>OH+CO+C2H3 8.0E11 0.0 0.0E0
C3H3+HCO=C3H4-A+CO 2.5E13 0.0 0.0E0
C2H5+C2H=C3H3+CH3 1.81E13 0.0 0.0E0
C3H3+O2=CH2CO+HCO 1.7E5 1.7 1.5E3

```
C3H3+OH=CH2O+C2H2    2.0E12 0.0 0.0E0
C3H3+OH=C2H3+HCO    1.0E13 0.0 0.0E0
C3H3+OH=C2H4+CO    1.0E13 0.0 0.0E0
CH3CHCO+OH=C2H5+CO2    1.73E12 0.0 -1.01E3
CH3CHCO+H=C2H5+CO    4.4E12 0.0 1.459E3
CH3CHCO+O=CH3CHO+CO    3.2E12 0.0 -4.37E2
CH3COCH3+H=C3H6OH2-1    8.0E12 0.0 9.5E3
C3H6OH2-1+O2=CH3COCH3+HO2    1.5E12 0.0 5.0E3
CH3COCH3=CH3CO+CH3    2.05E58 -12.796 1.000301E5
    PLOG/1.0E-2 2.05E58 -1.2796E1 1.000301E5/
    PLOG/1.0E-1 3.3E51 -1.0574E1 9.82212E4/
    PLOG/1.0E0 1.31E42 -7.657E0 9.46606E4/
    PLOG/1.0E1 2.16E33 -4.989E0 9.09165E4/
    PLOG/1.0E2 9.4E28 -3.669E0 8.90228E4/
C2H3+HCO=C2H3CHO    1.81E13 0.0 0.0E0
IC3H6CO+OH=IC3H7+CO2    1.73E12 0.0 -1.01E3
IC3H6CO+OH=C3H6OH2-1+CO    2.0E12 0.0 -1.01E3
C3H5-T+CH2O=C3H6+HCO    1.0E11 0.0 0.0E0
    PLOG/1.0E-3 1.11E7 1.09E0 1.8072E3/
    PLOG/1.0E-2 2.47E7 9.93E-1 1.9949E3/
    PLOG/1.0E-1 2.47E8 7.04E-1 2.5962E3/
    PLOG/1.0E0 1.42E10 2.09E-1 3.9342E3/
    PLOG/1.0E1 3.45E13 -7.26E-1 6.9443E3/
    PLOG/1.0E2 3.31E14 -8.66E-1 1.09657E4/
    PLOG/1.0E3 1.65E1 3.17E0 9.3998E3/
C5H81-3+OH=C2H3CHO+C2H5    1.0E12 0.0 0.0E0
END
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ARIES 82 Mechanism

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ELEMENTS
C H N O AR
HE
END
SPECIES
AR N2 HE H2 H
O2 O H2O OH OHV
H2O2 HO2 CO CO2 CH4
CH3 CH2 CH2(S) CH CHV
CH3O2H CH3O2 CH3O CH2OH CH2O
HCO HCOH HO2CHO O2CHO HOCHO
OCHO C2H6 C2H5 C2H5O2H C2H5O2
C2H4 C2H3 C2H3OO CHCHO C2H2
C2H C2H5O CH3CHO CH3CO CH2CHO
O2CH2CHO HO2CH2CO CH2CO HCCO CH3CO3H
CH3CO3 CH3CO2 C3H8 IC3H7 NC3H7
NC3H7O2 IC3H7O2H IC3H7O2 C3H6OOH1-2 C3H6OOH1-3
C3H6OOH2-1 C3H6OOH1-2O2 C3H6OOH1-3O2 C3KET12 C3KET13
C3H6 C3H5-A C3H5-T CH3CHCO C3H5O
AC3H5OOH C3H4-A C3H3 C3H2 C3H6OH2-1
CH3COCH3 CH3COCH2O C2H3CHO C2H5CHO IC3H6CO
C2H5CHCO C5H81-3
END

THERMO ALL
   300.000  1000.000  5000.000
AR               G-5-97AR  1               G     200.0    6000.0  1000.0      1
         2.5E0         0.0E0         0.0E0         0.0E0         0.0E0    2
     -7.45375E2   4.37967491E0         2.5E0         0.0E0         0.0E0    3
         0.0E0         0.0E0     -7.45375E2   4.37967491E0                   4
N2               G-8-02N   2               G     200.0    6000.0  1000.0      1
    2.95257637E0   1.3969004E-3 -4.92631603E-7 7.86010195E-11-4.60755204E-15    2
   -9.23948688E2   5.87188762E0   3.53100528E0 -1.23660988E-4 -5.02999433E-7    3
    2.43530612E-9-1.40881235E-12  -1.04697628E3   2.96747038E0                   4
HE               G-5-97HE  1               G     200.0    6000.0  1000.0      1
         2.5E0         0.0E0         0.0E0         0.0E0         0.0E0    2
     -7.45375E2  9.28723974E-1         2.5E0         0.0E0         0.0E0    3
         0.0E0         0.0E0     -7.45375E2  9.28723974E-1                   4
H2               TPIS78H   2               G     200.0    6000.0  1000.0      1
    2.93286575E0  8.26608026E-4 -1.46402364E-7 1.54100414E-11  -6.888048E-16    2
   -8.13065581E2  -1.02432865E0   2.34433112E0  7.98052075E-3  -1.9478151E-5    3
    2.01572094E-8-7.37611761E-12  -9.17935173E2  6.83010238E-1                   4
H                L-6-94H   1               G     200.0    6000.0  1000.0      1
         2.5E0         0.0E0         0.0E0         0.0E0         0.0E0    2
     2.547366E4  -4.4668285E-1         2.5E0         0.0E0         0.0E0    3
         0.0E0         0.0E0     2.547366E4  -4.4668285E-1                   4
O2               RUS-89O   2               G     200.0    6000.0  1000.0      1
    3.66096065E0  6.56365811E-4 -1.41149627E-7 2.05797935E-11-1.29913436E-15    2
   -1.21597718E3   3.41536279E0   3.78245636E0 -2.99673416E-3  9.84730201E-6    3
   -9.68129509E-9 3.24372837E-12  -1.06394356E3   3.65767573E0                   4
O                L-1-90O   1               G     200.0    6000.0  1000.0      1
    2.54363697E0 -2.73162486E-5  -4.1902952E-9 4.95481845E-12-4.79553694E-16    2
    2.9226012E4   4.92229457E0    3.1682671E0 -3.27931884E-3  6.64306396E-6    3
   -6.12806624E-9 2.11265971E-12   2.91222592E4   2.05193346E0                   4
H2O              L-5-89H   2O  1           G     200.0    6000.0  1000.0      1
    2.6770389E0   2.9731816E-3  -7.7376889E-7  9.4433514E-11 -4.2689991E-15    2
   -2.9885894E4      6.88255E0    4.1986352E0  -2.0364017E-3   6.5203416E-6    3
   -5.4879269E-9   1.771968E-12   -3.0293726E4  -8.4900901E-1                   4
OH               IU3-03H   1O  1           G     200.0    6000.0  1000.0      1
    2.83853033E0  1.10741289E-3 -2.94000209E-7 4.20698729E-11 -2.4228989E-15    2
    3.69780808E3   5.84494652E0   3.99198424E0 -2.40106655E-3  4.61664033E-6    3
   -3.87916306E-9 1.36319502E-12   3.36889836E3 -1.03998477E-1                   4
!UB REFIT 13-11-2018
OHV               -THERMH   1O  1           G     300.0    5000.0  1710.0      1
    2.8537604E0  1.02994334E-3 -2.32666477E-7 1.93750704E-11-3.15759847E-16    2
    5.03225473E4   5.76240468E0   3.41896226E0  3.19255801E-4 -3.08292717E-7    3
   3.64407494E-10-1.00195479E-13   5.00756946E4   2.51917016E0                   4
H2O2             T-8-03H   2O  2           G     200.0    6000.0  1000.0      1
    4.57977305E0  4.05326003E-3  -1.2984473E-6   1.982114E-10-1.13968792E-14    2
   -1.80071775E4  6.64970694E-1   4.31515149E0 -8.47390622E-4  1.76404323E-5    3
   -2.26762944E-8 9.08950158E-12  -1.77067437E4   3.27373319E0                   4
HO2              T-1-09H   1O  2           G     200.0    5000.0  1000.0      1
    4.17228741E0  1.88117627E-3 -3.46277286E-7 1.94657549E-11 1.76256905E-16    2
    3.10206839E1   2.95767672E0   4.30179807E0 -4.74912097E-3  2.11582905E-5    3
   -2.42763914E-8 9.29225225E-12   2.64018485E2   3.7166622E0                   4
CO               RUS-79O   1C  1           G     200.0    6000.0  1000.0      1
    3.0484859E0   1.3517281E-3  -4.8579405E-7  7.8853644E-11 -4.6980746E-15    2
   -1.4266117E4   6.0170977E0   3.5795335E0  -6.1035369E-4   1.0168143E-6    3
   9.0700586E-10 -9.0442449E-13   -1.4344086E4   3.5084093E0                   4
CO2              L-7-88O   2C  1           G     200.0    6000.0  1000.0      1
    4.6365111E0   2.7414569E-3  -9.9589759E-7  1.6038666E-10 -9.1619857E-15    2
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-4.9024904E4 -1.9348955E0 2.356813E0 8.9841299E-3 -7.1220632E-6 3
2.4573008E-9 -1.4288548E-13 -4.8371971E4 9.9009035E0 4
CH4 G-8-99H 4C 1 G 200.0 6000.0 1000.0 1
1.65326226E0 1.00263099E-2 -3.31661238E-6 5.36483138E-10-3.14696758E-14 2
-1.00095936E4 9.90506283E0 5.14911468E0 -1.36622009E-2 4.91453921E-5 3
-4.84246767E-8 1.66603441E-11 -1.02465983E4 -4.63848842E0 4
CH3 IU0702H 3C 1 G 200.0 6000.0 1000.0 1
2.9781206E0 5.797852E-3 -1.97558E-6 3.072979E-10 -1.7917416E-14 2
1.6509513E4 4.7224799E0 3.6571797E0 2.1265979E-3 5.4583883E-6 3
-6.6181003E-9 2.4657074E-12 1.6422716E4 1.6735354E0 4
CH2 IU3-03H 2C 1 G 200.0 6000.0 1000.0 1
3.14631886E0 3.03671259E-3 -9.96474439E-7 1.5048358E-10-8.57335515E-15 2
4.60412605E4 4.72341711E0 3.71757846E0 1.2739126E-3 2.17347251E-6 3
-3.488585E-9 1.65208866E-12 4.58723866E4 1.75297945E0 4
CH2(S) IU6-03H 2C 1 G 200.0 6000.0 1000.0 1
3.13501686E0 2.89593926E-3 -8.1666809E-7 1.13572697E-10-6.36262835E-15 2
5.05040504E4 4.06030621E0 4.19331325E0 -2.33105184E-3 8.15676451E-6 3
-6.62985981E-9 1.93233199E-12 5.03662246E4 -7.4673431E-1 4
CH IU3-03H 1C 1 G 200.0 6000.0 1000.0 1
2.5209369E0 1.7653639E-3 -4.614766E-7 5.9289675E-11 -3.3474501E-15 2
7.0946769E4 7.4051829E0 3.4897583E0 3.243216E-4 -1.6899751E-6 3
3.162842E-9 -1.4061803E-12 7.0612646E4 2.0842841E0 4
!UB REFIT 13-11-2018
CHV -THERMH 1C 1 G 300.0 5000.0 1365.0 1
2.21703785E0 2.15314038E-3 -5.71569209E-7 6.54441183E-11-2.66374894E-15 2
1.04414085E5 9.18247549E0 3.50775836E0 -4.57470019E-4 1.32602633E-6 3
-5.1421376E-10 5.82219975E-14 1.03920991E5 2.09911232E0 4
CH3O2H A-7-05H 4O 2C 1 G 200.0 6000.0 1000.0 1
7.76538058E0 8.61499712E-3 -2.98006935E-6 4.68638071E-10-2.75339255E-14 2
-1.82979984E4 -1.43992663E1 2.90540897E0 1.74994735E-2 5.2824363E-6 3
-2.52827275E-8 1.34368212E-11 -1.68894632E4 1.13741987E1 4
CH3O2 H 3O 2C 1 G 300.0 5000.0 1374.0 1
6.47970487E0 7.4440108E-3 -2.52348555E-6 3.89577296E-10-2.25182399E-14 2
-1.56285441E3 -8.19477074E0 1.97339205E0 1.5354234E-2 -6.37314891E-6 3
3.19930565E-10 2.82193915E-13 2.54278835E2 1.69194215E1 4
CH3O IU1-03H 3O 1C 1 G 200.0 6000.0 1000.0 1
4.75779238E0 7.44142474E-3 -2.69705176E-6 4.38090504E-10-2.63537098E-14 2
3.7811194E2 -1.96680028E0 3.71180502E0 -2.80463306E-3 3.76550971E-5 3
-4.73072089E-8 1.8658842E-11 1.2956976E3 6.57240864E0 4
CH2OH IU2-03H 3O 1C 1 G 200.0 6000.0 1000.0 1
5.0931437E0 5.9476126E-3 -2.0649746E-6 3.23008173E-10-1.88125902E-14 2
-4.0340964E3 -1.84691493E0 4.47834367E0 -1.3507031E-3 2.7848498E-5 3
-3.6486906E-8 1.4790745E-11 -3.5007289E3 3.309135E0 4
CH2O T-5-11H 2O 1C 1 G 200.0 6000.0 1000.0 1
3.16952665E0 6.1932056E-3 -2.25056366E-6 3.6597566E-10-2.20149458E-14 2
-1.45486831E4 6.04207898E0 4.79372312E0 -9.90833322E-3 3.7321999E-5 3
-3.79285237E-8 1.31772641E-11 -1.43791953E4 6.02798058E-1 4
HCO T-5-03H 1O 1C 1 G 200.0 6000.0 1000.0 1
3.92001542E0 2.52279324E-3 -6.71004164E-7 1.05615948E-10-7.43798261E-15 2
3.65342928E3 3.58077056E0 4.2375461E0 -3.32075257E-3 1.40030264E-5 3
-1.34239995E-8 4.37416208E-12 3.87241185E3 3.30834869E0 4
HCOH -MAR94H 2O 1C 1 G 300.0 5000.0 1398.0 1
9.18749272E0 1.52011152E-3 -6.27603516E-7 1.09727989E-10-6.89655128E-15 2
7.81364593E3 -2.73434214E1 -2.82157421E0 3.57331702E-2 -3.8086158E-5 3
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HO2CHO -THERMH 2O 3C 1 G 300.0 5000.0 1378.0 1
9.87503878E0 4.64663708E-3 -1.67230522E-6 2.68624413E-10-1.59595232E-14 2
-3.80502496E4 -2.24939155E1 2.42464726E0 2.1970638E-2 -1.68705546E-5 3
6.25612194E-9-9.11645843E-13 -3.54828006E4 1.75027796E1 4
O2CHO -THERMH 1O 3C 1 G 300.0 5000.0 1368.0 1
7.24075139E0 4.63312951E-3 -1.63693995E-6 2.59706693E-10-1.52964699E-14 2
-1.87027618E4 -6.49547212E0 3.96059309E0 1.06002279E-2 -5.25713351E-6 3
1.01716726E-9-2.87487602E-14 -1.73599383E4 1.17807483E1 4
HOCHO L-8-88H 2O 2C 1 G 200.0 6000.0 1000.0 1
4.6138316E0 6.4496364E-3 -2.2908251E-6 3.6716047E-10 -2.1873675E-14 2
-4.751485E4 8.4788383E-1 3.8983616E0 -3.5587795E-3 3.5520538E-5 3
-4.3849959E-8 1.7107769E-11 -4.6770609E4 7.3495397E0 4
OCHO ATCT-AH 1O 2C 1 G 200.0 6000.0 1000.0 1
4.14394211E0 5.59738818E-3 -1.99794019E-6 3.16179193E-10-1.85614483E-14 2
-1.72459887E4 5.07778617E0 4.68825921E0 -4.14871834E-3 2.5506601E-5 3
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C2H6 G-8-88H 6C 2 G 200.0 6000.0 1000.0 1
4.04666411E0 1.53538802E-2 -5.47039485E-6 8.77826544E-10-5.23167531E-14 2
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C2H5 -THERMH 5C 2 G 300.0 5000.0 1387.0 1
5.8878439E0 1.03076793E-2 -3.46844396E-6 5.32499257E-10-3.06512651E-14 2
1.15065499E4 -8.49651771E0 1.32730217E0 1.76656753E-2 -6.14926558E-6 3
-3.01143466E-10 4.38617775E-13 1.34284028E4 1.71789216E1 4
C2H5O2H H 6O 2C 2 G 300.0 5000.0 1390.0 1
1.04823538E1 1.34779879E-2 -4.62179078E-6 7.18618519E-10-4.17307436E-14 2
-2.46578171E4 -2.84294243E1 1.83755328E0 3.38053586E-2 -2.3754814E-5 3
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C2H5O2 H 5O 2C 2 G 300.0 5000.0 1389.0 1
9.5028257E0 1.20429839E-2 -4.09491581E-6 6.33049241E-10-3.66133788E-14 2
-7.37069391E3 -2.2171713E1 3.90351912E0 2.22599212E-2 -1.01610079E-5 3
1.71709751E-9 1.88166738E-14 -5.09654081E3 8.9872275E0 4
C2H4 H 4C 2 G 300.0 5000.0 1392.0 1
5.07061289E0 9.11140768E-3 -3.10506692E-6 4.80733851E-10-2.78321396E-14 2
3.66391217E3 -6.64501414E0 4.81118223E-1 1.8377806E-2 -9.99633565E-6 3
2.73211039E-9-3.01837289E-13 5.44386648E3 1.85867157E1 4
C2H3 H 3C 2 G 300.0 5000.0 1400.0 1
4.99675415E0 6.55838271E-3 -2.20921909E-6 3.39300272E-10-1.95316926E-14 2

3.34604382E4 -3.01451097E0 1.25545094E0 1.57481597E-2 -1.12218328E-5 3
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C2H3OO H 3O 2C 2 G 298.15 2000.0 1000.0 1
6.04483828E0 1.45511127E-2 -7.50974622E-6 1.8348828E-9-1.66689681E-13 2
1.01699244E4 -3.71144913E0 1.09784776E0 2.95333237E-2 -2.2774436E-5 3
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CHCHO H 2O 1C 2 G 298.15 2000.0 1000.0 1
4.9263291E0 9.71712147E-3 -5.5485598E-6 1.53068537E-9-1.64742462E-13 2
2.89499494E4 5.27874677E-1 2.33256751E0 1.62952986E-2 -9.72052177E-6 3
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C2H2 G-1-91H 2C 2 G 200.0 6000.0 1000.0 1
4.65878489E0 4.88396667E-3 -1.60828888E-6 2.46974544E-10-1.38605959E-14 2
2.57594042E4 -3.99838194E0 8.08679682E-1 2.33615762E-2 -3.55172234E-5 3
2.80152958E-8-8.50075165E-12 2.64289808E4 1.39396761E1 4
C2H T-5-10H 1C 2 G 200.0 6000.0 1000.0 1
3.66270248E0 3.82492252E-3 -1.366325E-6 2.1345504E-10-1.23216848E-14 2
6.7168379E4 3.92205792E0 2.89867676E0 1.32988489E-2 -2.80733327E-5 3
2.89484755E-8-1.07502351E-11 6.7061605E4 6.18547632E0 4
C2H5O H 5O 1C 2 G 300.0 5000.0 1467.0 1
8.19120635E0 1.10391986E-2 -3.75270536E-6 5.80275784E-10-3.35735146E-14 2
-5.66847208E3 -1.90131344E1 2.90353584E0 1.77256708E-2 -2.69624757E-6 3
-3.45830533E-9 1.25224784E-12 -3.2893029E3 1.13545591E1 4
CH3CHO L-8-88H 4O 1C 2 G 200.0 6000.0 1000.0 1
5.4041108E0 1.1723059E-2 -4.2263137E-6 6.8372451E-10 -4.0984863E-14 2
-2.2593122E4 -3.4807917E0 4.7294595E0 -3.1932858E-3 4.7534921E-5 3
-5.7458611E-8 2.1931112E-11 -2.1572878E4 4.1030159E0 4
CH3CO IU2-03H 3O 1C 2 G 200.0 6000.0 1000.0 1
5.3137165E0 9.1737793E-3 -3.3220386E-6 5.3947456E-10 -3.2452368E-14 2
-3.6450414E3 -1.6757558E0 4.0358705E0 8.7729487E-4 3.071001E-5 3
-3.9247565E-8 1.5296869E-11 -2.6820738E3 7.8617682E0 4
CH2CHO T03-10H 3O 1C 2 G 200.0 6000.0 1000.0 1
6.53928338E0 7.80238629E-3 -2.76413612E-6 4.42098906E-10 -2.6295429E-14 2
-1.18858659E3 -8.72091393E0 2.795026E0 1.01099472E-2 1.61750645E-5 3
-3.10303145E-8 1.39436139E-11 1.62944975E2 1.23646657E1 4
O2CH2CHO BOZ-03H 3O 3C 2 G 300.0 5000.0 1393.0 1
1.11807543E1 9.14479256E-3 -3.15089833E-6 4.91944238E-10 -2.8663918E-14 2
-1.55790331E4 -2.8789274E1 -1.29465843E0 4.44936393E-2 -4.26577074E-5 3
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HO2CH2CO BOZ-03H 3O 3C 2 G 300.0 5000.0 1386.0 1
1.04146322E1 1.12680116E-2 -5.17494839E-6 1.00333285E-9-6.68165911E-14 2
-1.40955672E4 -2.278944E1 2.22681686E0 3.5678138E-2 -3.26401909E-5 3
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!UB REFIT 13-11-2018
CH2CO -THERMH 2O 1C 2 G 300.0 5000.0 1400.0 1
6.32896692E0 5.44012978E-3 -1.82687969E-6 2.80010787E-10 -1.6096416E-14 2
-8.36526176E3 -9.53528539E0 2.35724171E0 1.62213064E-2 -1.34812364E-5 3
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HCCO T-4-09H 1O 1C 2 G 200.0 6000.0 1000.0 1
5.91479333E0 3.7140873E-3 -1.3013701E-6 2.06473345E-10-1.21476759E-14 2
1.93596301E4 -5.50567269E0 1.87607969E0 2.21205418E-2 -3.58869325E-5 3
3.05402541E-8-1.01281069E-11 2.0163384E4 1.3696829E1 4
CH3CO3H -THERMH 4O 3C 2 G 300.0 5000.0 1391.0 1
1.25060485E1 9.47789695E-3 -3.30402246E-6 5.19630793E-10-3.04233568E-14 2
-4.59856703E4 -3.79195947E1 2.24135876E0 3.37963514E-2 -2.53887482E-5 3
9.67583587E-9-1.49266157E-12 -4.24677831E4 1.70668133E1 4
CH3CO3 -THERMH 3O 3C 2 G 300.0 5000.0 1391.0 1
1.12522498E1 8.33652672E-3 -2.8901453E-6 4.52781734E-10-2.64354456E-14 2
-2.60238584E4 -2.96370457E1 3.60373432E0 2.70080341E-2 -2.08293438E-5 3
8.50541104E-9 -1.4384611E-12 -2.34205171E4 1.12014914E1 4
CH3CO2 -THERMH 3O 2C 2 G 300.0 5000.0 1395.0 1
8.54059736E0 8.32951214E-3 -2.8472201E-6 4.41927196E-10-2.56373394E-14 2
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6.24799508E-9-9.09516835E-13 -2.7233015E4 1.81405454E1 4
C3H8 H 8C 3 G 300.0 5000.0 1390.0 1
9.1554131E0 1.72574139E-2 -5.85614868E-6 9.04190155E-10-5.22523772E-14 2
-1.75762439E4 -2.7741851E1 2.4087847E-1 3.39548599E-2 -1.60930874E-5 3
2.83480628E-9 2.78195172E-14 -1.40362853E4 2.165008E1 4
IC3H7 H 7C 3 G 298.0 6000.0 1000.0 1
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7.55377821E3 -1.03686516E1 -8.97467137E-1 4.15744022E-2 -4.94778349E-5 3
4.56493655E-8-1.79085437E-11 9.93950407E3 2.92641758E1 4
NC3H7 H 7C 3 G 298.0 6000.0 1000.0 1
7.48614243E0 1.65769478E-2 -5.74876481E-6 9.04103694E-10-5.30867231E-14 2
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6.3699694E-8-2.29332581E-11 1.15130744E4 3.43669174E1 4
NC3H7O2 H 7O 2C 3 G 300.0 5000.0 1390.0 1
1.32753283E1 1.61303126E-2 -5.52348308E-6 8.58197168E-10-4.98172586E-14 2
-1.16032968E4 -4.15091215E1 2.13311681E0 3.96692045E-2 -2.37570127E-5 3
6.96020417E-9-7.82576856E-13 -7.46687112E3 1.92444565E1 4
IC3H7O2H H 8O 2C 3 G 300.0 5000.0 1405.0 1
1.44896107E1 1.68268026E-2 -5.67601391E-6 8.72850837E-10-5.02993991E-14 2
-3.06478491E4 -5.01352281E1 1.77384705E0 4.75813498E-2 -3.43745304E-5 3
1.31405381E-8-2.06922904E-12 -2.63458844E4 1.77669753E1 4
IC3H7O2 H 7O 2C 3 G 300.0 5000.0 1407.0 1
1.3526812E1 1.54306581E-2 -5.17464218E-6 7.92548669E-10-4.55415379E-14 2
-1.33946348E4 -4.40461451E1 2.58517502E0 4.16107259E-2 -2.92193877E-5 3
1.08614807E-8-1.66312005E-12 -9.67013161E3 1.447313E1 4
C3H6OOH1-2 H 7O 2C 3 G 300.0 5000.0 1387.0 1
1.38088686E1 1.4384565E-2 -4.74440961E-6 7.1930828E-10-4.10654123E-14 2
-5.14352831E3 -4.20210765E1 2.83631132E0 3.88229894E-2 -2.47944364E-5 3
7.85644898E-9 -9.586343E-13 -1.26002528E3 1.72549973E1 4
C3H6OOH1-3 H 7O 2C 3 G 300.0 5000.0 1401.0 1
1.39130757E1 1.40218463E-2 -4.55921149E-6 6.84182417E-10-3.87696213E-14 2

-3.65650518E3 -4.21532559E1 1.74271107E0 4.53733504E-2 -3.57580373E-5 3
1.48540053E-8-2.49981756E-12 2.32580844E2 2.20973041E1 4
C3H6OOH2-1 H 7O 2C 3 G 300.0 5000.0 1393.0 1
1.36645362E1 1.54329764E-2 -5.29285952E-6 8.23001262E-10-4.77931121E-14 2
-5.58295862E3 -4.28758364E1 2.38465746E0 4.42928555E-2 -3.50977087E-5 3
1.53695144E-8-2.81167824E-12 -1.80979612E3 1.69923285E1 4
C3H6OOH1-2O2 ----12H 7O 4C 3 G 300.0 5000.0 1404.0 1
1.9104498E1 1.440761E-2 -4.72127814E-6 7.12631642E-10 -4.0557849E-14 2
-2.5027051E4 -6.63747978E1 3.99085043E0 5.31865338E-2 -4.28597948E-5 3
1.77187019E-8-2.92768695E-12 -2.02143526E4 1.34150719E1 4
C3H6OOH1-3O2 ----12H 7O 4C 3 G 300.0 5000.0 1416.0 1
1.81661664E1 1.47644887E-2 -4.74842743E-6 7.06972467E-10-3.98305587E-14 2
-2.26256376E4 -5.93719393E1 5.5693335E0 4.68523421E-2 -3.58917784E-5 3
1.43314525E-8-2.29776083E-12 -1.86065694E4 7.18655005E0 4
C3KET12 H 6O 3C 3 G 300.0 5000.0 1385.0 1
1.7018776E1 1.32097361E-2 -4.67054741E-6 7.4141177E-10-4.36869787E-14 2
-4.23572589E4 -5.92615939E1 1.03882879E0 5.3418008E-2 -4.47684141E-5 3
1.9465168E-8-3.45055244E-12 -3.70308881E4 2.56511209E1 4
C3KET13 H 6O 3C 3 G 300.0 5000.0 1508.0 1
1.73612692E1 1.32330813E-2 -4.7533211E-6 7.62529227E-10-4.52613717E-14 2
-4.0624806E4 -6.17768199E1 4.74956819E0 3.14080991E-2 -6.83838427E-6 3
-5.67123901E-9 2.27686972E-12 -3.5192457E4 9.83753744E0 4
C3H6 H 6C 3 G 298.0 6000.0 1000.0 1
6.59032304E0 1.52592866E-2 -5.30369441E-6 8.35510888E-10-4.91215549E-14 2
-2.47481113E2 -1.15748238E1 -1.54606737E0 4.36553128E-2 -5.61392417E-5 3
4.98421927E-8-1.84798923E-11 2.07056233E3 2.99232495E1 4
C3H5-A H 5C 3 G 298.0 6000.0 1000.0 1
7.37604097E0 1.23449782E-2 -4.26463882E-6 6.69045835E-10-3.92202554E-14 2
1.7733296E4 -1.61758204E1 -3.32899442E0 5.38423469E-2 -7.65500752E-5 3
6.35512285E-8-2.14283003E-11 2.03420628E4 3.68038362E1 4
C3H5-T H 5C 3 G 300.0 5000.0 1376.0 1
7.69949212E0 1.17803985E-2 -4.07791749E-6 6.38119222E-10-3.72229675E-14 2
2.61747145E4 -1.6830589E1 2.29256998E0 1.98527646E-2 -6.42635654E-6 3
-5.90016395E-10 5.05491095E-13 2.85773377E4 1.39407124E1 4
CH3CHCO -THERMH 4O 1C 3 G 300.0 5000.0 1400.0 1
1.00219123E1 9.569663E-3 -3.26221644E-6 5.05231706E-10-2.92593257E-14 2
-1.42482738E4 -2.77829973E1 1.48380119E0 3.22203013E-2 -2.70250033E-5 3
1.20499164E-8-2.18365931E-12 -1.1527654E4 1.71552068E1 4
C3H5O -KPS12H 5O 1C 3 G 300.0 5000.0 1402.0 1
1.02638186E1 1.17609932E-2 -3.89837957E-6 5.92650815E-10-3.38867417E-14 2
7.25938472E3 -2.75108651E1 8.24068673E-1 3.46749909E-2 -2.51786795E-5 3
9.56781953E-9-1.48085302E-12 1.04203725E4 2.2828307E1 4
AC3H5OOH ---ITHH 6O 2C 3 G 298.0 6000.0 1000.0 1
1.20838649E1 1.47946591E-2 -5.13212591E-6 8.07504999E-10-4.74394983E-14 2
-1.02184463E4 -3.36434791E1 3.18124993E0 4.35233041E-2 -5.16277353E-5 3
4.32011427E-8-1.57714983E-11 -7.63521503E3 1.21725683E1 4
C3H4-A L-8-89H 4C 3 G 200.0 6000.0 1000.0 1
6.3168722E0 1.1133728E-2 -3.9629378E-6 6.3564238E-10 -3.787554E-14 2
2.0117495E4 -1.0995766E1 2.6130445E0 1.2122575E-2 1.853988E-5 3
-3.4525149E-8 1.5335079E-11 2.1541567E4 1.0226139E1 4
C3H3 T-7-11H 3C 3 G 200.0 6000.0 1000.0 1
7.14221719E0 7.61902211E-3 -2.6746003E-6 4.24914904E-10-2.51475443E-14 2
3.95709594E4 -1.2584869E1 1.35110873E0 3.27411291E-2 -4.73827407E-5 3
3.7631022E-8-1.18541128E-11 4.07679941E4 1.52058598E1 4
C3H2 T12-00H 2C 3 G 200.0 6000.0 1000.0 1
6.67324762E0 5.57728845E-3 -1.99180164E-6 3.20289156E-10-1.91216272E-14 2
7.57571184E4 -9.72894405E0 2.43417332E0 1.73013063E-2 -1.18294047E-5 3
1.02756396E-9 1.62626314E-12 7.69074892E4 1.2101223E1 4
C3H6OH2-1 -THERMH 7O 1C 3 G 300.0 5000.0 1392.0 1
1.12222277E1 1.36444398E-2 -4.51406709E-6 7.10523275E-10-4.22690392E-14 2
-1.75350136E4 -3.18911926E1 1.0967036E0 3.80727565E-2 -2.75022497E-5 3
1.07477493E-8-1.74895773E-12 -1.40764487E4 2.22475799E1 4
CH3COCH3 H 6O 1C 3 G 300.0 5000.0 1394.0 1
8.87619308E0 1.45700263E-2 -4.8482328E-6 7.38614777E-10-4.22831194E-14 2
-3.06046242E4 -2.12730484E1 2.20008426E0 2.74019559E-2 -1.31342003E-5 3
2.57150371E-9-6.21509091E-14 -2.79933966E4 1.55883508E1 4
CH3COCH2O -THERMH 5O 2C 3 G 300.0 5000.0 2002.0 1
9.84061707E0 1.59181106E-2 -5.85164644E-6 9.56160073E-10-5.75477263E-14 2
-2.11214823E4 -2.12330791E1 5.85960137E0 1.78954926E-2 7.41506398E-7 3
-5.40032753E-9 1.47393197E-12 -1.90714739E4 2.70987883E0 4
C2H3CHO -KPS12H 4O 1C 3 G 300.0 5000.0 1398.0 1
9.99155394E0 9.82348001E-3 -3.31203088E-6 5.09524422E-10 -2.9382189E-14 2
-1.25303509E4 -2.85168883E1 7.33844455E-1 3.17482671E-2 -2.29599468E-5 3
8.42104232E-9-1.23613478E-12 -9.38473548E3 2.10308851E1 4
C2H5CHO H 6O 1C 3 G 300.0 5000.0 1449.0 1
1.06224453E1 1.35569132E-2 -4.60754771E-6 7.12755462E-10-4.12631683E-14 2
-2.78692266E4 -3.16628752E1 2.18895588E0 2.58289987E-2 -6.04170058E-6 3
-3.70702654E-9 1.57131095E-12 -2.42671146E4 1.6149633E1 4
IC3H6CO -THERMH 6O 1C 4 G 300.0 5000.0 1397.0 1
1.32548232E1 1.40142787E-2 -4.78910215E-6 7.42924342E-10-4.30737566E-14 2
-2.00529779E4 -4.44810221E1 2.28039055E0 4.17016989E-2 -3.25089661E-5 3
1.37243419E-8-2.40573132E-12 -1.63939712E4 1.38187714E1 4
C2H5CHCO H 6O 1C 4 G 300.0 5000.0 1550.0 1
-2.04040652E2 2.9346688E-1 -1.15884523E-4 1.95253673E-8-1.19030791E-12 2
8.27380036E4 1.21233386E3 -2.28307043E1 1.70978191E-1 -3.53394379E-4 3
2.78221616E-7-6.77325074E-11 -1.04125457E4 1.31232921E2 4
C5H81-3 H 8C 5 G 300.0 5000.0 1385.0 1
1.29945372E1 1.92678312E-2 -6.58966712E-6 1.02295969E-9-5.93441369E-14 2
4.59040047E3 -4.35689825E1 1.54882436E0 4.15042709E-2 -2.1435989E-5 3
4.71145517E-9-2.42142508E-13 9.05636062E3 1.9566591E1 4
END

TRANSPORT

```
AR 0 136.5 3.33 0.0 0.0 0.0
N2 1 97.53 3.621 0.0 1.76 4.0
HE 0 10.2 2.576 0.0 0.0 0.0
H2 1 38.0 2.92 0.0 0.79 280.0
H 0 145.0 2.05 0.0 0.0 0.0
O2 1 107.4 3.458 0.0 1.6 3.8
O 0 80.0 2.75 0.0 0.0 0.0
H2O 2 572.4 2.605 1.844 0.0 4.0
OH 1 80.0 2.75 0.0 0.0 0.0
OHV 1 80.0 2.75 0.0 0.0 0.0
H2O2 2 107.4 3.458 0.0 0.0 3.8
HO2 2 107.4 3.458 0.0 0.0 1.0
CO 1 98.1 3.65 0.0 1.95 1.8
CO2 1 244.0 3.763 0.0 2.65 2.1
CH4 2 141.4 3.746 0.0 2.6 13.0
CH3 1 144.0 3.8 0.0 0.0 0.0
CH2 1 144.0 3.8 0.0 0.0 0.0
CH2(S) 1 144.0 3.8 0.0 0.0 0.0
CH 1 80.0 2.75 0.0 0.0 0.0
CHV 1 80.0 2.75 0.0 0.0 0.0
CH3O2H 2 481.8 3.626 0.0 0.0 1.0
CH3O2 2 481.8 3.626 0.0 0.0 1.0
CH3O 2 417.0 3.69 1.7 0.0 2.0
CH2OH 2 417.0 3.69 1.7 0.0 2.0
CH2O 2 498.0 3.59 0.0 0.0 2.0
HCO 2 498.0 3.59 0.0 0.0 0.0
HCOH 2 498.0 3.59 0.0 0.0 1.0
HO2CHO 2 436.0 3.97 0.0 0.0 2.0
O2CHO 2 436.0 3.97 0.0 0.0 2.0
HOCHO 2 436.0 3.97 0.0 0.0 2.0
OCHO 2 498.0 3.59 0.0 0.0 2.0
C2H6 2 247.5 4.35 0.0 0.0 1.5
C2H5 2 247.5 4.35 0.0 0.0 1.5
C2H5O2H 2 470.6 4.41 0.0 0.0 1.5
C2H5O2 2 470.6 4.41 0.0 0.0 1.5
C2H4 2 238.4 3.496 0.0 0.0 1.5
C2H3 2 265.3 3.721 0.0 0.0 1.0
C2H3OO 2 436.0 3.97 0.0 0.0 2.0
CHCHO 2 436.0 3.97 0.0 0.0 2.0
C2H2 1 265.3 3.721 0.0 0.0 2.5
C2H 1 265.3 3.721 0.0 0.0 2.5
C2H5O 2 470.6 4.41 0.0 0.0 1.5
CH3CHO 2 436.0 3.97 0.0 0.0 2.0
CH3CO 2 436.0 3.97 0.0 0.0 2.0
CH2CHO 2 436.0 3.97 0.0 0.0 2.0
O2CH2CHO 2 275.049 5.428 0.0 0.0 1.0
HO2CH2CO 2 279.007 5.505 1.3 0.0 1.0
CH2CO 2 436.0 3.97 0.0 0.0 2.0
HCCO 2 150.0 2.5 0.0 0.0 1.0
CH3CO3H 2 436.0 3.97 0.0 0.0 2.0
CH3CO3 2 436.0 3.97 0.0 0.0 2.0
CH3CO2 2 436.0 3.97 0.0 0.0 2.0
C3H8 2 303.4 4.81 0.0 0.0 1.0
IC3H7 2 303.4 4.81 0.0 0.0 1.0
NC3H7 2 303.4 4.81 0.0 0.0 1.0
NC3H7O2 2 481.5 4.997 1.7 0.0 1.0
IC3H7O2H 2 459.5 5.036 1.7 0.0 1.0
IC3H7O2 2 459.5 5.036 1.7 0.0 1.0
C3H6OOH1-2 2 435.2 4.662 2.7 0.0 1.0
C3H6OOH1-3 2 435.2 4.662 2.7 0.0 1.0
C3H6OOH2-1 2 435.2 4.662 2.7 0.0 1.0
C3H6OOH1-2O2 2 435.2 4.662 2.7 0.0 1.0
C3H6OOH1-3O2 2 435.2 4.662 2.7 0.0 1.0
C3KET12 2 464.2 5.009 2.6 0.0 1.0
C3KET13 2 464.2 5.009 2.6 0.0 1.0
C3H6 2 307.8 4.14 0.0 0.0 1.0
C3H5-A 2 316.0 4.22 0.0 0.0 1.0
C3H5-T 2 316.0 4.22 0.0 0.0 1.0
CH3CHCO 2 443.2 4.12 0.0 0.0 1.0
C3H5O 2 411.0 4.82 0.0 0.0 1.0
AC3H5OOH 2 481.5 4.997 1.7 0.0 1.0
C3H4-A 1 324.8 4.29 0.0 0.0 1.0
C3H3 1 324.8 4.29 0.0 0.0 1.0
C3H2 2 209.0 4.1 0.0 0.0 1.0
C3H6OH2-1 2 487.9 4.82 0.0 0.0 1.0
CH3COCH3 2 435.5 4.86 0.0 0.0 1.0
CH3COCH2O 2 447.639 5.086 0.0 0.0 0.0
C2H3CHO 2 428.8 4.958 2.9 0.0 1.0
C2H5CHO 2 435.2 4.662 2.7 0.0 1.0
IC3H6CO 2 436.4 5.352 0.0 0.0 1.0
C2H5CHCO 2 436.95 5.016 0.0 0.0 0.0
C5H81-3 2 408.0 5.2 0.0 0.0 1.0
END

REACTIONS MOLES CAL/MOLE
H2+M=2H+M    4.577E19 -1.4 1.044E5
   H2/2.5/
   H2O/12.0/
   CO/1.9/
   CO2/3.8/
   HE/0.83/
   CH4/2.0/
   C2H6/3.0/
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H2+O=H+OH    5.08E4 2.67 6.292E3
H2+OH=H+H2O    4.38E13 0.0 6.99E3
2O+M=O2+M    6.165E15 -0.5 0.0E0
   H2/2.5/
   H2O/12.0/
   AR/0.83/
   CO/1.9/
   CO2/3.8/
   HE/0.83/
   CH4/2.0/
   C2H6/3.0/
O2+H=O+OH    1.04E14 0.0 1.5286E4
H+OH+M=H2O+M    3.5E22 -2.0 0.0E0
   H2/0.73/
   H2O/3.65/
   CH4/2.0/
   C2H6/3.0/
   AR/0.38/
O+H2O=2OH    6.7E7 1.704 1.49868E4
O+H+M=OH+M    4.714E18 -1.0 0.0E0
   H2/2.5/
   H2O/12.0/
   AR/0.75/
   CO/1.5/
   CO2/2.0/
   HE/0.75/
   CH4/2.0/
   C2H6/3.0/
H+O+M=OHV+M    1.5E13 0.0 5.975E3
   H2/1.0/
   H2O/6.5/
   O2/0.4/
   N2/0.4/
   AR/0.35/
OHV+H2O=OH+H2O    5.93E12 0.5 -8.6E2
OHV+H2=OH+H2    2.95E12 0.5 -4.44E2
OHV+N2=OH+N2    1.08E11 0.5 -1.242E3
OHV+OH=2OH    6.01E12 0.5 -7.64E2
OHV+H=OH+H    1.31E12 0.5 -1.67E2
OHV+AR=OH+AR    1.69E12 0.0 4.135E3
OHV=OH    1.45E6 0.0 0.0E0
OHV+O2=OH+O2    2.1E12 0.5 -4.78E2
OHV+CO2=OH+CO2    2.75E12 0.5 -9.68E2
OHV+CO=OH+CO    3.23E12 0.5 -7.87E2
OHV+CH4=OH+CH4    3.36E12 0.5 -6.35E2
H2O2(+M)=2OH(+M)    2.0E12 0.9 4.8749E4
   H2O/7.65/
   CO2/1.6/
   N2/1.5/
   O2/1.2/
   HE/0.65/
   H2O2/7.7/
   H2/3.7/
   CO/2.8/
   LOW/2.49E24 -2.3E0 4.8749E4/
   TROE/4.3E-1 1.0E-30 1.0E30/
H2O2+H=H2O+OH    2.41E13 0.0 3.97E3
H2O2+H=H2+HO2    2.15E10 1.0 6.0E3
H2O2+O=OH+HO2    9.55E6 2.0 3.97E3
H2O2+OH=H2O+HO2    1.74E12 0.0 3.18E2
   DUP
H2O2+OH=H2O+HO2    7.59E13 0.0 7.269E3
   DUP
HO2+H=2OH    7.079E13 0.0 2.95E2
HO2+H=H2+O2    1.1402E10 1.0827 5.5378E2
HO2+O=OH+O2    3.25E13 0.0 0.0E0
HO2+OH=H2O+O2    2.456E13 0.0 -4.97E2
2HO2=H2O2+O2    1.0E14 0.0 1.1040883E4
   DUP
2HO2=H2O2+O2    1.9E11 0.0 -1.4089248E3
   DUP
H+O2(+M)=HO2(+M)    4.65E12 0.44 0.0E0
   H2/1.3/
   CO/1.9/
   CO2/3.8/
   HE/0.64/
   H2O/10.0/
   AR/0.5/
   CH4/2.0/
   C2H6/3.0/
   LOW/1.737E19 -1.23E0 0.0E0/
   TROE/6.7E-1 1.0E-30 1.0E30 1.0E30/
CO+O(+M)=CO2(+M)    1.362E10 0.0 2.384E3
   H2/2.0/
   H2O/12.0/
   CO/1.75/
   CO2/3.6/
   AR/0.7/
   HE/0.7/
   LOW/1.173E24 -2.79E0 4.191E3/
CO+OH=CO2+H    7.015E4 2.053 -3.557E2
   DUP
CO+OH=CO2+H    5.757E12 -0.664 3.318E2
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   DUP
CO+HO2=CO2+OH    1.57E5 2.18 1.794E4
CO+O2=CO2+O    1.119E12 0.0 4.77E4
H+CO2=OCHO    7.5E13 0.0 2.9E4
CH3+H(+M)=CH4(+M)    1.27E16 -0.63 3.83E2
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/2.477E33 -4.76E0 2.44E3/
   TROE/7.83E-1 7.4E1 2.941E3 6.964E3/
CH4+H=CH3+H2    6.14E5 2.5 9.587E3
CH4+O=CH3+OH    1.02E9 1.5 8.6E3
CH4+OH=CH3+H2O    5.83E4 2.6 2.19E3
CH4+HO2=CH3+H2O2    1.13E1 3.74 2.101E4
CH4+CH3O2=CH3+CH3O2H    9.6E-1 3.77 1.781E4
CH3+HO2=CH4+O2    1.16E5 2.23 -3.022E3
CH4+CH2=2CH3    2.46E6 2.0 8.27E3
CH2(S)+N2=CH2+N2    1.5E13 0.0 6.0E2
CH2(S)+AR=CH2+AR    9.0E12 0.0 6.0E2
CH2(S)+H2O=CH2+H2O    3.0E13 0.0 0.0E0
CH2(S)+CO=CH2+CO    9.0E12 0.0 0.0E0
CH2(S)+CO2=CH2+CO2    7.0E12 0.0 0.0E0
CH2(S)+O2=>H+OH+CO    2.8E13 0.0 0.0E0
CH2(S)+O2=CO+H2O    1.2E13 0.0 0.0E0
CH2(S)+O=CO+H2    1.5E13 0.0 0.0E0
CH2(S)+O=HCO+H    1.5E13 0.0 0.0E0
CH2(S)+H2=CH3+H    7.0E13 0.0 0.0E0
CH2(S)+H=CH+H2    3.0E13 0.0 0.0E0
CH2(S)+OH=CH2O+H    3.0E13 0.0 0.0E0
CH2(S)+CO2=CH2O+CO    1.4E13 0.0 0.0E0
CH2+H(+M)=CH3(+M)    2.5E16 -0.8 0.0E0
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/3.2E27 -3.14E0 1.23E3/
   TROE/6.8E-1 7.8E1 1.995E3 5.59E3/
CH2+O2=HCO+OH    1.06E13 0.0 1.5E3
CH2+O2=>CO2+2H    2.64E12 0.0 1.5E3
CH2+O=>CO+2H    5.0E13 0.0 0.0E0
CH2+H=CH+H2    3.0E13 0.0 0.0E0
CH2+OH=CH+H2O    1.13E7 2.0 3.0E3
CHV+AR=CH+AR    4.0E11 0.5 0.0E0
CHV+H2O=CH+H2O    5.3E13 0.0 0.0E0
CHV+CO=CH+CO    2.44E12 0.5 0.0E0
CHV+CO2=CH+CO2    2.41E-1 4.3 -1.694E3
CHV+O2=CH+O2    2.48E6 2.14 -1.72E3
CHV+H2=CH+H2    1.47E14 0.0 1.361E3
CHV+CH4=CH+CH4    1.73E13 0.0 1.67E2
CHV=CH    1.86E6 0.0 0.0E0
CHV+N2=CH+N2    3.03E2 3.4 -3.81E2
CH+O2=CO+OHV    4.04E13 0.0 0.0E0
CH+O2=HCO+O    3.3E13 0.0 0.0E0
CH+O=CO+H    5.7E13 0.0 0.0E0
CH+OH=HCO+H    3.0E13 0.0 0.0E0
CH+H2O=H+CH2O    1.774E16 -1.22 2.38E1
CH+CO2=HCO+CO    1.7E12 0.0 6.85E2
CH3+O2(+M)=CH3O2(+M)    7.812E9 0.9 0.0E0
   LOW/6.85E24 -3.0E0 0.0E0/
   TROE/6.0E-1 1.0E3 7.0E1 1.7E3/
CH3+O2=CH3O+O    7.546E12 0.0 2.832E4
CH3+O2=CH2O+OH    2.641E0 3.283 8.105E3
CH3+O=CH2O+H    5.54E13 0.05 -1.36E2
CH3+OH=CH2(S)+H2O    4.936E14 -0.669 -4.458E2
   PLOG/1.0E-2 4.936E14 -6.69E-1 -4.458E2/
   PLOG/1.0E-1 1.207E15 -7.78E-1 -1.756E2/
   PLOG/1.0E0 5.282E17 -1.518E0 1.772E3/
   PLOG/1.0E1 4.788E23 -3.155E0 7.003E3/
   PLOG/1.0E2 8.433E19 -1.962E0 8.244E3/
CH3+OH=CH2O+H2    3.502E5 1.441 -3.244E3
   PLOG/1.0E-2 3.502E5 1.441E0 -3.244E3/
   PLOG/1.0E-1 8.854E5 1.327E0 -2.975E3/
   PLOG/1.0E0 1.65E7 9.73E-1 -2.01E3/
   PLOG/1.0E1 5.374E9 2.87E-1 2.8E2/
   PLOG/1.0E2 9.494E18 -2.199E0 9.769E3/
CH3+OH=CH2OH+H    1.621E10 0.965 3.21E3
   PLOG/1.0E-2 1.621E10 9.65E-1 3.214E3/
   PLOG/1.0E-1 1.807E10 9.5E-1 3.247E3/
   PLOG/1.0E0 4.686E10 8.33E-1 3.566E3/
   PLOG/1.0E1 1.525E13 1.34E-1 5.641E3/
   PLOG/1.0E2 3.59E14 -1.86E-1 8.601E3/
CH3+OH=H+CH3O    1.186E9 1.016 1.194E4
   PLOG/1.0E-2 1.186E9 1.016E0 1.194E4/
   PLOG/1.0E-1 1.188E9 1.016E0 1.194E4/
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   PLOG/1.0E0 1.23E9 1.011E0 1.195E4/
   PLOG/1.0E1 1.798E9 9.65E-1 1.206E4/
   PLOG/1.0E2 5.242E10 5.51E-1 1.307E4/
CH3+OH=HCOH+H2    8.674E8 0.787 -3.046E3
   PLOG/1.0E-2 8.674E8 7.87E-1 -3.046E3/
   PLOG/1.0E-1 3.115E9 6.3E-1 -2.669E3/
   PLOG/1.0E0 1.557E11 1.56E-1 -1.368E3/
   PLOG/1.0E1 1.704E21 -2.641E0 6.412E3/
   PLOG/1.0E2 7.25E20 -2.402E0 9.639E3/
CH3+OH=CH2+H2O    4.293E4 2.568 3.9978E3
CH3+HO2=CH3O+OH    1.0E12 0.269 -6.875E2
CH3O2+O=CH3O+O2    3.6E13 0.0 0.0E0
CH3O2+H=CH3O+OH    9.6E13 0.0 0.0E0
CH3O2+HO2=CH3O2H+O2    2.47E11 0.0 -1.57E3
CH3O2+H2O2=CH3O2H+HO2    2.41E12 0.0 9.936E3
CH3O2+CH3=2CH3O    5.08E12 0.0 -1.411E3
2CH3O2=>O2+2CH3O    1.4E16 -1.61 1.86E3
H2+CH3O2=H+CH3O2H    1.5E14 0.0 2.603E4
CH3O2H=CH3O+OH    6.31E14 0.0 4.23E4
CH2OH+O2=CH2O+HO2    1.51E15 -1.0 0.0E0
   DUP
CH2OH+O2=CH2O+HO2    2.41E14 0.0 5.017E3
   DUP
CH2OH+H=CH2O+H2    6.0E12 0.0 0.0E0
CH2OH+HO2=CH2O+H2O2    1.2E13 0.0 0.0E0
CH2OH+HCO=2CH2O    1.8E14 0.0 0.0E0
CH2OH+OH=H2O+CH2O    2.4E13 0.0 0.0E0
CH2OH+O=OH+CH2O    4.2E13 0.0 0.0E0
CH3O+O2=CH2O+HO2    4.38E-19 9.5 -5.501E3
CH3O+H=CH2O+H2    2.0E13 0.0 0.0E0
CH3O+HO2=CH2O+H2O2    3.01E11 0.0 0.0E0
CH3O+CH3=CH2O+CH4    1.2E13 0.0 0.0E0
HCOH+O2=>CO2+H+OH    5.0E12 0.0 0.0E0
HCOH+O2=CO2+H2O    3.0E13 0.0 0.0E0
HCOH+O=>CO2+2H    5.0E13 0.0 0.0E0
HCOH+O=>CO+OH+H    3.0E13 0.0 0.0E0
HCOH+H=CH2O+H    2.0E14 0.0 0.0E0
HCOH+OH=HCO+H2O    2.0E13 0.0 0.0E0
HCO+H(+M)=CH2O(+M)    1.09E12 0.48 -2.6E2
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/1.35E24 -2.57E0 1.425E3/
   TROE/7.824E-1 2.71E2 2.755E3 6.57E3/
CO+H2(+M)=CH2O(+M)    4.3E7 1.5 7.96E4
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/5.07E27 -3.42E0 8.4348E4/
   TROE/9.32E-1 1.97E2 1.54E3 1.03E4/
CH2O+O2=HCO+HO2    8.07E15 0.0 5.342E4
CH2O+O=HCO+OH    6.26E9 1.15 2.26E3
CH2O+H=HCO+H2    5.74E7 1.9 2.74E3
CH2O+OH=HCO+H2O    7.82E7 1.63 -1.055E3
CH2O+HO2=HCO+H2O2    1.88E4 2.7 1.152E4
CH2O+CH3=HCO+CH4    3.83E1 3.36 4.312E3
CH2O+O2CHO=HCO+HO2CHO    1.99E12 0.0 1.166E4
CH2O+OCHO=HCO+HOCHO    5.6E12 0.0 1.36E4
CH2O+CH3O2=HCO+CH3O2H    1.99E12 0.0 1.166E4
HCO+M=H+CO+M    5.7E11 0.66 1.487E4
   H2/2.0/
   H2O/6.0/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
HCO+O2=CO+HO2    7.58E12 0.0 4.1E2
HCO+O=CO+OH    3.02E13 0.0 0.0E0
HCO+H=CO+H2    7.34E13 0.0 0.0E0
HCO+OH=CO+H2O    3.011E13 0.0 0.0E0
HCO+CH3=CO+CH4    2.65E13 0.0 0.0E0
2HCO=CO+CH2O    1.8E13 0.0 0.0E0
HCO+O=CO2+H    3.0E13 0.0 0.0E0
HCO+HO2=>CO2+H+OH    3.0E13 0.0 0.0E0
2HCO=>H2+2CO    3.0E12 0.0 0.0E0
CH2O+H(+M)=CH2OH(+M)    5.4E11 0.454 3.6E3
   H2/2.0/
   H2O/6.0/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   LOW/1.27E32 -4.82E0 6.53E3/
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    TROE/7.187E-1 1.03E2 1.291E3 4.16E3/
CH3O(+M)=CH2O+H(+M)    6.8E13 0.0 2.617E4
    H2/2.0/
    H2O/6.0/
    CO/1.5/
    CO2/2.0/
    CH4/2.0/
    C2H6/3.0/
    LOW/1.867E25 -3.0E0 2.4307E4/
    TROE/9.0E-1 2.5E3 1.3E3 1.0E99/
HCO+O2=O2CHO    1.2E11 0.0 -1.1E3
HOCHO=CO+H2O    2.45E12 0.0 6.047E4
HOCHO=CO2+H2    2.95E9 0.0 4.852E4
OCHO+HO2=HOCHO+O2    3.5E10 0.0 -3.275E3
OCHO+H2O2=HOCHO+HO2    2.4E12 0.0 1.0E4
HOCHO+H=>H2+CO2+H    4.24E6 2.1 4.868E3
HOCHO+H=>H2+CO+OH    6.03E13 -0.35 2.988E3
HOCHO+O=>CO+2OH    1.77E18 -1.9 2.975E3
HOCHO+OH=>H2O+CO2+H    2.62E6 2.06 9.16E2
HOCHO+OH=>H2O+CO+OH    1.85E7 1.51 -9.62E2
HOCHO+CH3=>CH4+CO+OH    3.9E-7 5.8 2.2E3
HOCHO+HO2=>H2O2+CO+OH    1.0E12 0.0 1.192E4
OCHO+OH=HO2CHO    2.0E13 0.0 0.0E0
2CH3(+M)=C2H6(+M)    2.277E15 -0.69 1.749E2
    H2O/5.0/
    CO/2.0/
    CO2/3.0/
    LOW/8.054E31 -3.75E0 9.816E2/
    TROE/0.0E0 5.7E2 1.0E30 1.0E30/
C2H5+H(+M)=C2H6(+M)    5.21E17 -0.99 1.58E3
    H2/2.0/
    H2O/6.0/
    AR/0.7/
    CO/1.5/
    CO2/2.0/
    CH4/2.0/
    C2H6/3.0/
    HE/0.7/
    LOW/1.99E41 -7.08E0 6.685E3/
    TROE/8.42E-1 1.25E2 2.219E3 6.882E3/
2CH3=H+C2H5    4.74E12 0.105 1.06643E4
    PLOG/1.0E-2 4.74E12 1.05E-1 1.06643E4/
    PLOG/1.0E-1 2.57E13 -9.6E-2 1.14061E4/
    PLOG/1.0E0 3.1E14 -3.62E-1 1.33725E4/
    PLOG/1.0E1 2.15E10 8.85E-1 1.35325E4/
    PLOG/1.0E2 1.032E2 3.23E0 1.12361E4/
C2H6+O2=C2H5+HO2    6.03E13 0.0 5.187E4
C2H6+O=C2H5+OH    3.55E6 2.4 5.83E3
C2H6+H=C2H5+H2    1.15E8 1.9 7.53E3
C2H6+OH=C2H5+H2O    1.48E7 1.9 9.5E2
C2H6+HO2=C2H5+H2O2    3.46E1 3.61 1.692E4
C2H6+CH=C2H5+CH2    1.1E14 0.0 -2.6E2
C2H6+CH2(S)=C2H5+CH3    1.2E14 0.0 0.0E0
C2H6+CH3=C2H5+CH4    5.55E-4 4.72 3.231E3
C2H6+CH3O2=C2H5+CH3O2H    1.94E1 3.64 1.71E4
C2H6+C2H5O2=C2H5+C2H5O2H    8.6E0 3.76 1.72E4
C2H4+H(+M)=C2H5(+M)    9.569E8 1.463 1.355E3
    H2/2.0/
    H2O/6.0/
    CH4/2.0/
    CO/1.5/
    CO2/2.0/
    C2H6/3.0/
    AR/0.7/
    LOW/1.419E39 -6.642E0 5.769E3/
    TROE/-5.69E-1 2.99E2 -9.147E3 1.524E2/
C2H5+H=C2H4+H2    2.0E12 0.0 0.0E0
2C2H4=C2H5+C2H3    4.82E14 0.0 7.153E4
C2H5+CH3=CH4+C2H4    1.18E4 2.45 -2.921E3
C2H5+O=CH3CHO+H    1.1E14 0.0 0.0E0
C2H5+HO2=C2H5O+OH    1.1E13 0.0 0.0E0
C2H5+CH3O2=C2H5O+CH3O    8.0E12 0.0 -1.0E3
C2H5+O2=C2H5O2    3.398E53 -13.9 9.279E3
    PLOG/4.0E-2 3.398E53 -1.39E1 9.279E3/
    PLOG/1.0E0 9.362E59 -1.528E1 1.424E4/
    PLOG/1.0E1 1.262E60 -1.491E1 1.624E4/
C2H5+O2=C2H4+HO2    2.094E9 0.49 -3.914E2
    PLOG/4.0E-2 2.094E9 4.9E-1 -3.914E2/
    PLOG/1.0E0 1.843E7 1.13E0 -7.206E2/
    PLOG/1.0E1 7.561E14 -1.01E0 4.749E3/
C2H5+O2=CH3CHO+OH    4.908E-6 4.76 2.543E2
    PLOG/4.0E-2 4.908E-6 4.76E0 2.543E2/
    PLOG/1.0E0 6.803E-2 3.57E0 2.643E3/
    PLOG/1.0E1 8.265E2 2.41E0 5.285E3/
C2H5O2=CH3CHO+OH    1.237E35 -9.42 3.636E4
    PLOG/4.0E-2 1.237E35 -9.42E0 3.636E4/
    PLOG/1.0E0 1.687E36 -9.22E0 3.87E4/
    PLOG/1.0E1 2.52E41 -1.02E1 4.371E4/
C2H5O2=C2H4+HO2    1.782E32 -7.1 3.284E4
    PLOG/4.0E-2 1.782E32 -7.1E0 3.284E4/
    PLOG/1.0E0 2.701E37 -8.47E0 3.584E4/
    PLOG/1.0E1 1.98E38 -8.46E0 3.79E4/
C2H5O2+HO2=C2H5O2H+O2    1.75E10 0.0 -3.275E3
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C2H5O2+CH2O=C2H5O2H+HCO    1.99E12 0.0 1.166E4
C2H5O2+CH4=C2H5O2H+CH3    1.81E11 0.0 1.848E4
C2H5O2+H2=C2H5O2H+H    1.5E14 0.0 2.603E4
C2H5O2H=C2H5O+OH    6.31E14 0.0 4.23E4
C2H3+H(+M)=C2H4(+M)    6.08E12 0.27 2.8E2
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/1.4E30 -3.86E0 3.32E3/
   TROE/7.82E-1 2.075E2 2.663E3 6.095E3/
C2H4+O2=C2H3+HO2    4.22E13 0.0 5.76231E4
C2H4+H=C2H3+H2    5.07E7 1.93 1.295E4
C2H4+OH=C2H3+H2O    2.23E4 2.745 2.2155E3
C2H4+CH3O2=C2H3+CH3O2H    8.59E0 3.754 2.7132E4
C2H4+C2H5O2=C2H3+C2H5O2H    8.59E0 3.754 2.7132E4
C2H4+CH3CO3=C2H3+CH3CO3H    1.13E13 0.0 3.043E4
C2H4+CH3=C2H3+CH4    9.76E2 2.947 1.5148E4
   DUP
C2H4+CH3=C2H3+CH4    8.13E-5 4.417 8.8358E3
   DUP
C2H4+O=CH3+HCO    7.453E6 1.88 1.83E2
C2H4+O=CH2CHO+H    6.098E6 1.88 1.83E2
CH+CH4=C2H4+H    6.0E13 0.0 0.0E0
CH2(S)+CH3=C2H4+H    2.0E13 0.0 0.0E0
C2H4+OH=CH3+CH2O    5.35E0 2.92 -1.7327E3
   PLOG/1.0E-2 5.35E0 2.92E0 -1.7327E3/
   PLOG/2.5E-2 3.19E1 2.71E0 -1.1723E3/
   PLOG/1.0E-1 5.55E2 2.36E0 -1.808E2/
   PLOG/1.0E0 1.78E5 1.68E0 2.0605E3/
   PLOG/1.0E1 2.37E9 5.6E-1 6.0067E3/
   PLOG/1.0E2 2.76E13 -5.0E-1 1.14551E4/
C2H4+OH=CH3CHO+H    2.37E-7 5.3 -2.0506E3
   PLOG/1.0E-2 2.37E-7 5.3E0 -2.0506E3/
   PLOG/2.5E-2 8.73E-5 4.57E0 -6.18E2/
   PLOG/1.0E-1 4.03E-1 3.54E0 1.8817E3/
   PLOG/1.0E0 2.38E-2 3.91E0 1.7227E3/
   PLOG/1.0E1 8.25E8 1.01E0 1.05073E4/
   PLOG/1.0E2 6.8E9 8.1E-1 1.38673E4/
C2H2+H(+M)=C2H3(+M)    1.71E10 1.266 2.709E3
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/6.346E31 -4.664E0 3.78E3/
   TROE/7.88E-1 -1.02E4 1.0E-30/
C2H3+O2=C2H3OO    4.07E27 -4.67 5.222E3
   DUP
   PLOG/1.0E-2 1.55E24 -5.45E0 9.662E3/
   PLOG/1.0E-1 3.48E56 -1.501E1 1.916E4/
   PLOG/3.16E-1 1.25E64 -1.697E1 2.129E4/
   PLOG/1.0E0 3.34E61 -1.579E1 2.015E4/
   PLOG/3.16E0 7.34E53 -1.311E1 1.73E4/
   PLOG/1.0E1 4.16E48 -1.121E1 1.6E4/
   PLOG/3.16E1 2.33E43 -9.38E0 1.481E4/
   PLOG/1.0E2 3.41E39 -8.04E0 1.436E4/
C2H3+O2=C2H3OO    4.07E27 -4.67 5.222E3
   DUP
   PLOG/1.0E-2 1.78E-9 4.15E0 -4.707E3/
   PLOG/1.0E-1 2.36E22 -4.52E0 2.839E3/
   PLOG/3.16E-1 2.0E26 -5.43E0 2.725E3/
   PLOG/1.0E0 6.13E28 -5.89E0 3.154E3/
   PLOG/3.16E0 2.14E29 -5.8E0 3.52E3/
   PLOG/1.0E1 3.48E28 -5.37E0 3.636E3/
   PLOG/3.16E1 3.32E27 -4.95E0 3.61E3/
   PLOG/1.0E2 1.03E27 -4.72E0 3.68E3/
C2H3+O2=CHCHO+OH    2.84E14 -0.8 7.232E3
   DUP
   PLOG/1.0E-2 3.91E11 -1.1E-1 2.131E3/
   PLOG/1.0E-1 1.13E9 5.5E-1 4.6E1/
   PLOG/3.16E-1 8.46E8 5.6E-1 7.0E-1/
   PLOG/1.0E0 2.75E14 -1.83E0 4.6E0/
   PLOG/3.16E0 2.58E20 -2.84E0 7.53E3/
   PLOG/1.0E1 9.18E14 -2.26E0 -4.0E-1/
   PLOG/3.16E1 6.11E25 -4.21E0 1.305E4/
   PLOG/1.0E2 1.65E30 -5.35E0 1.843E4/
C2H3+O2=CHCHO+OH    2.84E14 -0.8 7.232E3
   DUP
   PLOG/1.0E-2 9.91E11 -6.6E-1 -6.0E-1/
   PLOG/1.0E-1 6.94E14 -1.16E0 4.542E3/
   PLOG/3.16E-1 2.79E13 -7.2E-1 3.479E3/
   PLOG/1.0E0 4.99E11 -1.4E-1 1.995E3/
   PLOG/3.16E0 2.35E10 2.3E-1 1.573E3/
   PLOG/1.0E1 1.7E14 -8.2E-1 4.45E3/
   PLOG/3.16E1 1.42E11 5.0E-2 3.774E3/
```

PLOG/1.0E2 3.17E11 -2.0E-2 5.338E3/
C2H3+O2=CH2CHO+O 1.76E12 0.15 4.205E3
DUP
PLOG/1.0E-2 7.88E20 -2.67E0 6.742E3/
PLOG/1.0E-1 7.72E20 -2.67E0 6.713E3/
PLOG/3.16E-1 9.87E20 -2.7E0 6.724E3/
PLOG/1.0E0 7.1E20 -2.65E0 6.489E3/
PLOG/3.16E0 4.5E20 -2.53E0 6.406E3/
PLOG/1.0E1 1.76E23 -3.22E0 8.697E3/
PLOG/3.16E1 3.14E25 -3.77E0 1.153E4/
PLOG/1.0E2 1.02E26 -3.8E0 1.391E4/
C2H3+O2=CH2CHO+O 1.76E12 0.15 4.205E3
DUP
PLOG/1.0E-2 1.36E10 6.2E-1 -2.776E2/
PLOG/1.0E-1 1.42E10 6.2E-1 -2.477E2/
PLOG/3.16E-1 1.66E10 6.0E-1 -1.625E2/
PLOG/1.0E0 2.02E10 5.8E-1 3.84E1/
PLOG/3.16E0 9.75E9 6.7E-1 2.48E2/
PLOG/1.0E1 7.34E9 7.2E-1 7.781E2/
PLOG/3.16E1 1.57E9 9.2E-1 1.219E3/
PLOG/1.0E2 7.85E7 1.28E0 1.401E3/
C2H3+O2=C2H2+HO2 6.49E6 1.5 5.218E3
DUP
PLOG/1.0E-2 1.08E7 1.28E0 3.322E3/
PLOG/1.0E-1 7.75E6 1.33E0 3.216E3/
PLOG/3.16E-1 1.21E7 1.27E0 3.311E3/
PLOG/1.0E0 2.15E7 1.19E0 3.367E3/
PLOG/3.16E0 1.13E8 1.0E0 3.695E3/
PLOG/1.0E1 1.31E11 1.2E-1 5.872E3/
PLOG/3.16E1 1.19E9 8.2E-1 5.617E3/
PLOG/1.0E2 1.06E17 -1.45E0 1.223E4/
C2H3+O2=C2H2+HO2 6.49E6 1.5 5.218E3
DUP
PLOG/1.0E-2 4.76E1 2.75E0 -7.964E2/
PLOG/1.0E-1 5.16E1 2.73E0 -7.683E2/
PLOG/3.16E-1 5.55E1 2.73E0 -6.585E2/
PLOG/1.0E0 4.6E1 2.76E0 -4.928E2/
PLOG/3.16E0 3.75E0 3.07E0 -6.01E2/
PLOG/1.0E1 5.48E0 3.07E0 8.57E1/
PLOG/3.16E1 4.47E8 0.0E0 9.55E2/
PLOG/1.0E2 2.02E1 2.94E0 1.847E3/
C2H3+O2=CH2CO+OH 1.17E3 2.43 7.074E3
DUP
PLOG/1.0E-2 8.66E2 2.41E0 6.061E3/
PLOG/1.0E-1 8.91E2 2.41E0 6.078E3/
PLOG/3.16E-1 9.43E2 2.4E0 6.112E3/
PLOG/1.0E0 1.06E3 2.39E0 6.18E3/
PLOG/3.16E0 1.09E3 2.38E0 6.179E3/
PLOG/1.0E1 1.39E3 2.36E0 6.074E3/
PLOG/3.16E1 2.49E6 1.42E0 8.48E3/
PLOG/1.0E2 1.66E10 3.6E-1 1.201E4/
C2H3+O2=CH2CO+OH 1.17E3 2.43 7.074E3
DUP
PLOG/1.0E-2 1.82E-1 3.12E0 1.331E3/
PLOG/1.0E-1 2.07E-1 3.11E0 1.383E3/
PLOG/3.16E-1 2.71E-1 3.08E0 1.496E3/
PLOG/1.0E0 5.26E-1 3.01E0 1.777E3/
PLOG/3.16E0 1.37E0 2.9E0 2.225E3/
PLOG/1.0E1 4.19E-1 2.93E0 2.052E3/
PLOG/3.16E1 1.19E-4 4.21E0 2.043E3/
PLOG/1.0E2 1.3E-3 3.97E0 3.414E3/
C2H3+O2=CH2O+HCO 1.16E16 -1.13 3.791E3
DUP
PLOG/1.0E-2 2.49E36 -7.6E0 1.264E4/
PLOG/1.0E-1 2.43E36 -7.6E0 1.261E4/
PLOG/3.16E-1 1.95E36 -7.57E0 1.249E4/
PLOG/1.0E0 2.73E35 -7.32E0 1.182E4/
PLOG/3.16E0 1.43E36 -7.47E0 1.246E4/
PLOG/1.0E1 5.18E35 -7.2E0 1.343E4/
PLOG/3.16E1 3.19E20 -2.57E0 5.578E3/
PLOG/1.0E2 2.73E33 -6.28E0 1.6E4/
C2H3+O2=CH2O+HCO 1.16E16 -1.13 3.791E3
DUP
PLOG/1.0E-2 4.54E15 -1.28E0 5.153E2/
PLOG/1.0E-1 4.59E15 -1.28E0 5.13E2/
PLOG/3.16E-1 4.81E15 -1.29E0 5.206E2/
PLOG/1.0E0 6.08E15 -1.31E0 6.457E2/
PLOG/3.16E0 9.45E15 -1.36E0 1.066E3/
PLOG/1.0E1 2.56E15 -1.18E0 1.429E3/
PLOG/3.16E1 1.03E69 -1.923E1 1.476E4/
PLOG/1.0E2 4.21E10 1.9E-1 8.306E2/
C2H3+O2=>CH2O+H+CO 1.16E16 -1.13 3.791E3
DUP
PLOG/1.0E-2 5.82E36 -7.6E0 1.264E4/
PLOG/1.0E-1 5.66E36 -7.6E0 1.261E4/
PLOG/3.16E-1 4.55E36 -7.57E0 1.249E4/
PLOG/1.0E0 6.36E35 -7.32E0 1.182E4/
PLOG/3.16E0 3.35E36 -7.47E0 1.246E4/
PLOG/1.0E1 1.21E36 -7.2E0 1.343E4/
PLOG/3.16E1 7.43E20 -2.57E0 5.578E3/
PLOG/1.0E2 6.36E33 -6.28E0 1.6E4/
C2H3+O2=>CH2O+H+CO 1.16E16 -1.13 3.791E3
DUP

PLOG/1.0E-2 1.06E16 -1.28E0 5.153E2/
PLOG/1.0E-1 1.07E16 -1.28E0 5.13E2/
PLOG/3.16E-1 1.13E16 -1.29E0 5.206E2/
PLOG/1.0E0 1.42E16 -1.31E0 6.457E2/
PLOG/3.16E0 2.2E16 -1.36E0 1.066E3/
PLOG/1.0E1 5.98E15 -1.18E0 1.429E3/
PLOG/3.16E1 2.39E69 -1.923E1 1.476E4/
PLOG/1.0E2 9.81E10 1.9E-1 8.306E2/
C2H3+O2=CO+CH3O 3.09E13 -0.89 3.682E3
DUP
PLOG/1.0E-2 8.19E18 -2.66E0 3.201E3/
PLOG/1.0E-1 4.06E14 -1.32E0 8.858E2/
PLOG/3.16E-1 4.34E14 -1.33E0 9.006E2/
PLOG/1.0E0 1.03E11 -3.3E-1 -7.478E2/
PLOG/3.16E0 1.89E12 -3.0E0 -8.995E3/
PLOG/1.0E1 1.93E24 -5.63E0 1.8E0/
PLOG/3.16E1 1.1E18 -2.22E0 5.178E3/
PLOG/1.0E2 5.79E32 -6.45E0 1.681E4/
C2H3+O2=CO+CH3O 3.09E13 -0.89 3.682E3
DUP
PLOG/1.0E-2 1.29E9 1.8E-1 -1.717E3/
PLOG/1.0E-1 5.99E11 -2.93E0 -9.564E3/
PLOG/3.16E-1 2.91E11 -2.93E0 -1.012E4/
PLOG/1.0E0 5.77E21 -3.54E0 4.772E3/
PLOG/3.16E0 4.99E15 -1.62E0 1.849E3/
PLOG/1.0E1 9.33E16 -1.96E0 3.324E3/
PLOG/3.16E1 1.02E72 -2.069E1 1.586E4/
PLOG/1.0E2 1.1E9 3.1E-1 1.024E3/
C2H3+O2=CO2+CH3 6.16E13 -1.05 3.743E3
DUP
PLOG/1.0E-2 2.37E35 -7.76E0 1.263E4/
PLOG/1.0E-1 1.73E35 -7.72E0 1.252E4/
PLOG/3.16E-1 4.47E34 -7.55E0 1.214E4/
PLOG/1.0E0 7.25E31 -6.7E0 1.044E4/
PLOG/3.16E0 3.63E35 -7.75E0 1.283E4/
PLOG/1.0E1 2.09E35 -7.53E0 1.405E4/
PLOG/3.16E1 3.84E18 -2.44E0 5.408E3/
PLOG/1.0E2 1.21E32 -6.32E0 1.619E4/
C2H3+O2=CO2+CH3 6.16E13 -1.05 3.743E3
DUP
PLOG/1.0E-2 6.27E13 -1.16E0 4.063E2/
PLOG/1.0E-1 6.24E13 -1.16E0 4.014E2/
PLOG/3.16E-1 6.12E13 -1.16E0 3.97E2/
PLOG/1.0E0 5.32E13 -1.14E0 4.467E2/
PLOG/3.16E0 1.45E14 -1.26E0 9.877E2/
PLOG/1.0E1 5.02E13 -1.11E0 1.409E3/
PLOG/3.16E1 1.4E70 -2.011E1 1.543E4/
PLOG/1.0E2 9.21E8 2.5E-1 8.553E2/
C2H3OO=CHCHO+OH 5.89E36 -7.1 5.144E4
DUP
PLOG/1.0E-2 3.64E49 -1.213E1 6.742E4/
PLOG/1.0E-1 1.44E36 -9.92E0 4.122E4/
PLOG/3.16E-1 4.18E40 -1.053E1 4.367E4/
PLOG/1.0E0 3.79E46 -1.072E1 5.19E4/
PLOG/3.16E0 1.6E49 -1.124E1 5.415E4/
PLOG/1.0E1 2.38E51 -1.164E1 5.698E4/
PLOG/3.16E1 2.0E54 -1.222E1 6.184E4/
PLOG/1.0E2 9.54E195 -5.227E1 1.635E5/
C2H3OO=CHCHO+OH 5.89E36 -7.1 5.144E4
DUP
PLOG/1.0E-2 1.17E56 -1.481E1 6.07E4/
PLOG/1.0E-1 2.32E40 -9.39E0 5.042E4/
PLOG/3.16E-1 1.61E43 -9.99E0 5.029E4/
PLOG/1.0E0 2.33E124 -3.677E1 7.01E4/
PLOG/3.16E0 1.88E103 -2.949E1 6.541E4/
PLOG/1.0E1 5.96E86 -2.381E1 6.217E4/
PLOG/3.16E1 1.51E57 -1.394E1 5.539E4/
PLOG/1.0E2 1.79E34 -6.4E0 5.0E4/
C2H3OO=CH2CHO+O 1.22E29 -4.71 4.234E4
DUP
PLOG/1.0E-2 2.7E180 -4.819E1 1.693E5/
PLOG/1.0E-1 3.9E38 -8.69E0 4.277E4/
PLOG/3.16E-1 4.57E47 -1.121E1 4.705E4/
PLOG/1.0E0 7.62E81 -2.128E1 6.508E4/
PLOG/3.16E0 1.86E68 -1.683E1 6.068E4/
PLOG/1.0E1 2.02E55 -1.269E1 5.584E4/
PLOG/3.16E1 1.11E53 -1.179E1 5.669E4/
PLOG/1.0E2 4.3E48 -1.031E1 5.609E4/
C2H3OO=CH2CHO+O 1.22E29 -4.71 4.234E4
DUP
PLOG/1.0E-2 1.47E30 -6.64E0 4.111E4/
PLOG/1.0E-1 9.65E-12 5.96E0 2.289E4/
PLOG/3.16E-1 3.95E22 -3.71E0 3.627E4/
PLOG/1.0E0 2.39E33 -6.62E0 4.128E4/
PLOG/3.16E0 6.37E31 -5.96E0 4.126E4/
PLOG/1.0E1 2.13E29 -5.1E0 4.071E4/
PLOG/3.16E1 4.66E27 -4.5E0 4.053E4/
PLOG/1.0E2 5.99E25 -3.85E0 4.012E4/
C2H3OO=CH2CO+OH 1.55E24 -3.87 4.985E4
DUP
PLOG/1.0E-2 1.15E47 -1.228E1 7.533E4/
PLOG/1.0E-1 8.43E9 -2.06E0 3.372E4/
PLOG/3.16E-1 6.06E4 1.7E-1 3.422E4/

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    PLOG/1.0E0 1.51E19 -3.61E0 4.306E4/
    PLOG/3.16E0 2.13E33 -7.39E0 5.161E4/
    PLOG/1.0E1 4.44E36 -7.99E0 5.468E4/
    PLOG/3.16E1 1.19E37 -7.8E0 5.646E4/
    PLOG/1.0E2 9.08E35 -7.21E0 5.755E4/
C2H3OO=CH2CO+OH    1.55E24 -3.87 4.985E4
    DUP
    PLOG/1.0E-2 2.31E2 -7.3E-1 2.571E4/
    PLOG/1.0E-1 1.83E-23 7.84E0 2.019E4/
    PLOG/3.16E-1 3.82E63 -2.044E1 4.342E4/
    PLOG/1.0E0 3.18E27 -7.76E0 3.723E4/
    PLOG/3.16E0 2.32E-5 3.47E0 3.156E4/
    PLOG/1.0E1 1.06E-1 2.64E0 3.416E4/
    PLOG/3.16E1 5.62E2 1.7E0 3.645E4/
    PLOG/1.0E2 1.11E7 5.2E-1 3.867E4/
C2H3OO=CH2O+HCO    1.19E20 -2.29 3.017E4
    DUP
    PLOG/1.0E-2 1.66E174 -5.552E1 6.032E4/
    PLOG/1.0E-1 9.03E66 -1.725E1 4.812E4/
    PLOG/3.16E-1 1.82E43 -9.87E0 3.796E4/
    PLOG/1.0E0 8.64E33 -6.88E0 3.437E4/
    PLOG/3.16E0 7.29E171 -4.353E1 1.919E5/
    PLOG/1.0E1 1.03E32 -6.06E0 3.55E4/
    PLOG/3.16E1 1.85E34 -6.57E0 3.851E4/
    PLOG/1.0E2 5.7E29 -5.19E0 3.68E4/
C2H3OO=CH2O+HCO    1.19E20 -2.29 3.017E4
    DUP
    PLOG/1.0E-2 2.27E35 -7.97E0 3.128E4/
    PLOG/1.0E-1 2.08E26 -4.96E0 2.878E4/
    PLOG/3.16E-1 1.45E20 -3.08E0 2.663E4/
    PLOG/1.0E0 1.06E130 -3.938E1 5.47E4/
    PLOG/3.16E0 2.35E34 -6.87E0 3.57E4/
    PLOG/1.0E1 2.18E175 -5.378E1 6.85E4/
    PLOG/3.16E1 1.07E185 -5.422E1 8.899E4/
    PLOG/1.0E2 4.68E2 1.81E0 1.81E4/
C2H3OO=>CH2O+H+CO    1.19E20 -2.29 3.017E4
    DUP
    PLOG/1.0E-2 3.88E174 -5.552E1 6.032E4/
    PLOG/1.0E-1 2.11E67 -1.725E1 4.812E4/
    PLOG/3.16E-1 4.26E43 -9.87E0 3.796E4/
    PLOG/1.0E0 2.02E34 -6.88E0 3.437E4/
    PLOG/3.16E0 1.7E172 -4.353E1 1.919E5/
    PLOG/1.0E1 2.4E32 -6.06E0 3.55E4/
    PLOG/3.16E1 4.32E34 -6.57E0 3.851E4/
    PLOG/1.0E2 1.33E30 -5.19E0 3.68E4/
C2H3OO=>CH2O+H+CO    1.19E20 -2.29 3.017E4
    DUP
    PLOG/1.0E-2 5.29E35 -7.97E0 3.128E4/
    PLOG/1.0E-1 4.85E26 -4.96E0 2.878E4/
    PLOG/3.16E-1 3.37E20 -3.08E0 2.663E4/
    PLOG/1.0E0 2.46E130 -3.938E1 5.47E4/
    PLOG/3.16E0 5.49E34 -6.87E0 3.57E4/
    PLOG/1.0E1 5.09E175 -5.378E1 6.85E4/
    PLOG/3.16E1 2.49E185 -5.422E1 8.899E4/
    PLOG/1.0E2 1.09E3 1.81E0 1.81E4/
C2H3OO=>CH2O+H+CO    1.19E20 -2.29 3.017E4
    DUP
    PLOG/1.0E-2 5.2E33 -7.92E0 3.132E4/
    PLOG/1.0E-1 1.26E98 -2.709E1 6.406E4/
    PLOG/3.16E-1 1.8E33 -7.27E0 3.376E4/
    PLOG/1.0E0 3.83E33 -7.2E0 3.51E4/
    PLOG/3.16E0 1.28E79 -1.961E1 7.487E4/
    PLOG/1.0E1 4.07E32 -6.62E0 3.721E4/
    PLOG/3.16E1 6.86E44 -1.004E1 4.703E4/
    PLOG/1.0E2 3.25E4 1.694E0 2.33276E4/
C2H3OO=>CH2O+H+CO    1.19E20 -2.29 3.017E4
    DUP
    PLOG/1.0E-2 2.31E129 -4.186E1 4.585E4/
    PLOG/1.0E-1 2.42E28 -5.99E0 3.054E4/
    PLOG/3.16E-1 8.69E-50 1.663E1 -3.9E3/
    PLOG/1.0E0 1.19E-39 1.361E1 -1.317E3/
    PLOG/3.16E0 8.8E86 -2.308E1 6.101E4/
    PLOG/1.0E1 1.27E3 1.44E0 1.866E4/
    PLOG/3.16E1 1.97E17 -2.23E0 2.859E4/
    PLOG/1.0E2 1.0E-99 0.0E0 0.0E0/
C2H3+H=C2H2+H2    1.7E14 0.0 0.0E0
C2H3+OH=C2H2+H2O    3.011E13 0.0 0.0E0
C2H3+CH3=C2H2+CH4    3.92E11 0.0 0.0E0
2C2H3=C2H2+C2H4    9.6E11 0.0 0.0E0
C2H+H(+M)=C2H2(+M)    1.0E17 0.0 0.0E0
    H2/2.0/
    H2O/6.0/
    AR/0.7/
    CO/1.5/
    CO2/2.0/
    CH4/2.0/
    C2H6/3.0/
    HE/0.7/
    LOW/3.75E33 -4.8E0 1.9E3/
    TROE/6.46E-1 1.32E2 1.315E3 5.566E3/
C2H+H2=H+C2H2    4.9E5 2.5 5.6E2
C2H+O2=CO2+CHV    2.17E10 0.0 0.0E0
C2H+O2=HCO+CO    5.0E13 0.0 1.5E3
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C2H+O=CO+CHV    6.2E12 0.0 0.0E0
C2H+O=CO+CH    5.0E13 0.0 0.0E0
C2H+OH=H+HCCO    2.0E13 0.0 0.0E0
C2H2+O=CH2+CO    7.395E8 1.28 2.472E3
C2H2+O=HCCO+H    2.958E9 1.28 2.472E3
C2H2+HO2=CH2CO+OH    6.03E9 0.0 7.949E3
C2H2+CH2=C3H3+H    1.2E13 0.0 6.62E3
C2H2+CH2(S)=C3H3+H    2.0E13 0.0 0.0E0
C2H2+HCO=C2H3+CO    1.0E7 2.0 6.0E3
C2H2+HCCO=C3H3+CO    1.0E11 0.0 3.0E3
C2H2+OH=C2H+H2O    2.632E6 2.14 1.706E4
C2H2+OH=CH2CO+H    1.578E3 2.56 -8.445E2
   PLOG/1.0E-2 1.578E3 2.56E0 -8.445E2/
   PLOG/2.5E-2 1.518E4 2.28E0 -2.921E2/
   PLOG/1.0E-1 3.017E5 1.92E0 5.981E2/
   PLOG/1.0E0 7.528E6 1.55E0 2.106E3/
   PLOG/1.0E1 5.101E6 1.65E0 3.4E3/
   PLOG/1.0E2 1.457E4 2.45E0 4.477E3/
C2H2+OH=CH3+CO    4.757E5 1.68 -3.298E2
   PLOG/1.0E-2 4.757E5 1.68E0 -3.298E2/
   PLOG/2.5E-2 4.372E6 1.4E0 2.265E2/
   PLOG/1.0E-1 7.648E7 1.05E0 1.115E3/
   PLOG/1.0E0 1.277E9 7.3E-1 2.579E3/
   PLOG/1.0E1 4.312E8 9.2E-1 3.736E3/
   PLOG/1.0E2 8.25E5 1.77E0 4.697E3/
CH3CHO(+M)=CH3+HCO(+M)    2.45E22 -1.74 8.6355E4
   LOW/1.03E59 -1.13E1 9.59125E4/
   TROE/2.49E-3 7.181E2 6.089E0 3.78E3/
CH3CHO(+M)=CH4+CO(+M)    2.72E21 -1.74 8.6355E4
   LOW/1.144E58 -1.13E1 9.59125E4/
   TROE/2.49E-3 7.181E2 6.089E0 3.78E3/
CH3CHO+O2=CH3CO+HO2    3.01E13 0.0 3.915E4
CH3CHO+O=CH3CO+OH    5.94E12 0.0 1.868E3
CH3CHO+H=CH3CO+H2    1.31E5 2.58 1.22E3
CH3CHO+OH=CH3CO+H2O    3.37E12 0.0 -6.19E2
CH3CHO+HO2=CH3CO+H2O2    3.01E12 0.0 1.192E4
CH3CHO+CH3=CH3CO+CH4    7.08E-4 4.58 1.966E3
CH3CHO+C2H3=CH3CO+C2H4    1.65E1 3.17 9.3998E3
CH3CHO+CH3O2=CH3CO+CH3O2H    3.01E12 0.0 1.192E4
CH3CHO+CH3CO3=CH3CO+CH3CO3H    3.01E12 0.0 1.192E4
CH3CHO+H=CH2CHO+H2    2.72E3 3.1 5.21E3
CH3CHO+OH=CH2CHO+H2O    1.72E5 2.4 8.15E2
CH3CHO+OH=CH3+HOCHO    3.0E15 -1.076 0.0E0
CH3CO(+M)=CH3+CO(+M)    1.07E12 0.63 1.69E4
   LOW/5.65E18 -9.7E-1 1.46E4/
   TROE/6.29E-1 8.73E9 5.52E0 7.6E7/
CH3CO(+M)=CH2CO+H(+M)    9.413E7 1.917 4.49872E4
   LOW/1.516E51 -1.027E1 5.539E4/
   TROE/6.009E-1 8.103E9 6.677E2 5.0E9/
CH3CO+H=CH2CO+H2    2.0E13 0.0 0.0E0
CH3CO+O=CH2CO+OH    2.0E13 0.0 0.0E0
CH3CO+CH3=CH2CO+CH4    5.0E13 0.0 0.0E0
CH3CO+O2=CH3CO3    1.2E11 0.0 -1.1E3
CH2CHO(+M)=CH2CO+H(+M)    1.43E15 -0.15 4.56E4
   LOW/6.0E29 -3.8E0 4.34239E4/
   TROE/9.85E-1 3.93E2 9.8E9 5.0E9/
CH2CHO(+M)=CH3+CO(+M)    2.93E12 0.29 4.03E4
   LOW/9.52E33 -5.07E0 4.13E4/
   TROE/7.13E-17 1.15E3 4.99E9 1.79E9/
CH3CO3H=CH3CO2+OH    5.01E14 0.0 4.015E4
CH3CO3+CH2O=CH3CO3H+HCO    1.99E12 0.0 1.166E4
CH3CO3+C2H6=CH3CO3H+C2H5    1.7E13 0.0 2.046E4
CH3CO3+HO2=CH3CO3H+O2    1.75E10 0.0 -3.275E3
CH3CO3+H2O2=CH3CO3H+HO2    2.41E12 0.0 9.936E3
CH3CO3+CH4=CH3CO3H+CH3    1.81E11 0.0 1.848E4
CH3CO2+M=CH3+CO2+M    4.4E15 0.0 1.05E4
CH2CHO+O2=O2CH2CHO    1.58E77 -21.9 1.935E4
   PLOG/1.0E-2 1.58E77 -2.19E1 1.935E4/
   PLOG/1.0E-1 3.88E69 -1.884E1 1.924E4/
   PLOG/1.0E0 7.8E59 -1.54E1 1.765E4/
   PLOG/1.0E1 3.05E50 -1.22E1 1.563E4/
CH2CHO+O2=CH2CO+HO2    1.88E5 2.37 2.373E4
   PLOG/1.0E-2 1.88E5 2.37E0 2.373E4/
   PLOG/1.0E-1 1.88E5 2.37E0 2.737E4/
   PLOG/1.0E0 2.51E5 2.33E0 2.38E4/
   PLOG/1.0E1 7.05E7 1.63E0 2.529E4/
CH2CHO+O2=>CH2O+CO+OH    2.68E17 -1.84 6.53E3
   PLOG/1.0E-2 2.68E17 -1.84E0 6.53E3/
   PLOG/1.0E-1 1.52E20 -2.58E0 8.98E3/
   PLOG/1.0E0 1.65E19 -2.22E0 1.034E4/
   PLOG/1.0E1 8.953E13 -6.0E-1 1.012E4/
CH2CHO+O2=HO2CH2CO    3.64E65 -21.87 1.902E4
   PLOG/1.0E-2 3.64E65 -2.187E1 1.902E4/
   PLOG/1.0E-1 3.64E58 -1.9E1 1.909E4/
   PLOG/1.0E0 6.65E48 -1.555E1 1.746E4/
   PLOG/1.0E1 4.8E38 -1.214E1 1.496E4/
O2CH2CHO=HO2CH2CO    8.27E30 -6.65 2.45E4
   PLOG/1.0E-2 8.27E30 -6.65E0 2.45E4/
   PLOG/1.0E-1 1.73E26 -4.99E0 2.376E4/
   PLOG/1.0E0 9.03E19 -2.92E0 2.217E4/
   PLOG/1.0E1 1.43E16 -1.67E0 2.121E4/
O2CH2CHO=CH2CO+HO2    2.05E40 -13.31 5.215E4
   PLOG/1.0E-2 2.05E40 -1.331E1 5.215E4/
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   PLOG/1.0E-1 5.72E45 -1.4E1 5.22E4/
   PLOG/1.0E0 4.16E55 -1.576E1 5.508E4/
   PLOG/1.0E1 1.12E61 -1.604E1 6.001E4/
HO2CH2CO=>CO+CH2O+OH    2.36E17 -2.95 8.1E3
   PLOG/1.0E-2 2.36E17 -2.95E0 8.1E3/
   PLOG/1.0E-1 2.38E18 -2.95E0 8.1E3/
   PLOG/1.0E0 2.51E19 -2.95E0 8.11E3/
   PLOG/1.0E1 4.16E20 -3.02E0 8.24E3/
HO2CH2CO=CH2CO+HO2    1.12E7 -3.76 2.168E4
   PLOG/1.0E-2 1.12E7 -3.76E0 2.168E4/
   PLOG/1.0E-1 1.1E8 -3.76E0 2.168E4/
   PLOG/1.0E0 9.2E8 -3.73E0 2.163E4/
   PLOG/1.0E1 2.09E9 -3.55E0 2.122E4/
CH2+CO(+M)=CH2CO(+M)    8.1E11 0.0 0.0E0
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/2.69E33 -5.11E0 7.095E3/
   TROE/5.907E-1 2.75E2 1.226E3 5.185E3/
CH2CO+H=HCCO+H2    1.401E15 -0.171 8.7832E3
CH2CO+O=HCCO+OH    1.0E13 0.0 8.0E3
CH2CO+OH=HCCO+H2O    1.0E13 0.0 2.0E3
CH2CO+H=CH3+CO    7.704E13 -0.171 4.1832E3
CH+CH2O=H+CH2CO    9.46E13 0.0 -5.15E2
CH2CO+O=CH2+CO2    1.75E12 0.0 1.35E3
CH2CO+OH=CH2OH+CO    2.0E12 0.0 -1.01E3
CH2CO+CH2(S)=C2H4+CO    1.6E14 0.0 0.0E0
CH2CO+CH3=C2H5+CO    4.769E4 2.312 9.468E3
CH+CO+M=HCCO+M    7.57E22 -1.9 0.0E0
HCCO+OH=>H2+2CO    1.0E14 0.0 0.0E0
HCCO+O=>H+2CO    8.0E13 0.0 0.0E0
HCCO+CH=CO+C2H2    5.0E13 0.0 0.0E0
HCCO+H=CH2(S)+CO    1.0E14 0.0 0.0E0
HCCO+O2=>OH+2CO    1.91E11 -0.02 1.02E3
HCCO+O2=>CO2+CO+H    4.78E12 -0.142 1.15E3
CH3+CH2O=C2H5O    3.0E11 0.0 6.336E3
CH3CHO+H=C2H5O    4.61E7 1.71 7.09E3
C2H5O+O2=CH3CHO+HO2    4.28E10 0.0 1.097E3
C3H8(+M)=CH3+C2H5(+M)    1.29E37 -5.84 9.738E4
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/5.64E74 -1.574E1 9.8714E4/
   TROE/3.1E-1 5.0E1 3.0E3 9.0E3/
NC3H7+H=C3H8    1.0E14 0.0 0.0E0
IC3H7+H=C3H8    1.0E14 0.0 0.0E0
C3H8+IC3H7=NC3H7+C3H8    3.0E10 0.0 1.29E4
C3H8+O2=NC3H7+HO2    6.0E13 0.0 5.229E4
C3H8+H=NC3H7+H2    3.49E5 2.69 6.45E3
C3H8+O=NC3H7+OH    3.71E6 2.4 5.505E3
C3H8+OH=NC3H7+H2O    2.732E7 1.811 8.684E2
C3H8+HO2=NC3H7+H2O2    4.08E1 3.59 1.716E4
C3H8+CH3=NC3H7+CH4    9.04E-1 3.65 7.154E3
C3H8+C2H3=NC3H7+C2H4    1.0E11 0.0 1.04E4
C3H8+C2H5=NC3H7+C2H6    1.0E11 0.0 1.04E4
C3H8+C3H5-A=NC3H7+C3H6    7.94E11 0.0 2.05E4
C3H8+CH3O2=NC3H7+CH3O2H    1.386E0 3.97 1.828E4
C3H8+C2H5O2=NC3H7+C2H5O2H    1.386E0 3.97 1.828E4
C3H8+IC3H7O2=NC3H7+IC3H7O2H    1.7E13 0.0 2.046E4
C3H8+CH3CO3=NC3H7+CH3CO3H    1.7E13 0.0 2.046E4
C3H8+O2CHO=NC3H7+HO2CHO    5.52E4 2.55 1.648E4
C3H8+O2=IC3H7+HO2    2.0E13 0.0 4.964E4
C3H8+H=IC3H7+H2    1.3E6 2.4 4.471E3
C3H8+O=IC3H7+OH    5.49E5 2.5 3.14E3
C3H8+OH=IC3H7+H2O    9.1715E9 0.935 5.047E2
C3H8+HO2=IC3H7+H2O2    6.32E1 3.37 1.372E4
C3H8+CH3=IC3H7+CH4    6.4E4 2.17 7.52E3
C3H8+C2H3=IC3H7+C2H4    1.0E11 0.0 1.04E4
C3H8+C2H5=IC3H7+C2H6    1.0E11 0.0 1.04E4
C3H8+C3H5-A=IC3H7+C3H6    7.94E11 0.0 1.62E4
C3H8+CH3O2=IC3H7+CH3O2H    1.019E1 3.58 1.481E4
C3H8+C2H5O2=IC3H7+C2H5O2H    1.019E1 3.58 1.481E4
C3H8+CH3CO3=IC3H7+CH3CO3H    2.0E12 0.0 1.7E4
C3H8+O2CHO=IC3H7+HO2CHO    1.475E4 2.6 1.391E4
C3H8+IC3H7O2=IC3H7+IC3H7O2H    2.0E12 0.0 1.7E4
IC3H7+H=C2H5+CH3    2.0E13 0.0 0.0E0
IC3H7+OH=C3H6+H2O    2.41E13 0.0 0.0E0
IC3H7+O=CH3COCH3+H    4.818E13 0.0 0.0E0
IC3H7+O=CH3CHO+CH3    4.818E13 0.0 0.0E0
O2+NC3H7=HO2+C3H6    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 5.05E10 2.06E-2 5.01905E2/
   PLOG/1.0E-1 7.47E15 -1.45E0 4.1129E3/
   PLOG/1.0E0 1.18E19 -2.35E0 7.29953E3/
```

PLOG/1.0E1 2.63E0 3.46E0 2.48117E3/
PLOG/1.0E2 7.37E2 2.71E0 5.49647E3/
O2+IC3H7=HO2+C3H6 1.0E11 0.0 0.0E0
PLOG/1.0E-2 5.91E9 4.28E-1 -1.43857E3/
PLOG/1.0E-1 1.6E14 -8.45E-1 1.42377E3/
PLOG/1.0E0 4.05E18 -2.07E0 4.97147E3/
PLOG/1.0E1 4.91E17 -1.66E0 6.96404E3/
PLOG/1.0E2 9.84E7 1.34E0 5.37912E3/
O2+NC3H7=C3H6OOH1-2 1.0E11 0.0 0.0E0
PLOG/1.0E-2 2.97E15 -2.84E0 3.56751E3/
PLOG/1.0E-1 2.64E12 -1.58E0 3.36232E3/
PLOG/1.0E0 2.78E2 1.63E0 -4.92364E2/
PLOG/1.0E1 1.3E14 -1.73E0 5.16366E3/
PLOG/1.0E2 7.63E16 -2.3E0 9.03614E3/
O2+NC3H7=C3H6OOH1-3 1.0E11 0.0 0.0E0
DUP
PLOG/1.0E-2 3.09E146 -4.59E1 3.12822E4/
PLOG/1.0E-1 1.26E47 -1.24E1 8.20313E3/
PLOG/1.0E0 1.3E23 -4.03E0 5.08867E3/
PLOG/1.0E1 3.94E-18 8.88E0 -6.1997E3/
PLOG/1.0E2 6.58E-15 7.8E0 -3.43101E3/
O2+NC3H7=C3H6OOH1-3 1.0E11 0.0 0.0E0
DUP
PLOG/1.0E-2 6.19E8 8.78E-1 1.11866E4/
PLOG/1.0E-1 1.12E14 -5.31E-1 1.38975E4/
PLOG/1.0E0 2.07E14 -4.0E-1 1.51581E4/
PLOG/1.0E1 1.02E21 -2.26E0 1.8554E4/
PLOG/1.0E2 1.05E15 -4.86E-1 1.58767E4/
O2+IC3H7=C3H6OOH2-1 1.0E11 0.0 0.0E0
PLOG/1.0E-2 4.86E10 -1.56E0 -7.08183E2/
PLOG/1.0E-1 3.76E11 -1.48E0 4.70031E2/
PLOG/1.0E0 4.08E12 -1.45E0 2.16878E3/
PLOG/1.0E1 1.13E14 -1.5E0 5.25342E3/
PLOG/1.0E2 3.56E10 -1.16E-1 7.05645E3/
O2+NC3H7=NC3H7O2 1.0E11 0.0 0.0E0
PLOG/1.0E-2 9.2E8 4.05E-1 -4.39865E3/
PLOG/1.0E-1 1.45001E14 -9.84E-1 -1.7108E3/
PLOG/1.0E0 2.09001E13 -4.99E-1 -9.38423E2/
PLOG/1.0E1 1.15001E20 -2.42E0 2.45126E3/
PLOG/1.0E2 2.07001E16 -1.3E0 8.03419E2/
O2+IC3H7=IC3H7O2 1.0E11 0.0 0.0E0
PLOG/1.0E-2 7.33E5 1.33E0 -6.34564E3/
PLOG/1.0E-1 2.24E11 -1.05E-1 -3.69787E3/
PLOG/1.0E0 1.54E18 -2.02E0 -4.98567E2/
PLOG/1.0E1 6.74E27 -4.85E0 3.77982E3/
PLOG/1.0E2 1.67E29 -5.15E0 5.03645E3/
NC3H7O2=HO2+C3H6 1.0E11 0.0 0.0E0
PLOG/1.0E-2 4.3E53 -1.4E1 3.9526E4/
PLOG/1.0E-1 9.52E57 -1.5E1 4.26843E4/
PLOG/1.0E0 6.9E33 -7.03E0 3.65435E4/
PLOG/1.0E1 2.55E16 -1.22E0 3.24803E4/
PLOG/1.0E2 2.26E32 -6.22E0 3.79482E4/
IC3H7O2=C3H6+HO2 1.0E11 0.0 0.0E0
PLOG/1.0E-2 1.61E75 -2.06E1 4.6203E4/
PLOG/1.0E-1 1.72E66 -1.73E1 4.54589E4/
PLOG/1.0E0 4.03E56 -1.4E1 4.40102E4/
PLOG/1.0E1 1.29E40 -8.58E0 3.94186E4/
PLOG/1.0E2 6.4E25 -4.02E0 3.49139E4/
NC3H7O2=C3H6OOH1-2 1.0E11 0.0 0.0E0
PLOG/1.0E-2 9.48E20 -5.14E0 2.37097E4/
PLOG/1.0E-1 1.24E22 -4.93E0 2.64778E4/
PLOG/1.0E0 1.99E20 -3.92E0 2.76341E4/
PLOG/1.0E1 2.58E42 -1.03E1 3.76702E4/
PLOG/1.0E2 2.79E42 -1.01E1 3.91082E4/
NC3H7O2=C3H6OOH1-3 1.0E11 0.0 0.0E0
DUP
PLOG/1.0E-2 1.69E4 1.56E0 1.85703E4/
PLOG/1.0E-1 5.85E4 1.66E0 1.9612E4/
PLOG/1.0E0 1.5E3 2.32E0 1.97537E4/
PLOG/1.0E1 1.01E0 3.38E0 1.89948E4/
PLOG/1.0E2 3.39E0 3.23E0 1.92093E4/
NC3H7O2=C3H6OOH1-3 1.0E11 0.0 0.0E0
DUP
PLOG/1.0E-2 7.72E17 5.57E-4 4.03931E4/
PLOG/1.0E-1 7.02E18 -1.18E-3 4.69318E4/
PLOG/1.0E0 1.19E20 -7.68E-3 5.52238E4/
PLOG/1.0E1 1.26E23 -3.15E-2 7.54407E4/
PLOG/1.0E2 4.06E26 -3.66E-2 9.94007E4/
IC3H7O2=C3H6OOH2-1 1.0E11 0.0 0.0E0
PLOG/1.0E-2 6.0E33 -8.94E0 3.04423E4/
PLOG/1.0E-1 2.48E34 -8.62E0 3.29047E4/
PLOG/1.0E0 2.01E33 -7.75E0 3.48901E4/
PLOG/1.0E1 4.62E27 -5.55E0 3.50367E4/
PLOG/1.0E2 2.22E18 -2.35E0 3.32447E4/
C3H6OOH1-2=C3H6OOH1-3 1.0E11 0.0 0.0E0
PLOG/1.0E-2 6.24E-135 4.57E1 -1.94619E4/
PLOG/1.0E-1 3.0E-176 5.79E1 -4.04217E4/
PLOG/1.0E0 1.0E-15 1.02E1 2.85937E4/
PLOG/1.0E1 5.36E-85 3.1E1 5.35821E2/
PLOG/1.0E2 1.58E-133 4.51E1 -2.11265E4/
C3H6OOH1-2=HO2+C3H6 1.0E11 0.0 0.0E0
PLOG/1.0E-2 1.49E-15 9.24E0 1.89606E4/
PLOG/1.0E-1 2.9E-44 1.76E1 1.8887E3/

PLOG/1.0E0 1.08E31 -4.56E0 3.21226E4/
PLOG/1.0E1 1.16E-9 7.46E0 1.47457E4/
PLOG/1.0E2 1.27E-15 8.78E0 9.26654E3/
C3H6OOH1-3=HO2+C3H6 1.0E11 0.0 0.0E0
PLOG/1.0E-2 3.55E-90 2.75E1 -3.5057E4/
PLOG/1.0E-1 3.21E4 -3.42E-1 4.33923E3/
PLOG/1.0E0 1.97E26 -5.97E0 1.87428E4/
PLOG/1.0E1 1.6E10 -4.44E-1 1.75318E4/
PLOG/1.0E2 3.45E17 -2.82E0 2.15791E4/
C3H6OOH2-1=HO2+C3H6 1.0E11 0.0 0.0E0
PLOG/1.0E-2 1.27E-80 2.78E1 -1.57525E4/
PLOG/1.0E-1 3.07E-68 2.41E1 -1.36247E4/
PLOG/1.0E0 7.16E-48 1.81E1 -6.62037E3/
PLOG/1.0E1 5.04E-23 1.05E1 2.46501E3/
PLOG/1.0E2 1.04E23 -3.25E0 2.02479E4/
O2+C3H6OOH1-3=C3H6OOH1-3O2 1.0E11 0.0 0.0E0
PLOG/1.0E-2 2.95E42 -1.02E1 5.86236E3/
PLOG/1.0E-1 4.3E42 -9.88E0 7.52686E3/
PLOG/1.0E0 7.47E36 -7.85E0 6.72435E3/
PLOG/1.0E1 2.18E27 -4.75E0 4.02617E3/
PLOG/1.0E2 1.46E18 -1.85E0 1.00584E3/
O2+C3H6OOH1-2=C3H6OOH1-2O2 1.0E11 0.0 0.0E0
PLOG/1.0E-2 3.53E43 -1.06E1 5.58018E3/
PLOG/1.0E-1 1.73E44 -1.05E1 7.43582E3/
PLOG/1.0E0 5.07E40 -9.11E0 7.63329E3/
PLOG/1.0E1 4.23E32 -6.42E0 5.737E3/
PLOG/1.0E2 6.65E22 -3.28E0 2.69488E3/
O2+C3H6OOH2-1=C3H6OOH1-2O2 1.0E11 0.0 0.0E0
PLOG/1.0E-2 3.34E46 -1.2E1 9.04943E3/
PLOG/1.0E-1 5.37E42 -1.06E1 1.0094E4/
PLOG/1.0E0 2.82E34 -7.84E0 9.74812E3/
PLOG/1.0E1 8.14E26 -5.4E0 9.40736E3/
PLOG/1.0E2 5.55E9 -1.18E-1 4.98652E3/
O2+C3H6OOH1-3=OH+C3KET13 1.0E11 0.0 0.0E0
PLOG/1.0E-2 6.2E30 -6.23E0 5.24155E3/
PLOG/1.0E-1 2.42E32 -6.58E0 8.14472E3/
PLOG/1.0E0 3.7E27 -5.03E0 8.65443E3/
PLOG/1.0E1 3.58E15 -1.36E0 5.98573E3/
PLOG/1.0E2 6.32E0 3.02E0 1.62507E3/
O2+C3H6OOH1-3=HO2+AC3H5OOH 1.0E11 0.0 0.0E0
PLOG/1.0E-2 1.46E15 -1.27E0 3.27888E3/
PLOG/1.0E-1 2.53E20 -2.73E0 7.33277E3/
PLOG/1.0E0 2.77E20 -2.61E0 9.79694E3/
PLOG/1.0E1 3.08E11 1.79E-1 8.56997E3/
PLOG/1.0E2 6.76E-4 4.57E0 4.46375E3/
O2+C3H6OOH1-2=>2OH+CH3COCH2O 1.0E11 0.0 0.0E0
PLOG/1.0E-2 5.81E37 -9.43E0 8.6681E3/
PLOG/1.0E-1 6.21E39 -9.86E0 1.30868E4/
PLOG/1.0E0 4.55E37 -9.0E0 1.65229E4/
PLOG/1.0E1 1.97E26 -5.41E0 1.65377E4/
PLOG/1.0E2 7.15E2 1.7E0 1.11595E4/
O2+C3H6OOH1-2=OH+C3KET12 1.0E11 0.0 0.0E0
PLOG/1.0E-2 2.79E12 -8.55E-1 5.28159E2/
PLOG/1.0E-1 8.75E17 -2.4E0 4.56698E3/
PLOG/1.0E0 1.79E20 -2.96E0 7.84392E3/
PLOG/1.0E1 9.72E14 -1.26E0 8.21243E3/
PLOG/1.0E2 7.36E1 2.72E0 5.02039E3/
O2+C3H6OOH1-2=HO2+AC3H5OOH 1.0E11 0.0 0.0E0
PLOG/1.0E-2 6.32E10 1.66E-3 8.74545E2/
PLOG/1.0E-1 5.12E16 -1.68E0 4.87214E3/
PLOG/1.0E0 1.51E20 -2.59E0 8.51258E3/
PLOG/1.0E1 1.51E16 -1.27E0 9.3915E3/
PLOG/1.0E2 4.35E3 2.55E0 6.47735E3/
O2+C3H6OOH1-2=O2+C3H6OOH2-1 1.0E11 0.0 0.0E0
PLOG/1.0E-2 1.68E33 -7.31E0 8.13443E3/
PLOG/1.0E-1 4.31E38 -8.76E0 1.33994E4/
PLOG/1.0E0 8.96E39 -8.95E0 1.7948E4/
PLOG/1.0E1 3.58E31 -6.24E0 1.90919E4/
PLOG/1.0E2 1.02E10 3.04E-1 1.44948E4/
O2+C3H6OOH2-1=>2OH+CH3COCH2O 1.0E11 0.0 0.0E0
PLOG/1.0E-2 1.28E9 -4.11E-2 -1.69352E3/
PLOG/1.0E-1 1.26E16 -2.06E0 2.60312E3/
PLOG/1.0E0 6.7E22 -3.98E0 7.36021E3/
PLOG/1.0E1 2.35E21 -3.39E0 9.36049E3/
PLOG/1.0E2 1.13E10 1.17E-1 7.22707E3/
O2+C3H6OOH2-1=OH+C3KET12 1.0E11 0.0 0.0E0
PLOG/1.0E-2 8.11E18 -3.19E0 5.91089E3/
PLOG/1.0E-1 3.67E13 -1.44E0 6.96738E3/
PLOG/1.0E0 5.7E6 6.97E-1 7.67386E3/
PLOG/1.0E1 2.3E3 1.68E0 9.63139E3/
PLOG/1.0E2 5.91E-13 6.32E0 6.80779E3/
O2+C3H6OOH2-1=HO2+AC3H5OOH 1.0E11 0.0 0.0E0
PLOG/1.0E-2 1.83E15 -1.76E0 4.65656E3/
PLOG/1.0E-1 4.68E15 -1.86E0 6.59916E3/
PLOG/1.0E0 1.81E22 -3.78E0 1.18049E4/
PLOG/1.0E1 8.68E20 -3.2E0 1.53524E4/
PLOG/1.0E2 2.23E4 1.94E0 1.30748E4/
C3H6OOH1-2O2=OH+C3KET12 1.0E11 0.0 0.0E0
PLOG/1.0E-2 2.53E40 -9.91E0 3.26314E4/
PLOG/1.0E-1 2.54E37 -8.72E0 3.29095E4/
PLOG/1.0E0 1.12E31 -6.53E0 3.18066E4/
PLOG/1.0E1 1.98E21 -3.34E0 2.91378E4/
PLOG/1.0E2 1.95E10 1.54E-1 2.5612E4/

C3H6OOH1-2O2=HO2+AC3H5OOH 1.0E11 0.0 0.0E0
PLOG/1.0E-2 1.02E51 -1.28E1 3.93617E4/
PLOG/1.0E-1 1.2E50 -1.22E1 4.0662E4/
PLOG/1.0E0 1.15E45 -1.03E1 4.03316E4/
PLOG/1.0E1 3.13E35 -7.15E0 3.79395E4/
PLOG/1.0E2 7.71E23 -3.45E0 3.43005E4/
C3H6OOH1-3O2=C3KET13+OH 1.0E11 0.0 0.0E0
PLOG/1.0E-2 4.08E29 -6.39E0 2.34402E4/
PLOG/1.0E-1 2.49E25 -4.95E0 2.26125E4/
PLOG/1.0E0 1.01E19 -2.88E0 2.08036E4/
PLOG/1.0E1 4.46E11 -5.38E-1 1.84411E4/
PLOG/1.0E2 1.67E5 1.48E0 1.62379E4/
C3H6OOH1-3O2=HO2+AC3H5OOH 1.0E11 0.0 0.0E0
PLOG/1.0E-2 3.85E46 -1.14E1 3.78724E4/
PLOG/1.0E-1 5.56E44 -1.05E1 3.88355E4/
PLOG/1.0E0 3.87E37 -8.08E0 3.75223E4/
PLOG/1.0E1 6.42E26 -4.59E0 3.43972E4/
PLOG/1.0E2 1.96E16 -1.27E0 3.09174E4/
C3KET13=>CH2O+CH2CHO+OH 1.0E11 0.0 0.0E0
PLOG/1.0E-2 3.41E64 -1.59E1 5.57614E4/
PLOG/1.0E-1 1.97E61 -1.46E1 5.60115E4/
PLOG/1.0E0 1.07E54 -1.21E1 5.45628E4/
PLOG/1.0E1 5.29E43 -8.74E0 5.15685E4/
PLOG/1.0E2 4.06E33 -5.54E0 4.82254E4/
C3KET12=>CH3CHO+HCO+OH 1.0E11 0.0 0.0E0
PLOG/1.0E-2 5.2E64 -1.59E1 5.66501E4/
PLOG/1.0E-1 2.19E60 -1.42E1 5.64797E4/
PLOG/1.0E0 1.08E52 -1.15E1 5.45804E4/
PLOG/1.0E1 1.56E41 -7.97E0 5.1321E4/
PLOG/1.0E2 1.03E31 -4.76E0 4.79219E4/
IC3H7O2+H2=IC3H7O2H+H 3.01E13 0.0 2.603E4
IC3H7O2+HO2=IC3H7O2H+O2 1.75E10 0.0 -3.275E3
IC3H7O2+CH2O=IC3H7O2H+HCO 5.6E12 0.0 1.36E4
IC3H7O2+CH4=IC3H7O2H+CH3 1.12E13 0.0 2.464E4
IC3H7O2+CH3CHO=IC3H7O2H+CH3CO 2.8E12 0.0 1.36E4
IC3H7O2+C2H4=IC3H7O2H+C2H3 1.13E13 0.0 3.043E4
IC3H7O2+C2H6=IC3H7O2H+C2H5 1.7E13 0.0 2.046E4
CH2(S)+C2H4=C3H6 4.82E57 -14.3 1.71E4
DUP
PLOG/1.0E-2 4.82E57 -1.43E1 1.71E4/
PLOG/1.0E-1 3.84E59 -1.44E1 1.84E4/
PLOG/1.0E0 2.13E58 -1.35E1 2.04E4/
PLOG/1.0E1 8.48E52 -1.16E1 2.07E4/
PLOG/1.0E2 6.07E47 -9.85E0 2.21E4/
CH2(S)+C2H4=C3H6 4.82E57 -14.3 1.71E4
DUP
PLOG/1.0E-2 1.15E45 -1.11E1 6.1452E3/
PLOG/1.0E-1 1.83E45 -1.07E1 6.6385E3/
PLOG/1.0E0 1.3E40 -8.77E0 5.8638E3/
PLOG/1.0E1 2.27E32 -6.14E0 4.3179E3/
PLOG/1.0E2 1.28E24 -3.49E0 2.5299E3/
CH2(S)+C2H4=C3H5-A+H 8.2E19 -2.06 1.15E3
DUP
PLOG/1.0E-2 8.2E19 -2.06E0 1.15E3/
PLOG/1.0E-1 2.27E21 -2.44E0 2.65E3/
PLOG/1.0E0 4.44E35 -6.55E0 1.39E4/
PLOG/1.0E1 1.18E28 -4.09E0 1.4E4/
PLOG/1.0E2 6.51E26 -3.58E0 1.89E4/
CH2(S)+C2H4=C3H5-A+H 8.2E19 -2.06 1.15E3
DUP
PLOG/1.0E-2 1.08E7 1.62E0 -3.1746E3/
PLOG/1.0E-1 1.37E5 2.15E0 -3.7992E3/
PLOG/1.0E0 3.89E14 -4.2E-1 1.2376E3/
PLOG/1.0E1 2.45E10 6.7E-1 7.5093E2/
PLOG/1.0E2 1.81E2 2.97E0 -7.4603E2/
CH2(S)+C2H4=C2H3+CH3 1.77E19 -1.94 6.79E3
DUP
PLOG/1.0E-2 1.77E19 -1.94E0 6.79E3/
PLOG/1.0E-1 1.68E19 -1.8E0 4.31E3/
PLOG/1.0E0 4.16E24 -3.19E0 9.76E3/
PLOG/1.0E1 7.89E24 -3.07E0 1.39E4/
PLOG/1.0E2 7.36E29 -4.28E0 2.38E4/
CH2(S)+C2H4=C2H3+CH3 1.77E19 -1.94 6.79E3
DUP
PLOG/1.0E-2 4.3E12 1.9E-1 -1.1041E2/
PLOG/1.0E-1 2.26E11 5.4E-1 4.781E1/
PLOG/1.0E0 4.92E9 1.02E0 5.9977E2/
PLOG/1.0E1 1.47E8 1.33E0 1.2284E3/
PLOG/1.0E2 8.11E10 5.5E-1 5.5065E3/
C2H3+CH3=C3H5-A+H 4.12E29 -4.95 8.0E3
DUP
PLOG/1.0E-2 4.12E29 -4.95E0 8.0E3/
PLOG/1.0E-1 4.86E30 -5.03E0 1.13E4/
PLOG/1.0E0 5.3E29 -4.57E0 1.44E4/
PLOG/1.0E1 1.32E30 -4.54E0 1.93E4/
PLOG/1.0E2 5.16E28 -4.03E0 2.38E4/
C2H3+CH3=C3H5-A+H 4.12E29 -4.95 8.0E3
DUP
PLOG/1.0E-2 5.73E15 -7.7E-1 1.1959E3/
PLOG/1.0E-1 2.06E13 -7.4E-2 1.4287E3/
PLOG/1.0E0 4.48E10 6.0E-1 1.4216E3/
PLOG/1.0E1 4.1E6 1.71E0 1.0569E3/
PLOG/1.0E2 1.37E-1 3.91E0 -3.5355E2/

C3H6=C2H3+CH3 1.88E78 -18.7 1.3E5
DUP
PLOG/1.0E-2 1.88E78 -1.87E1 1.3E5/
PLOG/1.0E-1 8.73E76 -1.79E1 1.32E5/
PLOG/1.0E0 5.8E75 -1.72E1 1.34E5/
PLOG/1.0E1 8.12E71 -1.58E1 1.36E5/
PLOG/1.0E2 2.15E64 -1.34E1 1.35E5/
C3H6=C2H3+CH3 1.88E78 -18.7 1.3E5
DUP
PLOG/1.0E-2 1.69E59 -1.36E1 1.1329E5/
PLOG/1.0E-1 2.0E60 -1.37E1 1.1489E5/
PLOG/1.0E0 6.7E54 -1.18E1 1.1384E5/
PLOG/1.0E1 1.06E47 -9.27E0 1.1151E5/
PLOG/1.0E2 7.29E38 -6.7E0 1.0874E5/
C3H6=C3H5-A+H 9.16E74 -17.6 1.2E5
DUP
PLOG/1.0E-2 9.16E74 -1.76E1 1.2E5/
PLOG/1.0E-1 1.73E70 -1.6E1 1.2E5/
PLOG/1.0E0 1.08E71 -1.59E1 1.2486E5/
PLOG/1.0E1 6.4E65 -1.42E1 1.25E5/
PLOG/1.0E2 8.05E56 -1.15E1 1.22E5/
C3H6=C3H5-A+H 9.16E74 -17.6 1.2E5
DUP
PLOG/1.0E-2 2.98E54 -1.23E1 1.012E5/
PLOG/1.0E-1 1.37E43 -8.87E0 9.6365E4/
PLOG/1.0E0 6.28E42 -8.51E0 9.8004E4/
PLOG/1.0E1 4.73E35 -6.26E0 9.5644E4/
PLOG/1.0E2 4.34E28 -4.06E0 9.3114E4/
C3H5-T+H=C3H6 4.96E60 -15.2 1.8E4
DUP
PLOG/1.0E-2 4.96E60 -1.52E1 1.8E4/
PLOG/1.0E-1 3.2E62 -1.51E1 2.01E4/
PLOG/1.0E0 2.31E60 -1.4E1 2.19E4/
PLOG/1.0E1 3.69E54 -1.2E1 2.21E4/
PLOG/1.0E2 1.15E50 -1.04E1 2.33E4/
C3H5-T+H=C3H6 4.96E60 -15.2 1.8E4
DUP
PLOG/1.0E-2 1.49E48 -1.2E1 7.2033E3/
PLOG/1.0E-1 6.76E46 -1.11E1 7.6299E3/
PLOG/1.0E0 1.09E40 -8.66E0 6.4478E3/
PLOG/1.0E1 2.38E31 -5.73E0 4.506E3/
PLOG/1.0E2 5.69E25 -3.83E0 3.2504E3/
C3H5-T+H=C3H5-A+H 2.11E17 -1.08 1.29E3
DUP
PLOG/1.0E-2 2.11E17 -1.08E0 1.29E3/
PLOG/1.0E-1 9.05E29 -4.91E0 8.54E3/
PLOG/1.0E0 2.98E30 -4.79E0 1.2E4/
PLOG/1.0E1 8.22E28 -4.14E0 1.54E4/
PLOG/1.0E2 2.28E29 -4.12E0 2.09E4/
C3H5-T+H=C3H5-A+H 2.11E17 -1.08 1.29E3
DUP
PLOG/1.0E-2 6.41E3 2.61E0 -3.7784E3/
PLOG/1.0E-1 5.19E14 -3.0E-1 1.0904E3/
PLOG/1.0E0 8.17E11 4.9E-1 1.1846E3/
PLOG/1.0E1 2.79E9 1.09E0 1.1875E3/
PLOG/1.0E2 6.75E3 2.7E0 3.738E2/
C3H5-T+H=C2H3+CH3 3.31E16 -0.69 5.2E3
DUP
PLOG/1.0E-2 3.31E16 -6.9E-1 5.2E3/
PLOG/1.0E-1 9.04E16 -8.1E-1 4.8E3/
PLOG/1.0E0 2.01E24 -2.86E0 1.09E4/
PLOG/1.0E1 2.75E26 -3.31E0 1.58E4/
PLOG/1.0E2 3.15E32 -4.83E0 2.6E4/
C3H5-T+H=C2H3+CH3 3.31E16 -0.69 5.2E3
DUP
PLOG/1.0E-2 8.04E13 -1.4E-1 1.15E3/
PLOG/1.0E-1 7.17E10 6.7E-1 6.738E2/
PLOG/1.0E0 9.97E8 1.36E0 1.5964E3/
PLOG/1.0E1 7.41E7 1.57E0 2.1088E3/
PLOG/1.0E2 2.7E12 3.2E-1 6.7918E3/
C3H6+H=C3H5-A+H2 3.644E5 2.455 4.3612E3
C3H6+O2=C3H5-A+HO2 5.96E19 -1.67 4.61921E4
C3H6+O=C3H5-A+OH 5.24E11 0.7 5.884E3
C3H6+OH=C3H5-A+H2O 4.46E6 2.072 1.0508E3
C3H6+HO2=C3H5-A+H2O2 3.07E-2 4.403 1.35472E4
C3H6+CH3=C3H5-A+CH4 2.21E0 3.5 5.675E3
C3H6+CH3O2=C3H5-A+CH3O2H 7.68E-2 4.403 1.35472E4
C3H6+C2H5=C3H5-A+C2H6 1.0E11 0.0 9.8E3
C3H6+C2H5O2=C3H5-A+C2H5O2H 7.68E-2 4.403 1.35472E4
C3H6+CH3CO3=C3H5-A+CH3CO3H 7.68E-2 4.403 1.35472E4
C3H6+IC3H7O2=C3H5-A+IC3H7O2H 7.68E-2 4.403 1.35472E4
C3H6+H=C3H5-T+H2 1.498E2 3.381 8.9095E3
C3H6+O=C3H5-T+OH 6.03E10 0.7 7.632E3
C3H6+OH=C3H5-T+H2O 1.8E6 1.979 2.2352E3
C3H6+HO2=C3H5-T+H2O2 1.56E4 2.82 2.44279E4
C3H6+O2=C3H5-T+HO2 1.0E13 0.0 5.877E4
C3H6+CH3=C3H5-T+CH4 8.4E-1 3.5 1.166E4
C3H6+O=C2H4+CH2O 2.11E12 0.36357832 3.6251147E3
PLOG/1.0E-1 3.239515E10 8.6277366E-1 2.1012156E3/
PLOG/1.0E0 3.7102143E10 8.4675413E-1 2.152084E3/
PLOG/1.0E1 6.4621495E10 7.7988106E-1 2.3372114E3/
PLOG/3.0E1 1.79581E11 6.5836787E-1 2.7279312E3/
PLOG/1.0E2 2.11E12 3.6357832E-1 3.6251147E3/

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C3H6+O=C2H5+HCO    4.5392427E9 0.46990082 3.3909714E3
   PLOG/1.0E-1 3.81938E20 -2.8445151E0 2.2008093E3/
   PLOG/1.0E0 6.782E23 -3.7431204E0 5.0411938E3/
   PLOG/1.0E1 5.78554E21 -3.0582581E0 6.6882314E3/
   PLOG/3.0E1 4.41563E16 -1.5513902E0 5.3826196E3/
   PLOG/1.0E2 4.5392427E9 4.6990082E-1 3.3909714E3/
C3H6+O=CH3+CH2CHO    6.118106E10 0.72471172 1.7372183E3
   PLOG/1.0E-1 7.1169661E8 1.2452729E0 -2.2913843E2/
   PLOG/1.0E0 2.7972334E9 1.0825886E0 2.8259222E2/
   PLOG/1.0E1 1.8003295E10 8.6375535E-1 1.0689554E3/
   PLOG/3.0E1 3.3952128E10 7.9012293E-1 1.3842371E3/
   PLOG/1.0E2 6.118106E10 7.2471172E-1 1.7372183E3/
C3H6+O=H2+CH3CHCO    2.92162E11 -0.46592912 -7.2082123E2
   PLOG/1.0E-1 4.34829E14 -1.3823626E0 3.2638251E2/
   PLOG/1.0E0 5.03596E17 -2.2524612E0 2.2980547E3/
   PLOG/1.0E1 1.88555E14 -1.2406751E0 9.8652802E2/
   PLOG/3.0E1 1.45046E14 -1.2325199E0 8.0590204E2/
   PLOG/1.0E2 2.92162E11 -4.6592912E-1 -7.2082123E2/
C3H6+O=CO+C2H6    2.8063963E10 -0.15197791 8.5133477E3
   PLOG/1.0E-1 3.30559E19 -3.0550032E0 4.0607322E3/
   PLOG/1.0E0 4.47648E13 -1.2992022E0 2.5097214E3/
   PLOG/1.0E1 7.29311E16 -2.0833492E0 7.7710391E3/
   PLOG/3.0E1 2.2306699E1 2.136199E0 -3.9348716E3/
   PLOG/1.0E2 2.8063963E10 -1.5197791E-1 8.5133477E3/
C3H6+O=H2+C2H4+CO    1.9064245E5 1.4148871 1.8470398E3
   PLOG/1.0E-1 1.40605E19 -2.7684405E0 1.5882145E3/
   PLOG/1.0E0 1.42188E22 -3.5758173E0 4.455772E3/
   PLOG/1.0E1 4.5976E19 -2.7595153E0 6.0180806E3/
   PLOG/3.0E1 5.57149E13 -1.0280579E0 4.2239531E3/
   PLOG/1.0E2 1.9064245E5 1.4148871E0 1.8470398E3/
C3H6+O=C2H5CHO    8.41666E38 -8.3907213 1.0066773E4
   PLOG/1.0E-1 4.71689E24 -5.1135931E0 7.6513763E1/
   PLOG/1.0E0 1.04304E54 -1.3354402E1 1.4363056E4/
   PLOG/1.0E1 4.4714E47 -1.1098352E1 1.3584807E4/
   PLOG/3.0E1 8.32695E45 -1.0515912E1 1.3147347E4/
   PLOG/1.0E2 8.41666E38 -8.3907213E0 1.0066773E4/
C3H6+H=NC3H7    1.0E0 1.0 0.0E0
   DUP
   PLOG/1.3E-3 7.99E81 -2.3161E1 2.2239E4/
   PLOG/4.0E-2 4.24E68 -1.8427E1 1.9665E4/
   PLOG/1.0E0 1.04E49 -1.15E1 1.5359E4/
   PLOG/1.0E1 6.2E41 -8.892E0 1.4637E4/
   PLOG/1.0E2 4.22E27 -4.39E0 9.3458E3/
C3H6+H=NC3H7    1.0E0 1.0 0.0E0
   DUP
   PLOG/1.3E-3 1.85E26 -5.83E0 3.8658E3/
   PLOG/4.0E-2 2.82E30 -6.49E0 5.4708E3/
   PLOG/1.0E0 3.78E28 -5.57E0 5.6251E3/
   PLOG/1.0E1 1.46E25 -4.28E0 5.2478E3/
   PLOG/1.0E2 1.0E-10 0.0E0 0.0E0/
C3H6+H=C2H4+CH3    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.3E-3 1.54E9 1.35E0 2.542E3/
   PLOG/4.0E-2 7.88E10 8.7E-1 3.5996E3/
   PLOG/1.0E0 2.67E12 4.7E-1 5.4311E3/
   PLOG/1.0E1 9.25E22 -2.6E0 1.2898E4/
   PLOG/1.0E2 1.32E23 -2.42E0 1.65E4/
C3H6+H=C2H4+CH3    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.3E-3 1.0E-10 0.0E0 0.0E0/
   PLOG/4.0E-2 1.0E-10 0.0E0 0.0E0/
   PLOG/1.0E0 1.0E-10 0.0E0 0.0E0/
   PLOG/1.0E1 1.24E5 2.52E0 3.6791E3/
   PLOG/1.0E2 2.51E3 2.91E0 3.9809E3/
C3H6+H=IC3H7    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.3E-3 1.35E44 -1.068E1 8.1964E3/
   PLOG/4.0E-2 2.11E57 -1.423E1 1.5147E4/
   PLOG/1.0E0 3.26E61 -1.494E1 2.0161E4/
   PLOG/1.0E1 5.3E56 -1.312E1 2.0667E4/
   PLOG/1.0E2 1.11E50 -1.08E1 2.0202E4/
C3H6+H=IC3H7    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.3E-3 2.17E130 -3.258E1 1.3614E5/
   PLOG/4.0E-2 2.25E29 -5.84E0 4.2419E3/
   PLOG/1.0E0 1.06E30 -5.63E0 5.6134E3/
   PLOG/1.0E1 6.11E26 -4.44E0 5.1823E3/
   PLOG/1.0E2 2.73E23 -3.26E0 4.597E3/
C2H4+CH3=NC3H7    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.3E-3 8.67E48 -1.254E1 1.8206E4/
   PLOG/4.0E-2 1.06E49 -1.204E1 2.0001E4/
   PLOG/1.0E0 7.67E47 -1.117E1 2.2366E4/
   PLOG/1.0E1 1.81E45 -1.003E1 2.3769E4/
   PLOG/1.0E2 2.04E40 -8.25E0 2.4214E4/
C2H4+CH3=NC3H7    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.3E-3 1.12E43 -1.13E1 1.308E4/
   PLOG/4.0E-2 7.28E39 -9.88E0 1.3164E4/
   PLOG/1.0E0 2.6E33 -7.46E0 1.2416E4/
   PLOG/1.0E1 3.85E27 -5.38E0 1.1455E4/
   PLOG/1.0E2 1.66E21 -3.17E0 1.0241E4/
C3H5-A+H=C3H4-A+H2    1.232E3 3.035 2.582E3
```

```
C3H5-A+OH=C3H4-A+H2O    6.0E12 0.0 0.0E0
C3H5-A+CH3=C3H4-A+CH4    3.0E12 -0.32 -1.31E2
C3H5-A+C2H5=C3H4-A+C2H6    4.0E11 0.0 0.0E0
C3H5-A+C2H3=C3H4-A+C2H4    1.0E12 0.0 0.0E0
2C3H4-A=C3H5-A+C3H3    5.0E14 0.0 6.47467E4
2C3H5-A=C3H4-A+C3H6    9.55E40 -9.3 1.247E4
   PLOG/1.0E0 4.77E40 -9.3E0 1.247E4/
   PLOG/4.0E0 3.97E32 -6.8E0 9.18E3/
   PLOG/1.0E1 1.46E28 -5.5E0 7.41E3/
C3H5-A+C2H5=C2H4+C3H6    4.0E11 0.0 0.0E0
C3H5-A+HCO=C3H6+CO    6.0E13 0.0 0.0E0
C3H5-T+O=CH3+CH2CO    6.0E13 0.0 0.0E0
C3H5-T+OH=>CH3+CH2CO+H    5.0E12 0.0 0.0E0
C3H5-T+HO2=>CH3+CH2CO+OH    2.0E13 0.0 0.0E0
C3H5-T+HCO=C3H6+CO    9.0E13 0.0 0.0E0
C3H5-A+O=C2H3CHO+H    6.0E13 0.0 0.0E0
C3H5-A+OH=>C2H3CHO+2H    5.3E37 -6.71 2.9306E4
   PLOG/1.0E-1 5.3E37 -6.71E0 2.9306E4/
   PLOG/1.0E0 4.2E32 -5.16E0 3.0126E4/
   PLOG/1.0E1 1.6E20 -1.56E0 2.633E4/
C3H5-A+O2=C3H4-A+HO2    4.99E15 -1.4 2.2428E4
   PLOG/1.0E0 4.99E15 -1.4E0 2.2428E4/
   PLOG/1.0E1 2.18E21 -2.85E0 3.0755E4/
C3H5-A+O2=CH3CO+CH2O    1.19E15 -1.01 2.0128E4
   PLOG/1.0E0 1.19E15 -1.01E0 2.0128E4/
   PLOG/1.0E1 7.14E15 -1.21E0 2.1046E4/
C3H5-A+O2=C2H3CHO+OH    1.82E13 -0.41 2.2859E4
   PLOG/1.0E0 1.82E13 -4.1E-1 2.2859E4/
   PLOG/1.0E1 2.47E13 -4.5E-1 2.3017E4/
C3H5-T+O2=CH3CO+CH2O    2.55E20 -2.608 1.5657E3
C3H5-T+O2=C3H4-A+HO2    3.59E10 -0.27 -4.136E2
C3H5-A+HO2=C3H5O+OH    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 1.02E13 -1.58E-1 -1.417E3/
   PLOG/1.0E-1 4.98E14 -6.42E-1 -3.491E2/
   PLOG/1.0E0 7.77E17 -1.52E0 2.3792E3/
   PLOG/1.0E1 2.93E15 -6.84E-1 3.6153E3/
   PLOG/1.0E2 1.64E4 2.74E0 1.1444E3/
C3H5-A+HO2=AC3H5OOH    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 1.91E31 -7.23E0 1.3362E3/
   PLOG/1.0E-1 6.31E42 -1.03E1 5.5689E3/
   PLOG/1.0E0 1.03E45 -1.06E1 7.8515E3/
   PLOG/1.0E1 2.79E37 -7.92E0 6.4979E3/
   PLOG/1.0E2 1.44E32 -6.01E0 6.0536E3/
C3H5-A+HO2=C2H3CHO+H2O    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 1.09E0 3.01E0 -3.4211E3/
   PLOG/1.0E-1 6.35E1 2.5E0 -2.3414E3/
   PLOG/1.0E0 6.05E5 1.39E0 5.951E2/
   PLOG/1.0E1 3.1E5 1.59E0 2.6776E3/
   PLOG/1.0E2 5.07E-5 4.59E0 9.275E2/
AC3H5OOH=C2H3CHO+H2O    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 1.99E50 -1.27E1 5.35319E4/
   PLOG/1.0E-1 4.72E47 -1.15E1 5.43609E4/
   PLOG/1.0E0 1.5E40 -8.84E0 5.31792E4/
   PLOG/1.0E1 2.54E28 -5.0E0 4.99194E4/
   PLOG/1.0E2 1.48E16 -1.12E0 4.59493E4/
AC3H5OOH=C3H5O+OH    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 1.49E58 -1.39E1 5.42669E4/
   PLOG/1.0E-1 1.8E54 -1.24E1 5.41938E4/
   PLOG/1.0E0 3.36E46 -9.81E0 5.24685E4/
   PLOG/1.0E1 2.39E36 -6.54E0 4.9429E4/
   PLOG/1.0E2 1.28E27 -3.61E0 4.63331E4/
C3H5O=C2H3+CH2O    1.0E11 0.0 0.0E0
   PLOG/1.0E-3 7.26E6 1.82E-1 1.78155E4/
   PLOG/1.0E-2 6.97E16 -2.5E0 2.08787E4/
   PLOG/1.0E-1 6.64E23 -4.23E0 2.3565E4/
   PLOG/1.0E0 1.07E26 -4.56E0 2.46229E4/
   PLOG/1.0E1 6.5E29 -5.37E0 2.6645E4/
   PLOG/1.0E2 4.63E31 -5.59E0 2.89153E4/
   PLOG/1.0E3 8.52E25 -3.61E0 2.78634E4/
C3H5O=C2H3CHO+H    1.0E11 0.0 0.0E0
   PLOG/1.0E-3 3.0E15 -2.31E0 1.46679E4/
   PLOG/1.0E-2 1.5E22 -3.96E0 1.8283E4/
   PLOG/1.0E-1 1.95E23 -3.99E0 1.91433E4/
   PLOG/1.0E0 1.15E25 -4.24E0 2.03112E4/
   PLOG/1.0E1 1.76E28 -4.89E0 2.27652E4/
   PLOG/1.0E2 1.41E27 -4.28E0 2.37706E4/
   PLOG/1.0E3 2.57E20 -2.06E0 2.20401E4/
C3H5O=C2H4+HCO    1.0E11 0.0 0.0E0
   PLOG/1.0E-3 6.62E16 -2.84E0 1.3197E4/
   PLOG/1.0E-2 1.26E20 -3.53E0 1.54692E4/
   PLOG/1.0E-1 2.13E21 -3.64E0 1.65845E4/
   PLOG/1.0E0 1.07E24 -4.16E0 1.8985E4/
   PLOG/1.0E1 8.42E25 -4.4E0 2.23826E4/
   PLOG/1.0E2 1.86E21 -2.73E0 2.36588E4/
   PLOG/1.0E3 4.75E8 1.14E0 2.09225E4/
C2H3+CH2O=C2H3CHO+H    1.0E11 0.0 0.0E0
   PLOG/1.0E-3 2.6E4 2.26E0 1.5103E3/
   PLOG/1.0E-2 5.13E4 2.17E0 1.6755E3/
   PLOG/1.0E-1 3.99E5 1.91E0 2.2183E3/
   PLOG/1.0E0 1.75E7 1.45E0 3.428E3/
   PLOG/1.0E1 1.35E9 9.33E-1 5.173E3/
   PLOG/1.0E2 2.24E11 3.57E-1 8.0013E3/
   PLOG/1.0E3 6.01E5 2.09E0 7.8956E3/
```

C2H3+CH2O=C2H4+HCO 1.0E11 0.0 0.0E0
PLOG/1.0E-3 1.11E7 1.09E0 1.8072E3/
PLOG/1.0E-2 2.47E7 9.93E-1 1.9949E3/
PLOG/1.0E-1 2.47E8 7.04E-1 2.5962E3/
PLOG/1.0E0 1.42E10 2.09E-1 3.9342E3/
PLOG/1.0E1 3.45E13 -7.26E-1 6.9443E3/
PLOG/1.0E2 3.31E14 -8.66E-1 1.09657E4/
PLOG/1.0E3 1.65E1 3.17E0 9.3998E3/
C3H5-A+CH3O2=C3H5O+CH3O 1.0E11 0.0 0.0E0
PLOG/1.0E-2 3.33E12 -1.58E-1 -1.417E3/
PLOG/1.0E-1 1.66E14 -6.42E-1 -3.491E2/
PLOG/1.0E0 2.595E17 -1.52E0 2.3792E3/
PLOG/1.0E1 9.78E14 -6.84E-1 3.6153E3/
PLOG/1.0E2 5.47E3 2.74E0 1.1444E3/
C3H6+OH=CH3CHO+CH3 6.93E5 1.49 -5.36E2
PLOG/1.3E-3 6.93E5 1.49E0 -5.36E2/
PLOG/1.0E-2 5.94E3 2.01E0 -5.6E2/
PLOG/1.3E-2 1.1E3 2.22E0 -6.8E2/
PLOG/2.5E-2 1.07E2 2.5E0 -7.59E2/
PLOG/1.0E-1 7.83E-1 3.1E0 -9.19E2/
PLOG/1.315E-1 3.07E-1 3.22E0 -9.46E2/
PLOG/1.0E0 3.16E-4 4.05E0 -1.144E3/
PLOG/1.0E1 7.59E-6 4.49E0 -6.8E2/
PLOG/1.0E2 5.45E-5 4.22E0 1.141E3/
C3H6+OH=C3H6OH2-1 5.1E54 -20.7 3.2402E4
DUP
PLOG/1.3E-3 2.14E59 -1.584E1 1.1594E4/
PLOG/1.0E-2 2.43E59 -1.551E1 1.2898E4/
PLOG/1.3E-2 9.3E58 -1.534E1 1.2913E4/
PLOG/2.5E-2 8.83E57 -1.493E1 1.2936E4/
PLOG/1.0E-1 4.5E55 -1.404E1 1.2945E4/
PLOG/1.315E-1 1.33E55 -1.385E1 1.2887E4/
PLOG/1.0E0 5.18E49 -1.204E1 1.1493E4/
PLOG/1.0E1 2.14E41 -9.35E0 8.921E3/
PLOG/1.0E2 7.65E31 -6.31E0 6.088E3/
C3H6+OH=C3H6OH2-1 5.1E54 -20.7 3.2402E4
DUP
PLOG/1.3E-3 7.68E77 -2.07E1 3.2402E4/
PLOG/1.0E-2 9.13E76 -2.0E1 3.3874E4/
PLOG/1.3E-2 3.55E75 -1.958E1 3.2874E4/
PLOG/2.5E-2 1.23E73 -1.879E1 3.1361E4/
PLOG/1.0E-1 3.45E67 -1.701E1 2.7909E4/
PLOG/1.315E-1 2.41E66 -1.664E1 2.7162E4/
PLOG/1.0E0 6.5E58 -1.417E1 2.3079E4/
PLOG/1.0E1 2.53E53 -1.223E1 2.2976E4/
PLOG/1.0E2 4.78E47 -1.023E1 2.3772E4/
C3H4-A=C3H3+H 1.32E31 -4.749 9.20795E4
PLOG/1.0E0 1.32E31 -4.749E0 9.20795E4/
PLOG/1.0E1 3.65E25 -2.95E0 9.06249E4/
C3H4-A+H=C3H3+H2 6.625E3 3.095 5.522E3
C3H4-A+O2=C3H3+HO2 4.0E13 0.0 4.132E4
C3H4-A+OH=C3H3+H2O 1.482E5 2.492 1.8072E3
C3H4-A+CH3=C3H3+CH4 1.3E12 0.0 7.7E3
C3H4-A+HO2=C3H3+H2O2 3.58E-2 4.17 9.6328E3
C3H4-A+CH3O2=C3H3+CH3O2H 7.161E-2 4.17 9.6328E3
C3H4-A+C3H5-A=C3H3+C3H6 2.0E11 0.0 7.7E3
C3H4-A+H=C3H5-A 2.21E61 -15.25 2.0076E4
DUP
PLOG/1.0E-3 2.21E61 -1.525E1 2.0076E4/
PLOG/3.9E-2 1.24E52 -1.202E1 1.7839E4/
PLOG/1.0E0 4.67E51 -1.145E1 2.134E4/
PLOG/1.0E1 3.75E48 -1.027E1 2.2511E4/
PLOG/1.0E2 4.23E43 -8.61E0 2.2522E4/
C3H4-A+H=C3H5-A 2.21E61 -15.25 2.0076E4
DUP
PLOG/1.0E-3 2.8E38 -8.67E0 8.035E3/
PLOG/3.9E-2 9.33E36 -8.19E0 7.462E3/
PLOG/1.0E0 3.32E30 -5.78E0 6.913E3/
PLOG/1.0E1 2.29E26 -4.32E0 6.163E3/
PLOG/1.0E2 4.38E21 -2.71E0 5.187E3/
C3H4-A+H=C3H5-T 6.44E102 -27.51 5.1768E4
DUP
PLOG/1.0E-3 6.44E102 -2.751E1 5.1768E4/
PLOG/3.9E-2 1.55E53 -1.31E1 1.4472E4/
PLOG/1.0E0 1.9E53 -1.259E1 1.6726E4/
PLOG/1.0E1 7.95E51 -1.182E1 1.8286E4/
PLOG/1.0E2 4.21E52 -1.164E1 2.2262E4/
C3H4-A+H=C3H5-T 6.44E102 -27.51 5.1768E4
DUP
PLOG/1.0E-3 1.1E54 -1.429E1 1.0809E4/
PLOG/3.9E-2 9.88E44 -1.121E1 8.212E3/
PLOG/1.0E0 2.81E40 -9.42E0 7.85E3/
PLOG/1.0E1 2.6E35 -7.57E0 7.147E3/
PLOG/1.0E2 9.88E29 -5.53E0 6.581E3/
C3H4-A+H=CH3+C2H2 3.74E1 3.35 5.78E1
DUP
PLOG/1.0E-3 1.23E8 1.53E0 4.737E3/
PLOG/3.9E-2 2.72E9 1.2E0 6.834E3/
PLOG/1.0E0 1.26E20 -1.83E0 1.5003E4/
PLOG/1.0E1 1.68E16 -6.0E-1 1.4754E4/
PLOG/1.0E2 1.37E17 -7.9E-1 1.7603E4/
C3H4-A+H=CH3+C2H2 3.74E1 3.35 5.78E1
DUP

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    PLOG/1.0E-3 1.0E-10 0.0E0 0.0E0/
    PLOG/3.9E-2 1.0E-10 0.0E0 0.0E0/
    PLOG/1.0E0 1.23E4 2.68E0 6.335E3/
    PLOG/1.0E1 3.31E8 1.14E0 8.886E3/
    PLOG/1.0E2 1.28E6 1.71E0 9.774E3/
C3H5-A=C3H5-T    3.9E59 -15.42 7.54E4
    PLOG/1.0E-1 3.9E59 -1.542E1 7.54E4/
    PLOG/1.0E0 7.06E56 -1.408E1 7.5868E4/
    PLOG/2.0E0 4.8E55 -1.359E1 7.5949E4/
    PLOG/5.0E0 4.86E53 -1.281E1 7.5883E4/
    PLOG/1.0E1 6.4E51 -1.212E1 7.57E4/
    PLOG/1.0E2 2.8E43 -9.27E0 7.4E4/
C2H2+CH3=C3H5-T    6.8E20 -4.16 1.8E4
    PLOG/1.0E-1 6.8E20 -4.16E0 1.8E4/
    PLOG/1.0E0 4.99E22 -4.39E0 1.885E4/
    PLOG/2.0E0 6.0E23 -4.6E0 1.9571E4/
    PLOG/5.0E0 7.31E25 -5.06E0 2.115E4/
    PLOG/1.0E1 9.3E27 -5.55E0 2.29E4/
    PLOG/1.0E2 3.8E36 -7.58E0 3.13E4/
C2H2+CH3=C3H5-A    8.2E53 -13.32 3.32E4
    PLOG/1.0E-1 8.2E53 -1.332E1 3.32E4/
    PLOG/1.0E0 2.68E53 -1.282E1 3.573E4/
    PLOG/2.0E0 3.64E52 -1.246E1 3.6127E4/
    PLOG/5.0E0 1.04E51 -1.189E1 3.6476E4/
    PLOG/1.0E1 4.4E49 -1.14E1 3.67E4/
    PLOG/1.0E2 3.8E44 -9.63E0 3.76E4/
C3H4-A+O=C2H4+CO    2.0E7 1.8 1.0E3
C3H4-A+O=C2H2+CH2O    3.0E-3 4.61 -4.243E3
C3H4-A+HO2=>C2H4+CO+OH    1.0E11 0.0 1.4E4
C3H4-A+HO2=>CH2CO+CH2+OH    4.0E12 0.0 1.9E4
C3H4-A+C2H=C2H2+C3H3    1.0E13 0.0 0.0E0
C3H3+O=CH2O+C2H    2.0E13 0.0 0.0E0
C3H3+HO2=>OH+CO+C2H3    8.0E11 0.0 0.0E0
C3H3+HCO=C3H4-A+CO    2.5E13 0.0 0.0E0
C2H5+C2H=C3H3+CH3    1.81E13 0.0 0.0E0
C3H3+O2=CH2CO+HCO    1.7E5 1.7 1.5E3
C3H3+H=C3H2+H2    2.14E5 2.52 7.453E3
C3H3+OH=C3H2+H2O    2.0E13 0.0 8.0E3
C3H3+OH=CH2O+C2H2    2.0E12 0.0 0.0E0
C3H3+OH=C2H3+HCO    1.0E13 0.0 0.0E0
C3H3+OH=C2H4+CO    1.0E13 0.0 0.0E0
CH3CHCO+OH=C2H5+CO2    1.73E12 0.0 -1.01E3
CH3CHCO+H=C2H5+CO    4.4E12 0.0 1.459E3
CH3CHCO+O=CH3CHO+CO    3.2E12 0.0 -4.37E2
C3H5O+O2=C2H3CHO+HO2    1.0E12 0.0 6.0E3
CH3COCH3+H=C3H6OH2-1    8.0E12 0.0 9.5E3
C3H6OH2-1+O2=CH3COCH3+HO2    1.5E12 0.0 5.0E3
CH3COCH3=CH3CO+CH3    2.05E58 -12.796 1.000301E5
    PLOG/1.0E-2 2.05E58 -1.2796E1 1.000301E5/
    PLOG/1.0E-1 3.3E51 -1.0574E1 9.82212E4/
    PLOG/1.0E0 1.31E42 -7.657E0 9.46606E4/
    PLOG/1.0E1 2.16E33 -4.989E0 9.09165E4/
    PLOG/1.0E2 9.4E28 -3.669E0 8.90228E4/
CH3COCH2O=CH3CO+CH2O    5.872E20 -2.4218 1.05358E4
C2H3+HCO=C2H3CHO    1.81E13 0.0 0.0E0
C2H5+HCO=C2H5CHO    1.81E13 0.0 0.0E0
IC3H6CO+OH=IC3H7+CO2    1.73E12 0.0 -1.01E3
IC3H6CO+OH=C3H6OH2-1+CO    2.0E12 0.0 -1.01E3
C3H5-T+CH2O=C3H6+HCO    1.0E11 0.0 0.0E0
    PLOG/1.0E-3 1.11E7 1.09E0 1.8072E3/
    PLOG/1.0E-2 2.47E7 9.93E-1 1.9949E3/
    PLOG/1.0E-1 2.47E8 7.04E-1 2.5962E3/
    PLOG/1.0E0 1.42E10 2.09E-1 3.9342E3/
    PLOG/1.0E1 3.45E13 -7.26E-1 6.9443E3/
    PLOG/1.0E2 3.31E14 -8.66E-1 1.09657E4/
    PLOG/1.0E3 1.65E1 3.17E0 9.3998E3/
C2H5CHCO+OH=NC3H7+CO2    3.73E12 0.0 -1.01E3
C2H5CHCO+H=NC3H7+CO    4.4E12 0.0 1.459E3
C2H5CHCO+O=C3H6+CO2    3.2E12 0.0 -4.37E2
C5H81-3+OH=C2H3CHO+C2H5    1.0E12 0.0 0.0E0
END
```

APPENDIX G

IG Blend Mechanism

```
ELEMENTS
C H N O AR
HE
END
SPECIES
AR N2 HE H2 H
O2 O H2O OH OHV
H2O2 HO2 CO CO2 CH4
CH3 CH2 CH2(S) CH CHV
CH3O2H CH3O2 CH3OH CH3O CH2OH
CH2O HCO HCOH HO2CHO O2CHO
HOCHO OCHO C2H6 C2H5 C2H4
C2H3 CHCHO C2H2 C2H CH3CHO
C2H3OH CH2CO HCCO C3H3 C3H2
C3H6OH2-1 C4H3-I C5H6 HOCH2O C2H5O2H
C2H5O2 C2H3OO H2CC C2H5O SC2H4OH
O2C2H4OH C2H4O1-2 CH3CO CH2CHO CH3CO3H
CH3CO3 CH3CO2 C3H8 C3H6OOH2-1 C3H6OOH2-1O2
C3H6O1-2 C3H6 C3H5-A CH3CHCO SC3H5OH
C2H3CHO C2H5CHO C4H10 C4H8-1 C4H71-2
C5H81-3 IC3H7 NC3H7 NC3H7O2 IC3H7O2H
IC3H7O2 C3H6OOH1-2 C3H6OOH1-3 C3H6OOH1-3O2 C3KET13
CH3CHCHO C3H5O AC3H5OOH IC3H7O CH2CH2CHO
C2H5CHCO
END

THERMO ALL
   300.000  1000.000  5000.000
AR                G-5-97AR  1               G     200.0    6000.0  1000.0      1
         2.5E0         0.0E0         0.0E0         0.0E0         0.0E0    2
     -7.45375E2   4.37967491E0         2.5E0         0.0E0         0.0E0    3
         0.0E0         0.0E0     -7.45375E2   4.37967491E0                   4
N2                G-8-02N   2               G     200.0    6000.0  1000.0      1
    2.95257637E0   1.3969004E-3 -4.92631603E-7 7.86010195E-11-4.60755204E-15    2
   -9.23948688E2   5.87188762E0   3.53100528E0 -1.23660988E-4 -5.02999433E-7    3
    2.43530612E-9-1.40881235E-12  -1.04697628E3   2.96747038E0                   4
HE                G-5-97HE  1               G     200.0    6000.0  1000.0      1
         2.5E0         0.0E0         0.0E0         0.0E0         0.0E0    2
     -7.45375E2  9.28723974E-1         2.5E0         0.0E0         0.0E0    3
         0.0E0         0.0E0     -7.45375E2  9.28723974E-1                   4
H2                TPIS78H   2               G     200.0    6000.0  1000.0      1
    2.93286575E0  8.26608026E-4 -1.46402364E-7 1.54100414E-11  -6.888048E-16    2
   -8.13065581E2  -1.02432865E0   2.34433112E0  7.98052075E-3  -1.9478151E-5    3
    2.01572094E-8-7.37611761E-12  -9.17935173E2  6.83010238E-1                   4
H                 L-6-94H   1               G     200.0    6000.0  1000.0      1
         2.5E0         0.0E0         0.0E0         0.0E0         0.0E0    2
     2.547366E4  -4.4668285E-1         2.5E0         0.0E0         0.0E0    3
         0.0E0         0.0E0     2.547366E4  -4.4668285E-1                   4
O2                RUS-89O   2               G     200.0    6000.0  1000.0      1
    3.66096065E0  6.56365811E-4 -1.41149627E-7 2.05797935E-11-1.29913436E-15    2
   -1.21597718E3   3.41536279E0   3.78245636E0 -2.99673416E-3  9.84730201E-6    3
   -9.68129509E-9 3.24372837E-12  -1.06394356E3   3.65767573E0                   4
O                 L-1-90O   1               G     200.0    6000.0  1000.0      1
    2.54363697E0 -2.73162486E-5  -4.1902952E-9 4.95481845E-12-4.79553694E-16    2
     2.9226012E4   4.92229457E0    3.1682671E0 -3.27931884E-3  6.64306396E-6    3
   -6.12806624E-9 2.11265971E-12   2.91222592E4   2.05193346E0                   4
H2O               L-5-89H   2O  1           G     200.0    6000.0  1000.0      1
     2.6770389E0   2.9731816E-3  -7.7376889E-7  9.4433514E-11 -4.2689991E-15    2
    -2.9885894E4      6.88255E0    4.1986352E0  -2.0364017E-3   6.5203416E-6    3
    -5.4879269E-9   1.771968E-12   -3.0293726E4  -8.4900901E-1                   4
OH                IU3-03H   1O  1           G     200.0    6000.0  1000.0      1
    2.83853033E0  1.10741289E-3 -2.94000209E-7 4.20698729E-11 -2.4228989E-15    2
    3.69780808E3   5.84494652E0   3.99198424E0 -2.40106655E-3  4.61664033E-6    3
   -3.87916306E-9 1.36319502E-12   3.36889836E3 -1.03998477E-1                   4
!UB REFIT 13-11-2018
OHV               -THERMH   1O  1           G     300.0    5000.0  1710.0      1
     2.8537604E0  1.02994334E-3 -2.32666477E-7 1.93750704E-11-3.15759847E-16    2
    5.03225473E4   5.76240468E0   3.41896226E0  3.19255801E-4 -3.08292717E-7    3
   3.64407494E-10-1.00195479E-13   5.00756946E4   2.51917016E0                   4
H2O2              T-8-03H   2O  2           G     200.0    6000.0  1000.0      1
    4.57977305E0  4.05326003E-3  -1.2984473E-6   1.982114E-10-1.13968792E-14    2
   -1.80071775E4  6.64970694E-1   4.31515149E0 -8.47390622E-4  1.76404323E-5    3
   -2.26762944E-8 9.08950158E-12  -1.77067437E4   3.27373319E0                   4
HO2               T-1-09H   1O  2           G     200.0    5000.0  1000.0      1
    4.17228741E0  1.88117627E-3 -3.46277286E-7 1.94657549E-11 1.76256905E-16    2
    3.10206839E1   2.95767672E0   4.30179807E0 -4.74912097E-3  2.11582905E-5    3
   -2.42763914E-8 9.29225225E-12   2.64018485E2   3.7166622E0                   4
CO                RUS-79O   1C  1           G     200.0    6000.0  1000.0      1
    3.0484859E0   1.3517281E-3  -4.8579405E-7  7.8853644E-11 -4.6980746E-15    2
   -1.4266117E4   6.0170977E0   3.5795335E0  -6.1035369E-4   1.0168143E-6    3
   9.0700586E-10 -9.0442449E-13   -1.4344086E4   3.5084093E0                   4
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CO2               L-7-88O  2C  1         G     200.0    6000.0  1000.0      1
   4.6365111E0  2.7414569E-3 -9.9589759E-7  1.6038666E-10 -9.1619857E-15    2
  -4.9024904E4  -1.9348955E0     2.356813E0   8.9841299E-3  -7.1220632E-6    3
   2.4573008E-9 -1.4288548E-13   -4.8371971E4    9.9009035E0                 4
CH4               G-8-99H  4C  1         G     200.0    6000.0  1000.0      1
  1.65326226E0  1.00263099E-2 -3.31661238E-6 5.36483138E-10-3.14696758E-14    2
 -1.00095936E4   9.90506283E0   5.14911468E0 -1.36622009E-2  4.91453921E-5    3
 -4.84246767E-8 1.66603441E-11  -1.02465983E4  -4.63848842E0                 4
CH3               IU0702H  3C  1         G     200.0    6000.0  1000.0      1
   2.9781206E0   5.797852E-3   -1.97558E-6   3.072979E-10 -1.7917416E-14    2
   1.6509513E4   4.7224799E0   3.6571797E0   2.1265979E-3   5.4583883E-6    3
 -6.6181003E-9  2.4657074E-12    1.6422716E4    1.6735354E0                 4
CH2               IU3-03H  2C  1         G     200.0    6000.0  1000.0      1
  3.14631886E0  3.03671259E-3 -9.96474439E-7  1.5048358E-10-8.57335515E-15    2
  4.60412605E4  4.72341711E0   3.71757846E0   1.2739126E-3  2.17347251E-6    3
  -3.488585E-9 1.65208866E-12   4.58723866E4   1.75297945E0                 4
CH2(S)            IU6-03H  2C  1         G     200.0    6000.0  1000.0      1
  3.13501686E0  2.89593926E-3  -8.1666809E-7 1.13572697E-10-6.36262835E-15    2
  5.05040504E4  4.06030621E0   4.19331325E0 -2.33105184E-3  8.15676451E-6    3
 -6.62985981E-9 1.93233199E-12   5.03662246E4  -7.4673431E-1                 4
CH                IU3-03H  1C  1         G     200.0    6000.0  1000.0      1
   2.5209369E0   1.7653639E-3   -4.614766E-7  5.9289675E-11 -3.3474501E-15    2
   7.0946769E4   7.4051829E0   3.4897583E0   3.243216E-4  -1.6899751E-6    3
   3.162842E-9 -1.4061803E-12    7.0612646E4   2.0842841E0                 4
!UB REFIT 13-11-2018
CHV               -THERMH  1C  1         G     300.0    5000.0  1365.0      1
  2.21703785E0  2.15314038E-3 -5.71569209E-7 6.54441183E-11-2.66374894E-15    2
  1.04414085E5   9.18247549E0   3.50775836E0 -4.57470019E-4  1.32602633E-6    3
 -5.1421376E-10 5.82219975E-14   1.03920991E5   2.09911232E0                 4
CH3O2H            A-7-05H  4O  2C  1     G     200.0    6000.0  1000.0      1
  7.76538058E0  8.61499712E-3 -2.98006935E-6 4.68638071E-10-2.75339255E-14    2
 -1.82979984E4  -1.43992663E1   2.90540897E0  1.74994735E-2   5.2824363E-6    3
 -2.52827275E-8 1.34368212E-11  -1.68894632E4   1.13741987E1                 4
CH3O2               H  3O  2C  1     G     300.0    5000.0  1374.0      1
  6.47970487E0   7.4440108E-3 -2.52348555E-6 3.89577296E-10-2.25182399E-14    2
 -1.56285441E3  -8.19477074E0   1.97339205E0   1.5354234E-2 -6.37314891E-6    3
 3.19930565E-10 2.82193915E-13   2.54278835E2   1.69194215E1                 4
CH3OH             T06-02H  4O  1C  1     G     200.0    6000.0  1000.0      1
  3.52726795E0  1.03178783E-2 -3.62892944E-6 5.77448016E-10-3.42182632E-14    2
 -2.60028834E4  5.16758693E0   5.65851051E0 -1.62983419E-2  6.91938156E-5    3
 -7.58372926E-8  2.8042755E-11  -2.56119736E4 -8.97330508E-1                 4
CH3O              IU1-03H  3O  1C  1     G     200.0    6000.0  1000.0      1
  4.75779238E0  7.44142474E-3 -2.69705176E-6 4.38090504E-10-2.63537098E-14    2
   3.7811194E2  -1.96680028E0   3.71180502E0 -2.80463306E-3  3.76550971E-5    3
 -4.73072089E-8  1.8658842E-11    1.2956976E3   6.57240864E0                 4
CH2OH             IU2-03H  3O  1C  1     G     200.0    6000.0  1000.0      1
   5.0931437E0   5.9476126E-3  -2.0649746E-6 3.23008173E-10-1.88125902E-14    2
  -4.0340964E3  -1.84691493E0   4.47834367E0  -1.3507031E-3   2.7848498E-5    3
  -3.6486906E-8  1.4790745E-11   -3.5007289E3    3.309135E0                 4
CH2O              T-5-11H  2O  1C  1     G     200.0    6000.0  1000.0      1
  3.16952665E0   6.1932056E-3 -2.25056366E-6  3.6597566E-10-2.20149458E-14    2
 -1.45486831E4   6.04207898E0   4.79372312E0 -9.90833322E-3   3.7321999E-5    3
 -3.79285237E-8 1.31772641E-11  -1.43791953E4  6.02798058E-1                 4
HCO               T-5-03H  1O  1C  1     G     200.0    6000.0  1000.0      1
  3.92001542E0  2.52279324E-3 -6.71004164E-7 1.05615948E-10-7.43798261E-15    2
   3.6534292 8E3   3.58077056E0   4.2375461E0 -3.32075257E-3  1.40030264E-5    3
 -1.34239995E-8 4.37416208E-12   3.87241185E3   3.30834869E0                 4
HCOH              -MAR94H  2O  1C  1     G     300.0    5000.0  1398.0      1
  9.18749272E0  1.52011152E-3 -6.27603516E-7 1.09727989E-10-6.89655128E-15    2
  7.81364593E3  -2.73434214E1  -2.82157421E0  3.57331702E-2  -3.8086158E-5    3
 1.86205951E-8-3.45957838E-12   1.12956672E4   3.48487757E1                 4
HO2CHO            -THERMH  2O  3C  1     G     300.0    5000.0  1378.0      1
  9.87503878E0  4.64663708E-3 -1.67230522E-6 2.68624413E-10-1.59595232E-14    2
 -3.80502496E4  -2.24939155E1   2.42464726E0   2.1970638E-2 -1.68705546E-5    3
  6.25612194E-9-9.11645843E-13  -3.54828006E4   1.75027796E1                 4
O2CHO             -THERMH  1O  3C  1     G     300.0    5000.0  1368.0      1
  7.24075139E0  4.63312951E-3 -1.63693995E-6 2.59706693E-10-1.52964699E-14    2
 -1.87027618E4  -6.49547212E0   3.96059309E0  1.06002279E-2 -5.25713351E-6    3
  1.01716726E-9-2.87487602E-14  -1.73599383E4   1.17807483E1                 4
HOCHO             L-8-88H  2O  2C  1     G     200.0    6000.0  1000.0      1
   4.6138316E0   6.4496364E-3  -2.2908251E-6  3.6716047E-10 -2.1873675E-14    2
   -4.751485E4   8.4788383E-1   3.8983616E0  -3.5587795E-3   3.5520538E-5    3
  -4.3849959E-8  1.7107769E-11   -4.6770609E4   7.3495397E0                 4
OCHO              ATCT-AH  1O  2C  1     G     200.0    6000.0  1000.0      1
  4.14394211E0  5.59738818E-3 -1.99794019E-6 3.16179193E-10-1.85614483E-14    2
 -1.72459887E4   5.07778617E0   4.68825921E0 -4.14871834E-3   2.5506601E-5    3
  -2.844739E-8  1.04422559E-11  -1.69867041E4   4.2842648E0                 4
C2H6              G-8-88H  6C  2         G     200.0    6000.0  1000.0      1
  4.04666411E0  1.53538802E-2 -5.47039485E-6 8.77826544E-10-5.23167531E-14    2
 -1.24473499E4 -9.68698313E-1   4.29142572E0 -5.50154901E-3  5.99438458E-5    3
 -7.08466469E-8 2.68685836E-11  -1.15222056E4   2.66678994E0                 4
C2H5              -THERMH  5C  2         G     300.0    5000.0  1387.0      1
   5.8878439E0  1.03076793E-2 -3.46844396E-6 5.32499257E-10-3.06512651E-14    2
  1.15065499E4  -8.49651771E0   1.32730217E0  1.76656753E-2 -6.14926558E-6    3
-3.01143466E-10 4.38617775E-13   1.34284028E4   1.71789216E1                 4
C2H4                H  4C  2         G     300.0    5000.0  1392.0      1
  5.07061289E0  9.11140768E-3 -3.10506692E-6 4.80733851E-10-2.78321396E-14    2
  3.66391217E3  -6.64501414E0  4.81118223E-1   1.8377806E-2 -9.99633565E-6    3
  2.73211039E-9-3.01837289E-13   5.44386648E3   1.85867157E1                 4
C2H3                H  3C  2         G     300.0    5000.0  1400.0      1
  4.99675415E0  6.55838271E-3 -2.20921909E-6 3.39300272E-10-1.95316926E-14    2
  3.34604382E4  -3.01451097E0   1.25545094E0  1.57481597E-2 -1.12218328E-5    3
  4.50915682E-9-7.74861577E-13   3.47435574E4   1.69664043E1                 4
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CHCHO               H  2O  1C  2    G   298.15    2000.0  1000.0      1
   4.9263291E0  9.71712147E-3  -5.5485598E-6  1.53068537E-9-1.64742462E-13    2
   2.89499494E4  5.27874677E-1   2.33256751E0  1.62952986E-2 -9.72052177E-6    3
 5.15124155E-10 1.03836514E-12   2.96585452E4   1.39904923E1                   4
C2H2           G-1-91H  2C  2        G    200.0    6000.0  1000.0      1
   4.65878489E0  4.88396667E-3 -1.60828888E-6 2.46974544E-10-1.38605959E-14    2
   2.57594042E4  -3.99838194E0  8.08679682E-1  2.33615762E-2 -3.55172234E-5    3
   2.80152958E-8-8.50075165E-12   2.64289808E4   1.39396761E1                   4
C2H            T-5-10H  1C  2        G    200.0    6000.0  1000.0      1
   3.66270248E0  3.82492252E-3   -1.366325E-6  2.1345504E-10-1.23216848E-14    2
    6.7168379E4   3.92205792E0   2.89867676E0  1.32988489E-2 -2.80733327E-5    3
   2.89484755E-8-1.07502351E-11    6.7061605E4   6.18547632E0                   4
CH3CHO          L-8-88H  4O  1C  2    G    200.0    6000.0  1000.0      1
   5.4041108E0   1.1723059E-2  -4.2263137E-6  6.8372451E-10 -4.0984863E-14    2
  -2.2593122E4   -3.4807917E0    4.7294595E0  -3.1932858E-3   4.7534921E-5    3
  -5.7458611E-8  2.1931112E-11   -2.1572878E4    4.1030159E0                   4
C2H3OH          -THERMH  4O  1C  2    G    300.0    5000.0  1410.0      1
   8.32598158E0  8.03387281E-3 -2.63928405E-6 3.98410726E-10-2.26551155E-14    2
  -1.83221436E4  -2.02080305E1  -1.2797226E-1  3.38506073E-2 -3.30644935E-5    3
   1.64858739E-8-3.19935455E-12   -1.59914544E4   2.30438601E1                   4
!UB REFIT 13-11-2018
CH2CO           -THERMH  2O  1C  2    G    300.0    5000.0  1400.0      1
   6.32896692E0  5.44012978E-3 -1.82687969E-6 2.80010787E-10 -1.6096416E-14    2
  -8.36526176E3  -9.53528539E0   2.35724171E0  1.62213064E-2 -1.34812364E-5    3
   6.11939897E-9-1.13613089E-12   -7.11393356E3   1.12990053E1                   4
HCCO            T-4-09H  1O  1C  2    G    200.0    6000.0  1000.0      1
   5.91479333E0   3.7140873E-3  -1.3013701E-6 2.06473345E-10-1.21476759E-14    2
   1.93596301E4  -5.50567269E0   1.87607969E0  2.21205418E-2 -3.58869325E-5    3
   3.05402541E-8-1.01281069E-11    2.0163384E4   1.3696829E1                   4
C3H3            T-7-11H  3C  3        G    200.0    6000.0  1000.0      1
   7.14221719E0  7.61902211E-3  -2.6746003E-6 4.24914904E-10-2.51475443E-14    2
   3.95709594E4   -1.2584869E1   1.35110873E0  3.27411291E-2 -4.73827407E-5    3
   3.7631022E-8-1.18541128E-11   4.07679941E4   1.52058598E1                   4
C3H2            T12-00H  2C  3        G    200.0    6000.0  1000.0      1
   6.67324762E0  5.57728845E-3 -1.99180164E-6 3.20289156E-10-1.91216272E-14    2
   7.57571184E4  -9.72894405E0   2.43417332E0  1.73013063E-2 -1.18294047E-5    3
   1.02756396E-9  1.62626314E-12   7.69074892E4   1.2101223E1                   4
C3H6OH2-1       -THERMH  7O  1C  3    G    300.0    5000.0  1392.0      1
   1.12222277E1  1.36444398E-2 -4.51406709E-6 7.10523275E-10-4.22690392E-14    2
  -1.75350136E4  -3.18911926E1   1.0967036E0  3.80727565E-2 -2.75022497E-5    3
   1.07477493E-8-1.74895773E-12  -1.40764487E4   2.22475799E1                   4
C4H3-I          AB1-93H  3C  4        G    300.0    3000.0  1000.0      1
   9.0978165E0   9.2207119E-3  -3.3878441E-6  4.9160498E-10  -1.452978E-14    2
   5.6600574E4   -1.9802597E1   2.0830412E0   4.0834274E-2  -6.2159685E-5    3
   5.1679358E-8 -1.7029184E-11   5.8005129E4   1.3617462E1                   4
C5H6            T-1-90H  6C  5        G    200.0    6000.0  1000.0      1
   9.9757848E0   1.8905543E-2  -6.8411461E-6   1.109934E-9 -6.6680236E-14    2
   1.1081693E4   -3.2209454E1   8.6108957E-1   1.4804031E-2   7.2108895E-5    3
  -1.1338055E-7  4.8689972E-11   1.4801755E4   2.1353453E1                   4
HOCH2O          -THERMH  3O  2C  1    G    300.0    5000.0  1452.0      1
   6.39521515E0  7.43673043E-3 -2.50422354E-6 3.84879712E-10-2.21778689E-14    2
  -2.4110884E4  -6.63865583E0   4.11183145E0  7.53850697E-3   3.7733737E-6    3
  -5.38746005E-9 1.45615887E-12  -2.28023001E4   7.46807254E0                   4
C2H5O2H           H  6O  2C  2    G    300.0    5000.0  1390.0      1
   1.04823538E1  1.34779879E-2 -4.62179078E-6 7.18618519E-10-4.17307436E-14    2
  -2.46578171E4  -2.84294243E1   1.83755328E0  3.38053586E-2  -2.3754814E-5    3
   9.31974865E-9-1.58003428E-12  -2.15814086E4   1.80977584E1                   4
C2H5O2            H  5O  2C  2    G    300.0    5000.0  1389.0      1
   9.5028257E0  1.20429839E-2 -4.09491581E-6 6.33049241E-10-3.66133788E-14    2
  -7.37069391E3   -2.2171713E1   3.90351912E0  2.22599212E-2 -1.01610079E-5    3
   1.71709751E-9  1.88166738E-14  -5.09654081E3   8.9872275E0                   4
C2H3OO            H  3O  2C  2    G   298.15    2000.0  1000.0      1
   6.04483828E0  1.45511127E-2 -7.50974622E-6   1.8348828E-9-1.66689681E-13    2
   1.01699244E4  -3.71144913E0   1.09784776E0  2.95333237E-2  -2.2774436E-5    3
   7.20559155E-9-3.07929092E-13   1.13996101E4   2.13563583E1                   4
H2CC            L12-89H  2C  2        G    200.0    6000.0  1000.0      1
    4.278034E0   4.7562804E-3  -1.6301009E-6  2.5462806E-10 -1.4886379E-14    2
   4.8316688E4   6.4023701E-1   3.2815483E0   6.9764791E-3   -2.3855244E-6    3
  -1.2104432E-9  9.8189545E-13   4.8621794E4    5.920391E0                   4
C2H5O             H  5O  1C  2    G    300.0    5000.0  1467.0      1
   8.19120635E0  1.10391986E-2 -3.75270536E-6 5.80275784E-10-3.35735146E-14    2
  -5.66847208E3  -1.90131344E1   2.90353584E0  1.77256708E-2 -2.69624757E-6    3
  -3.45830533E-9 1.25224784E-12   -3.2893029E3   1.13545591E1                   4
SC2H4OH           H  5O  1C  2    G    300.0    5000.0  1385.0      1
   8.15007136E0  1.02549305E-2 -3.40137764E-6 5.17509965E-10-2.96128942E-14    2
  -1.05014386E4  -1.73134615E1   1.46281093E0  2.39193995E-2 -1.30667185E-5    3
   3.10615465E-9-1.85896007E-13   -8.00790323E3   1.92547092E1                   4
O2C2H4OH        -THERMH  5O  3C  2    G    300.0    5000.0  1506.0      1
   1.27503881E1  1.11514325E-2 -3.83473891E-6 5.98155829E-10-3.48372108E-14    2
  -2.52770876E4  -3.54317608E1    7.040098E0  1.59564166E-2  2.21097416E-6    3
  -7.05197355E-9  2.08266026E-12  -2.24524432E4  -1.75361758E0                   4
C2H4O1-2        L-8-88H  4O  1C  2    G    200.0    6000.0  1000.0      1
   5.4887641E0   1.204619E-2  -4.3336931E-6  7.0028311E-10 -4.1949088E-14    2
  -9.1804251E3   -7.0799605E0   3.7590532E0   -9.441218E-3   8.0309721E-5    3
  -1.0080788E-7  4.0039921E-11   -7.5608143E3   7.8497475E0                   4
CH3CO           IU2-03H  3O  1C  2    G    200.0    6000.0  1000.0      1
   5.3137165E0   9.1737793E-3  -3.3220386E-6  5.3947456E-10 -3.2452368E-14    2
  -3.6450414E3   -1.6757558E0   4.0358705E0   8.7729487E-4   3.071001E-5    3
  -3.9247565E-8  1.5296869E-11   -2.6820738E3   7.8617682E0                   4
CH2CHO          T03-10H  3O  1C  2    G    200.0    6000.0  1000.0      1
   6.53928338E0  7.80238629E-3 -2.76413612E-6 4.42098906E-10 -2.6295429E-14    2
  -1.18858659E3  -8.72091393E0    2.795026E0  1.01099472E-2  1.61750645E-5    3
  -3.10303145E-8 1.39436139E-11   1.62944975E2   1.23646657E1                   4
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CH3CO3H          -THERMH  4O  3C  2    G    300.0    5000.0  1391.0      1
  1.25060485E1 9.47789695E-3 -3.30402246E-6 5.19630793E-10-3.04233568E-14    2
 -4.59856703E4 -3.79195947E1   2.24135876E0  3.37963514E-2 -2.53887482E-5    3
  9.67583587E-9-1.49266157E-12 -4.24677831E4   1.70668133E1                  4
CH3CO3           -THERMH  3O  3C  2    G    300.0    5000.0  1391.0      1
  1.12522498E1 8.33652672E-3  -2.8901453E-6 4.52781734E-10-2.64354456E-14    2
 -2.60238584E4 -2.96370457E1   3.60373432E0  2.70080341E-2 -2.08293438E-5    3
  8.50541104E-9 -1.4384611E-12  -2.34205171E4   1.12014914E1                  4
CH3CO2           -THERMH  3O  2C  2    G    300.0    5000.0  1395.0      1
  8.54059736E0  8.32951214E-3  -2.8472201E-6 4.41927196E-10-2.56373394E-14    2
 -2.97290678E4 -2.03883545E1   1.37440768E0  2.49115604E-2 -1.74308894E-5    3
  6.24799508E-9-9.09516835E-13   -2.7233015E4   1.81405454E1                  4
C3H8             H  8C  3        G    300.0    5000.0  1390.0      1
   9.1554131E0  1.72574139E-2 -5.85614868E-6 9.04190155E-10-5.22523772E-14    2
 -1.75762439E4   -2.7741851E1   2.4087847E-1  3.39548599E-2 -1.60930874E-5    3
  2.83480628E-9 2.78195172E-14  -1.40362853E4   2.165008E1                   4
C3H6OOH2-1       H  7O  2C  3    G    300.0    5000.0  1393.0      1
  1.36645362E1  1.54329764E-2 -5.29285952E-6 8.23001262E-10-4.77931121E-14    2
 -5.58295862E3  -4.28758364E1   2.38465746E0  4.42928555E-2 -3.50977087E-5    3
  1.53695144E-8-2.81167824E-12  -1.80979612E3   1.69923285E1                  4
C3H6OOH2-1O2     ----12H  7O  4C  3    G    300.0    5000.0  1404.0      1
   1.9104498E1   1.440761E-2 -4.72127814E-6 7.12631642E-10 -4.0557849E-14    2
  -2.5027051E4  -6.63747978E1   3.99085043E0  5.31865338E-2 -4.28597948E-5    3
  1.77187019E-8-2.92768695E-12  -2.02143526E4   1.34150719E1                  4
C3H6O1-2         A01-05H  6O  1C  3    G    200.0    6000.0  1000.0      1
  8.01491079E0  1.73919953E-2 -6.26027968E-6  1.01188256E-9-6.06239111E-14    2
 -1.51980838E4  -1.88279964E1   3.42806676E0  6.25176642E-3  6.13196311E-5    3
 -8.60387185E-8 3.51371393E-11  -1.28446646E4   1.04244994E1                  4
C3H6             H  6C  3        G    298.0    6000.0  1000.0      1
  6.59032304E0  1.52592866E-2 -5.30369441E-6 8.35510888E-10-4.91215549E-14    2
 -2.47481113E2  -1.15748238E1  -1.54606737E0  4.36553128E-2 -5.61392417E-5    3
  4.98421927E-8-1.84798923E-11   2.07056233E3   2.99232495E1                  4
C3H5-A           H  5C  3        G    298.0    6000.0  1000.0      1
  7.37604097E0  1.23449782E-2 -4.26463882E-6 6.69045835E-10-3.92202554E-14    2
   1.7733296E4  -1.61758204E1  -3.32899442E0  5.38423469E-2 -7.65500752E-5    3
  6.35512285E-8-2.14283003E-11   2.03420628E4   3.68038362E1                  4
CH3CHCO          -THERMH  4O  1C  3    G    300.0    5000.0  1400.0      1
  1.00219123E1   9.569663E-3 -3.26221644E-6 5.05231706E-10-2.92593257E-14    2
 -1.42482738E4  -2.77829973E1   1.48380119E0  3.22203013E-2 -2.70250033E-5    3
  1.20499164E-8-2.18365931E-12   -1.1527654E4   1.71552068E1                  4
SC3H5OH          H  6O  1C  3    G    300.0    5000.0  1404.0      1
  1.11222064E1   1.2774541E-2 -4.25315532E-6 6.48216484E-10 -3.7119085E-14    2
 -2.36690795E4  -3.41335182E1 -3.53977226E-2  4.34969453E-2 -3.74479918E-5    3
  1.70906074E-8-3.13775054E-12  -2.02502608E4   2.41528201E1                  4
C2H3CHO          -KPS12H  4O  1C  3    G    300.0    5000.0  1398.0      1
  9.99155394E0  9.82348001E-3 -3.31203088E-6 5.09524422E-10 -2.9382189E-14    2
 -1.25303509E4  -2.85168883E1   7.33844455E-1  3.17482671E-2 -2.29599468E-5    3
  8.42104232E-9-1.23613478E-12  -9.38473548E3   2.10308851E1                  4
C2H5CHO          H  6O  1C  3    G    300.0    5000.0  1449.0      1
  1.06224453E1  1.35569132E-2 -4.60754771E-6 7.12755462E-10-4.12631683E-14    2
 -2.78692266E4  -3.16628752E1   2.18895588E0  2.58289987E-2 -6.04170058E-6    3
 -3.70702654E-9 1.57131095E-12  -2.42671146E4   1.6149633E1                  4
C4H10            H  10C  4        G    300.0    5000.0  1392.0      1
  1.24923813E1  2.15951935E-2 -7.34277611E-6  1.13529859E-9-6.56730149E-14    2
 -2.17598985E4  -4.41546866E1 -9.20862487E-2  4.69703816E-2 -2.54761945E-5    3
  6.35894738E-9-5.16005946E-13  -1.69556758E4   2.49101571E1                  4
C4H8-1           H  8C  4        G    300.0    5000.0  1388.0      1
  1.10189295E1  1.82714177E-2 -6.21801907E-6 9.62038611E-10-5.56791341E-14    2
 -5.80998818E3  -3.47942287E1   1.62599556E-1  4.01052746E-2 -2.18038592E-5    3
  5.47070727E-9-4.54073315E-13  -1.65402601E3   2.48169258E1                  4
!CWZ ADDED FROM YL CALCULATION
C4H71-2          H  7C  4        G   298.15    2000.0  1000.0      1
  4.57642739E0  2.64291321E-2 -1.13345708E-5  1.98119158E-9-6.72515039E-14    2
  2.51643094E4   3.76340541E0   1.82636932E0  3.22499538E-2 -1.22966874E-5    3
 -2.55680795E-9 2.36210103E-12   2.59732915E4   1.83256985E1                  4
C5H81-3          H  8C  5        G    300.0    5000.0  1385.0      1
  1.29945372E1  1.92678312E-2 -6.58966712E-6  1.02295969E-9-5.93441369E-14    2
  4.59040047E3  -4.35689825E1   1.54882436E0  4.15042709E-2  -2.1435989E-5    3
  4.71145517E-9-2.42142508E-13   9.05636062E3   1.9566591E1                  4
IC3H7            H  7C  3        G    298.0    6000.0  1000.0      1
  6.70775549E0  1.74048076E-2 -6.07615926E-6 9.60084351E-10 -5.6565649E-14    2
  7.55377821E3  -1.03686516E1 -8.97467137E-1  4.15744022E-2 -4.94778349E-5    3
  4.56493655E-8-1.79085437E-11   9.93950407E3   2.92641758E1                  4
NC3H7            H  7C  3        G    298.0    6000.0  1000.0      1
  7.48614243E0  1.65769478E-2 -5.74876481E-6 9.04103694E-10-5.30867231E-14    2
  8.93710008E3  -1.42595379E1  -2.20120865E0  5.29641653E-2 -7.23640506E-5    3
  6.3699694E-8-2.29332581E-11   1.15130744E4   3.43669174E1                  4
NC3H7O2          H  7O  2C  3    G    300.0    5000.0  1390.0      1
  1.32753283E1  1.61303126E-2 -5.52348308E-6 8.58197168E-10-4.98172586E-14    2
 -1.16032968E4  -4.15091215E1   2.13311681E0  3.96692045E-2 -2.37570127E-5    3
  6.96020417E-9-7.82576856E-13  -7.46687112E3   1.92444565E1                  4
IC3H7O2H         H  8O  2C  3    G    300.0    5000.0  1405.0      1
  1.44896107E1  1.68268026E-2 -5.67601391E-6 8.72850837E-10-5.02993991E-14    2
 -3.06478491E4  -5.01352281E1   1.77384705E0  4.75813498E-2 -3.43745304E-5    3
  1.31405381E-8-2.06922904E-12  -2.63458844E4   1.77669753E1                  4
IC3H7O2          H  7O  2C  3    G    300.0    5000.0  1407.0      1
   1.3526812E1  1.54306581E-2 -5.17464218E-6 7.92548669E-10-4.55415379E-14    2
 -1.33946348E4  -4.40461451E1   2.58517502E0  4.16107259E-2 -2.92193877E-5    3
  1.08614807E-8-1.66312005E-12  -9.67013161E3   1.447313E1                   4
C3H6OOH1-2       H  7O  2C  3    G    300.0    5000.0  1387.0      1
  1.38088686E1  1.4384565E-2 -4.74440961E-6  7.1930828E-10-4.10654123E-14    2
 -5.14352831E3  -4.20210765E1   2.83631132E0  3.88229894E-2 -2.47944364E-5    3
  7.85644898E-9  -9.586343E-13  -1.26002528E3   1.72549973E1                  4
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C3H6OOH1-3              H   7O   2C   3    G     300.0    5000.0  1401.0      1
  1.39130757E1  1.40218463E-2 -4.55921149E-6 6.84182417E-10-3.87696213E-14    2
 -3.65650518E3  -4.21532559E1   1.74271107E0  4.53733504E-2 -3.57580373E-5    3
  1.48540053E-8-2.49981756E-12   2.32580844E2   2.20973041E1                  4
C3H6OOH1-3O2      ----12H   7O   4C   3    G     300.0    5000.0  1416.0      1
  1.81661664E1  1.47644887E-2 -4.74842743E-6 7.06972467E-10-3.98305587E-14    2
 -2.26256376E4  -5.93719393E1   5.5693335E0  4.68523421E-2 -3.58917784E-5    3
  1.43314525E-8-2.29776083E-12  -1.86065694E4   7.18655005E0                  4
C3KET13                 H   6O   3C   3    G     300.0    5000.0  1508.0      1
  1.73612692E1  1.32330813E-2  -4.7533211E-6 7.62529227E-10-4.52613717E-14    2
  -4.0624806E4  -6.17768199E1   4.74956819E0  3.14080991E-2 -6.83838427E-6    3
 -5.67123901E-9 2.27686972E-12   -3.5192457E4   9.83753744E0                  4
CH3CHCHO                H   5O   1C   3    G     300.0    5000.0  1424.0      1
  1.06781476E1  1.12805711E-2 -3.89010759E-6 6.07617268E-10-3.54120848E-14    2
 -7.73234209E3  -3.24971238E1   1.47166733E0  2.69251618E-2 -1.00248013E-5    3
 -1.13421435E-9 1.03416658E-12  -4.04142023E3   1.88722472E1                  4
C3H5O             -KPS12H   5O   1C   3    G     300.0    5000.0  1402.0      1
  1.02638186E1  1.17609932E-2 -3.89837957E-6 5.92650815E-10-3.38867417E-14    2
  7.25938472E3  -2.75108651E1  8.24068673E-1  3.46749909E-2 -2.51786795E-5    3
  9.56781953E-9-1.48085302E-12   1.04203725E4    2.2828307E1                  4
AC3H5OOH          ---ITHH   6O   2C   3    G     298.0    6000.0  1000.0      1
  1.20838649E1  1.47946591E-2 -5.13212591E-6 8.07504999E-10-4.74394983E-14    2
 -1.02184463E4  -3.36434791E1   3.18124993E0  4.35233041E-2 -5.16277353E-5    3
  4.32011427E-8-1.57714983E-11  -7.63521503E3   1.21725683E1                  4
IC3H7O                  H   7O   1C   3    G     300.0    5000.0  1527.0      1
  1.19648494E1  1.42943974E-2 -4.71413211E-6 7.14027066E-10-4.07161162E-14    2
 -1.17519389E4  -3.88860959E1   2.3610841E0  3.45650027E-2 -1.94579631E-5    3
  4.71536901E-9-2.64704937E-13  -8.28791395E3   1.33112436E1                  4
CH2CH2CHO               H   5O   1C   3    G     300.0    5000.0  1437.0      1
  1.00673122E1  1.14971005E-2 -3.90137798E-6 6.03029101E-10-3.48958224E-14    2
 -2.75080876E3  -2.58818404E1   2.55799036E0  2.23391941E-2 -4.89741478E-6    3
 -3.58874384E-9  1.4717503E-12   4.53127696E2   1.67016285E1                  4
C2H5CHCO                H   6O   1C   4    G     300.0    5000.0  1550.0      1
 -2.04040652E2   2.9346688E-1 -1.15884523E-4  1.95253673E-8-1.19030791E-12    2
  8.27380036E4   1.21233386E3  -2.28307043E1  1.70978191E-1 -3.53394379E-4    3
  2.78221616E-7-6.77325074E-11  -1.04125457E4   1.31232921E2                  4
END

TRANSPORT
AR 0 136.5 3.33 0.0 0.0 0.0
N2 1 97.53 3.621 0.0 1.76 4.0
HE 0 10.2 2.576 0.0 0.0 0.0
H2 1 38.0 2.92 0.0 0.79 280.0
H 0 145.0 2.05 0.0 0.0 0.0
O2 1 107.4 3.458 0.0 1.6 3.8
O 0 80.0 2.75 0.0 0.0 0.0
H2O 2 572.4 2.605 1.844 0.0 4.0
OH 1 80.0 2.75 0.0 0.0 0.0
OHV 1 80.0 2.75 0.0 0.0 0.0
H2O2 2 107.4 3.458 0.0 0.0 3.8
HO2 2 107.4 3.458 0.0 0.0 1.0
CO 1 98.1 3.65 0.0 1.95 1.8
CO2 1 244.0 3.763 0.0 2.65 2.1
CH4 2 141.4 3.746 0.0 2.6 13.0
CH3 1 144.0 3.8 0.0 0.0 0.0
CH2 1 144.0 3.8 0.0 0.0 0.0
CH2(S) 1 144.0 3.8 0.0 0.0 0.0
CH 1 80.0 2.75 0.0 0.0 0.0
CHV 1 80.0 2.75 0.0 0.0 0.0
CH3O2H 2 481.8 3.626 0.0 0.0 1.0
CH3O2 2 481.8 3.626 0.0 0.0 1.0
CH3OH 2 481.8 3.626 0.0 0.0 1.0
CH3O 2 417.0 3.69 1.7 0.0 2.0
CH2OH 2 417.0 3.69 1.7 0.0 2.0
CH2O 2 498.0 3.59 0.0 0.0 2.0
HCO 2 498.0 3.59 0.0 0.0 0.0
HCOH 2 498.0 3.59 0.0 0.0 1.0
HO2CHO 2 436.0 3.97 0.0 0.0 2.0
O2CHO 2 436.0 3.97 0.0 0.0 2.0
HOCHO 2 436.0 3.97 0.0 0.0 2.0
OCHO 2 498.0 3.59 0.0 0.0 2.0
C2H6 2 247.5 4.35 0.0 0.0 1.5
C2H5 2 247.5 4.35 0.0 0.0 1.5
C2H4 2 238.4 3.496 0.0 0.0 1.5
C2H3 2 265.3 3.721 0.0 0.0 1.0
CHCHO 2 436.0 3.97 0.0 0.0 2.0
C2H2 1 265.3 3.721 0.0 0.0 2.5
C2H 1 265.3 3.721 0.0 0.0 2.5
CH3CHO 2 436.0 3.97 0.0 0.0 2.0
C2H3OH 2 470.6 4.41 0.0 0.0 1.5
CH2CO 2 436.0 3.97 0.0 0.0 2.0
HCCO 2 150.0 2.5 0.0 0.0 1.0
C3H3 1 324.8 4.29 0.0 0.0 1.0
C3H2 2 209.0 4.1 0.0 0.0 1.0
C3H6OH2-1 2 487.9 4.82 0.0 0.0 1.0
C4H3-I 2 357.0 5.18 0.0 0.0 1.0
C5H6 1 408.0 5.2 0.0 0.0 1.0
HOCH2O 2 470.6 4.41 0.0 0.0 1.5
C2H5O2H 2 470.6 4.41 0.0 0.0 1.5
C2H5O2 2 470.6 4.41 0.0 0.0 1.5
C2H3OO 2 436.0 3.97 0.0 0.0 2.0
H2CC 2 209.0 4.1 0.0 0.0 2.5
C2H5O 2 470.6 4.41 0.0 0.0 1.5
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SC2H4OH 2 470.6 4.41 0.0 0.0 1.5
O2C2H4OH 2 523.2 5.664 1.7 0.0 1.0
C2H4O1-2 2 436.0 3.97 0.0 0.0 2.0
CH3CO 2 436.0 3.97 0.0 0.0 2.0
CH2CHO 2 436.0 3.97 0.0 0.0 2.0
CH3CO3H 2 436.0 3.97 0.0 0.0 2.0
CH3CO3 2 436.0 3.97 0.0 0.0 2.0
CH3CO2 2 436.0 3.97 0.0 0.0 2.0
C3H8 2 303.4 4.81 0.0 0.0 1.0
C3H6OOH2-1 2 435.2 4.662 2.7 0.0 1.0
C3H6OOH2-1O2 2 435.2 4.662 2.7 0.0 1.0
C3H6O1-2 2 403.6 4.968 2.0 0.0 1.0
C3H6 2 307.8 4.14 0.0 0.0 1.0
C3H5-A 2 316.0 4.22 0.0 0.0 1.0
CH3CHCO 2 443.2 4.12 0.0 0.0 1.0
SC3H5OH 2 304.276 5.45 0.0 0.0 1.0
C2H3CHO 2 428.8 4.958 2.9 0.0 1.0
C2H5CHO 2 435.2 4.662 2.7 0.0 1.0
C4H10 2 350.9 5.206 0.0 0.0 1.0
C4H8-1 2 355.0 4.65 0.0 0.0 1.0
C4H71-2 2 357.1 4.72 0.0 0.0 1.0
C5H81-3 2 408.0 5.2 0.0 0.0 1.0
IC3H7 2 303.4 4.81 0.0 0.0 1.0
NC3H7 2 303.4 4.81 0.0 0.0 1.0
NC3H7O2 2 481.5 4.997 1.7 0.0 1.0
IC3H7O2H 2 459.5 5.036 1.7 0.0 1.0
IC3H7O2 2 459.5 5.036 1.7 0.0 1.0
C3H6OOH1-2 2 435.2 4.662 2.7 0.0 1.0
C3H6OOH1-3 2 435.2 4.662 2.7 0.0 1.0
C3H6OOH1-3O2 2 435.2 4.662 2.7 0.0 1.0
C3KET13 2 464.2 5.009 2.6 0.0 1.0
CH3CHCHO 2 387.86 4.687 0.0 0.0 0.0
C3H5O 2 411.0 4.82 0.0 0.0 1.0
AC3H5OOH 2 481.5 4.997 1.7 0.0 1.0
IC3H7O 2 459.5 5.036 1.7 0.0 1.0
CH2CH2CHO 2 424.6 4.82 0.0 0.0 1.0
C2H5CHCO 2 436.95 5.016 0.0 0.0 0.0
END

REACTIONS MOLES CAL/MOLE
H2+M=2H+M    4.577E19 -1.4 1.044E5
   H2/2.5/
   H2O/12.0/
   CO/1.9/
   CO2/3.8/
   HE/0.83/
   CH4/2.0/
   C2H6/3.0/
H2+O=H+OH    5.08E4 2.67 6.292E3
H2+OH=H+H2O    4.38E13 0.0 6.99E3
2O+M=O2+M    6.165E15 -0.5 0.0E0
   H2/2.5/
   H2O/12.0/
   AR/0.83/
   CO/1.9/
   CO2/3.8/
   HE/0.83/
   CH4/2.0/
   C2H6/3.0/
O2+H=O+OH    1.04E14 0.0 1.5286E4
H+OH+M=H2O+M    3.5E22 -2.0 0.0E0
   H2/0.73/
   H2O/3.65/
   CH4/2.0/
   C2H6/3.0/
   AR/0.38/
O+H2O=2OH    6.7E7 1.704 1.49868E4
O+H+M=OH+M    4.714E18 -1.0 0.0E0
   H2/2.5/
   H2O/12.0/
   AR/0.75/
   CO/1.5/
   CO2/2.0/
   HE/0.75/
   CH4/2.0/
   C2H6/3.0/
H+O+M=OHV+M    1.5E13 0.0 5.975E3
   H2/1.0/
   H2O/6.5/
   O2/0.4/
   N2/0.4/
   AR/0.35/
OHV+H2O=OH+H2O    5.93E12 0.5 -8.6E2
OHV+H2=OH+H2    2.95E12 0.5 -4.44E2
OHV+N2=OH+N2    1.08E11 0.5 -1.242E3
OHV+OH=2OH    6.01E12 0.5 -7.64E2
OHV+H=OH+H    1.31E12 0.5 -1.67E2
OHV+AR=OH+AR    1.69E12 0.0 4.135E3
OHV=OH    1.45E6 0.0 0.0E0
OHV+O2=OH+O2    2.1E12 0.5 -4.78E2
OHV+CO2=OH+CO2    2.75E12 0.5 -9.68E2
OHV+CO=OH+CO    3.23E12 0.5 -7.87E2
OHV+CH4=OH+CH4    3.36E12 0.5 -6.35E2
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```
H2O2(+M)=2OH(+M)    2.0E12 0.9 4.8749E4
   H2O/7.65/
   CO2/1.6/
   N2/1.5/
   O2/1.2/
   HE/0.65/
   H2O2/7.7/
   H2/3.7/
   CO/2.8/
   LOW/2.49E24 -2.3E0 4.8749E4/
   TROE/4.3E-1 1.0E-30 1.0E30/
H2O2+H=H2O+OH    2.41E13 0.0 3.97E3
H2O2+H=H2+HO2    2.15E10 1.0 6.0E3
H2O2+O=OH+HO2    9.55E6 2.0 3.97E3
H2O2+OH=H2O+HO2    1.74E12 0.0 3.18E2
   DUP
H2O2+OH=H2O+HO2    7.59E13 0.0 7.269E3
   DUP
HO2+H=2OH    7.079E13 0.0 2.95E2
HO2+H=H2+O2    1.1402E10 1.0827 5.5378E2
HO2+O=OH+O2    3.25E13 0.0 0.0E0
HO2+OH=H2O+O2    2.456E13 0.0 -4.97E2
2HO2=H2O2+O2    1.0E14 0.0 1.1040883E4
   DUP
2HO2=H2O2+O2    1.9E11 0.0 -1.4089248E3
   DUP
H+O2(+M)=HO2(+M)    4.65E12 0.44 0.0E0
   H2/1.3/
   CO/1.9/
   CO2/3.8/
   HE/0.64/
   H2O/10.0/
   AR/0.5/
   CH4/2.0/
   C2H6/3.0/
   LOW/1.737E19 -1.23E0 0.0E0/
   TROE/6.7E-1 1.0E-30 1.0E30 1.0E30/
CO+O(+M)=CO2(+M)    1.362E10 0.0 2.384E3
   H2/2.0/
   H2O/12.0/
   CO/1.75/
   CO2/3.6/
   AR/0.7/
   HE/0.7/
   LOW/1.173E24 -2.79E0 4.191E3/
CO+OH=CO2+H    7.015E4 2.053 -3.557E2
   DUP
CO+OH=CO2+H    5.757E12 -0.664 3.318E2
   DUP
CO+HO2=CO2+OH    1.57E5 2.18 1.794E4
CO+O2=CO2+O    1.119E12 0.0 4.77E4
H+CO2=OCHO    7.5E13 0.0 2.9E4
CH3+H(+M)=CH4(+M)    1.27E16 -0.63 3.83E2
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/2.477E33 -4.76E0 2.44E3/
   TROE/7.83E-1 7.4E1 2.941E3 6.964E3/
CH4+H=CH3+H2    6.14E5 2.5 9.587E3
CH4+O=CH3+OH    1.02E9 1.5 8.6E3
CH4+OH=CH3+H2O    5.83E4 2.6 2.19E3
CH4+HO2=CH3+H2O2    1.13E1 3.74 2.101E4
CH4+CH3O2=CH3+CH3O2H    9.6E-1 3.77 1.781E4
CH3+HO2=CH4+O2    1.16E5 2.23 -3.022E3
CH4+CH2=2CH3    2.46E6 2.0 8.27E3
CH2(S)+N2=CH2+N2    1.5E13 0.0 6.0E2
CH2(S)+AR=CH2+AR    9.0E12 0.0 6.0E2
CH2(S)+H2O=CH2+H2O    3.0E13 0.0 0.0E0
CH2(S)+CO=CH2+CO    9.0E12 0.0 0.0E0
CH2(S)+CO2=CH2+CO2    7.0E12 0.0 0.0E0
CH2(S)+O2=>H+OH+CO    2.8E13 0.0 0.0E0
CH2(S)+O2=CO+H2O    1.2E13 0.0 0.0E0
CH2(S)+O=CO+H2    1.5E13 0.0 0.0E0
CH2(S)+O=HCO+H    1.5E13 0.0 0.0E0
CH2(S)+H2=CH3+H    7.0E13 0.0 0.0E0
CH2(S)+H=CH+H2    3.0E13 0.0 0.0E0
CH2(S)+OH=CH2O+H    3.0E13 0.0 0.0E0
CH2(S)+CO2=CH2O+CO    1.4E13 0.0 0.0E0
CH2+H(+M)=CH3(+M)    2.5E16 -0.8 0.0E0
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/3.2E27 -3.14E0 1.23E3/
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   TROE/6.8E-1 7.8E1 1.995E3 5.59E3/
CH2+O2=HCO+OH    1.06E13 0.0 1.5E3
CH2+O2=>CO2+2H    2.64E12 0.0 1.5E3
CH2+O=>CO+2H    5.0E13 0.0 0.0E0
CH2+H=CH+H2    3.0E13 0.0 0.0E0
CH2+OH=CH+H2O    1.13E7 2.0 3.0E3
CHV+AR=CH+AR    4.0E11 0.5 0.0E0
CHV+H2O=CH+H2O    5.3E13 0.0 0.0E0
CHV+CO=CH+CO    2.44E12 0.5 0.0E0
CHV+CO2=CH+CO2    2.41E-1 4.3 -1.694E3
CHV+O2=CH+O2    2.48E6 2.14 -1.72E3
CHV+H2=CH+H2    1.47E14 0.0 1.361E3
CHV+CH4=CH+CH4    1.73E13 0.0 1.67E2
CHV=CH    1.86E6 0.0 0.0E0
CHV+N2=CH+N2    3.03E2 3.4 -3.81E2
CH+O2=CO+OHV    4.04E13 0.0 0.0E0
CH+O2=HCO+O    3.3E13 0.0 0.0E0
CH+O=CO+H    5.7E13 0.0 0.0E0
CH+OH=HCO+H    3.0E13 0.0 0.0E0
CH+H2O=H+CH2O    1.774E16 -1.22 2.38E1
CH+CO2=HCO+CO    1.7E12 0.0 6.85E2
CH3+O2(+M)=CH3O2(+M)    7.812E9 0.9 0.0E0
   LOW/6.85E24 -3.0E0 0.0E0/
   TROE/6.0E-1 1.0E3 7.0E1 1.7E3/
CH3+O2=CH3O+O    7.546E12 0.0 2.832E4
CH3+O2=CH2O+OH    2.641E0 3.283 8.105E3
CH3+O=CH2O+H    5.54E13 0.05 -1.36E2
CH3+OH=CH2(S)+H2O    4.936E14 -0.669 -4.458E2
   PLOG/1.0E-2 4.936E14 -6.69E-1 -4.458E2/
   PLOG/1.0E-1 1.207E15 -7.78E-1 -1.756E2/
   PLOG/1.0E0 5.282E17 -1.518E0 1.772E3/
   PLOG/1.0E1 4.788E23 -3.155E0 7.003E3/
   PLOG/1.0E2 8.433E19 -1.962E0 8.244E3/
CH3+OH=CH2O+H2    3.502E5 1.441 -3.244E3
   PLOG/1.0E-2 3.502E5 1.441E0 -3.244E3/
   PLOG/1.0E-1 8.854E5 1.327E0 -2.975E3/
   PLOG/1.0E0 1.65E7 9.73E-1 -2.01E3/
   PLOG/1.0E1 5.374E9 2.87E-1 2.8E2/
   PLOG/1.0E2 9.494E18 -2.199E0 9.769E3/
CH3+OH=CH2OH+H    1.621E10 0.965 3.21E3
   PLOG/1.0E-2 1.621E10 9.65E-1 3.214E3/
   PLOG/1.0E-1 1.807E10 9.5E-1 3.247E3/
   PLOG/1.0E0 4.686E10 8.33E-1 3.566E3/
   PLOG/1.0E1 1.525E13 1.34E-1 5.641E3/
   PLOG/1.0E2 3.59E14 -1.86E-1 8.601E3/
CH3+OH=H+CH3O    1.186E9 1.016 1.194E4
   PLOG/1.0E-2 1.186E9 1.016E0 1.194E4/
   PLOG/1.0E-1 1.188E9 1.016E0 1.194E4/
   PLOG/1.0E0 1.23E9 1.011E0 1.195E4/
   PLOG/1.0E1 1.798E9 9.65E-1 1.206E4/
   PLOG/1.0E2 5.242E10 5.51E-1 1.307E4/
CH3+OH=HCOH+H2    8.674E8 0.787 -3.046E3
   PLOG/1.0E-2 8.674E8 7.87E-1 -3.046E3/
   PLOG/1.0E-1 3.115E9 6.3E-1 -2.669E3/
   PLOG/1.0E0 1.557E11 1.56E-1 -1.368E3/
   PLOG/1.0E1 1.704E21 -2.641E0 6.412E3/
   PLOG/1.0E2 7.25E20 -2.402E0 9.639E3/
CH3+OH=CH2+H2O    4.293E4 2.568 3.9978E3
CH3+HO2=CH3O+OH    1.0E12 0.269 -6.875E2
CH3O2+O=CH3O+O2    3.6E13 0.0 0.0E0
CH3O2+H=CH3O+OH    9.6E13 0.0 0.0E0
CH3O2+OH=CH3OH+O2    6.0E13 0.0 0.0E0
CH3O2+HO2=CH3O2H+O2    2.47E11 0.0 -1.57E3
CH3O2+H2O2=CH3O2H+HO2    2.41E12 0.0 9.936E3
CH3O2+CH3=2CH3O    5.08E12 0.0 -1.411E3
2CH3O2=>CH2O+CH3OH+O2    3.11E14 -1.61 -1.051E3
2CH3O2=>O2+2CH3O    1.4E16 -1.61 1.86E3
H2+CH3O2=H+CH3O2H    1.5E14 0.0 2.603E4
CH3O2H=CH3O+OH    6.31E14 0.0 4.23E4
CH3OH(+M)=CH3+OH(+M)    2.084E18 -0.615 9.25406E4
   LOW/1.5E43 -6.995E0 9.79922E4/
   TROE/-4.748E-1 3.558E4 1.116E3 9.023E3/
CH3OH(+M)=CH2(S)+H2O(+M)    3.121E18 -1.017 9.1712E4
   LOW/1.43E47 -8.227E0 9.94171E4/
   TROE/2.545E0 3.29E3 4.732E4 4.711E4/
CH3OH(+M)=CH2OH+H(+M)    7.896E-3 5.038 8.44674E4
   LOW/3.39E42 -7.244E0 1.052303E5/
   TROE/-7.391E1 3.705E4 4.15E4 5.22E3/
CH3OH+H=CH3O+H2    1.99E5 2.56 1.03E4
CH3OH+H=CH2OH+H2    3.07E5 2.55 5.44E3
CH3OH+O=CH3O+OH    3.88E4 2.5 3.08E3
CH3OH+O=CH2OH+OH    3.88E5 2.5 3.08E3
CH3OH+OH=CH3O+H2O    1.5E2 3.03 -7.63E2
CH3OH+OH=CH2OH+H2O    3.08E4 2.65 -8.067E2
CH3OH+O2=CH3O+HO2    3.58E4 2.27 4.27645E4
CH3OH+O2=CH2OH+HO2    3.58E5 2.27 4.27645E4
CH3OH+HO2=CH3O+H2O2    1.22E12 0.0 2.00707E4
CH3OH+HO2=CH2OH+H2O2    3.26E13 0.0 1.87822E4
CH3OH+CH3=CH2OH+CH4    2.13E-1 3.953 7.0551E3
CH3OH+CH3=CH3O+CH4    3.22E3 2.425 8.5795E3
CH3OH+HCO=CH2OH+CH2O    9.63E3 2.9 1.311E4
CH3OH+CH3O=CH2OH+CH3OH    3.0E11 0.0 4.074E3
CH3OH+CH3O2=CH2OH+CH3O2H    1.81E12 0.0 1.371E4
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CH2OH+O2=CH2O+HO2    1.51E15 -1.0 0.0E0
   DUP
CH2OH+O2=CH2O+HO2    2.41E14 0.0 5.017E3
   DUP
CH2OH+H=CH2O+H2    6.0E12 0.0 0.0E0
CH2OH+HO2=CH2O+H2O2    1.2E13 0.0 0.0E0
CH2OH+HCO=2CH2O    1.8E14 0.0 0.0E0
CH2OH+HCO=CH3OH+CO    1.0E13 0.0 0.0E0
CH2OH+CH3O=CH2O+CH3OH    2.4E13 0.0 0.0E0
CH2OH+OH=H2O+CH2O    2.4E13 0.0 0.0E0
CH2OH+O=OH+CH2O    4.2E13 0.0 0.0E0
2CH2OH=CH2O+CH3OH    3.0E12 0.0 0.0E0
CH3O+O2=CH2O+HO2    4.38E-19 9.5 -5.501E3
CH3O+H=CH2O+H2    2.0E13 0.0 0.0E0
CH3O+HO2=CH2O+H2O2    3.01E11 0.0 0.0E0
CH3O+CH3=CH2O+CH4    1.2E13 0.0 0.0E0
2CH3O=CH3OH+CH2O    6.03E13 0.0 0.0E0
HCOH+O2=>CO2+H+OH    5.0E12 0.0 0.0E0
HCOH+O2=CO2+H2O    3.0E13 0.0 0.0E0
HCOH+O=>CO2+2H    5.0E13 0.0 0.0E0
HCOH+O=>CO+OH+H    3.0E13 0.0 0.0E0
HCOH+H=CH2O+H    2.0E14 0.0 0.0E0
HCOH+OH=HCO+H2O    2.0E13 0.0 0.0E0
HCO+H(+M)=CH2O(+M)    1.09E12 0.48 -2.6E2
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/1.35E24 -2.57E0 1.425E3/
   TROE/7.824E-1 2.71E2 2.755E3 6.57E3/
CO+H2(+M)=CH2O(+M)    4.3E7 1.5 7.96E4
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/5.07E27 -3.42E0 8.4348E4/
   TROE/9.32E-1 1.97E2 1.54E3 1.03E4/
CH2O+O2=HCO+HO2    8.07E15 0.0 5.342E4
CH2O+O=HCO+OH    6.26E9 1.15 2.26E3
CH2O+H=HCO+H2    5.74E7 1.9 2.74E3
CH2O+OH=HCO+H2O    7.82E7 1.63 -1.055E3
CH2O+HO2=HCO+H2O2    1.88E4 2.7 1.152E4
CH2O+CH3=HCO+CH4    3.83E1 3.36 4.312E3
CH2O+O2CHO=HCO+HO2CHO    1.99E12 0.0 1.166E4
CH2O+OCHO=HCO+HOCHO    5.6E12 0.0 1.36E4
CH2O+CH3O=HCO+CH3OH    6.62E11 0.0 2.294E3
CH2O+CH3O2=HCO+CH3O2H    1.99E12 0.0 1.166E4
HCO+M=H+CO+M    5.7E11 0.66 1.487E4
   H2/2.0/
   H2O/6.0/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
HCO+O2=CO+HO2    7.58E12 0.0 4.1E2
HCO+O=CO+OH    3.02E13 0.0 0.0E0
HCO+H=CO+H2    7.34E13 0.0 0.0E0
HCO+OH=CO+H2O    3.011E13 0.0 0.0E0
HCO+CH3=CO+CH4    2.65E13 0.0 0.0E0
2HCO=CO+CH2O    1.8E13 0.0 0.0E0
HCO+O=CO2+H    3.0E13 0.0 0.0E0
HCO+HO2=>CO2+H+OH    3.0E13 0.0 0.0E0
2HCO=>H2+2CO    3.0E12 0.0 0.0E0
CH2O+H(+M)=CH2OH(+M)    5.4E11 0.454 3.6E3
   H2/2.0/
   H2O/6.0/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   LOW/1.27E32 -4.82E0 6.53E3/
   TROE/7.187E-1 1.03E2 1.291E3 4.16E3/
CH3O(+M)=CH2O+H(+M)    6.8E13 0.0 2.617E4
   H2/2.0/
   H2O/6.0/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   LOW/1.867E25 -3.0E0 2.4307E4/
   TROE/9.0E-1 2.5E3 1.3E3 1.0E99/
HCO+O2=O2CHO    1.2E11 0.0 -1.1E3
HOCHO=CO+H2O    2.45E12 0.0 6.047E4
HOCHO=CO2+H2    2.95E9 0.0 4.852E4
OCHO+HO2=HOCHO+O2    3.5E10 0.0 -3.275E3
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OCHO+H2O2=HOCHO+HO2    2.4E12 0.0 1.0E4
HOCHO+H=>H2+CO2+H    4.24E6 2.1 4.868E3
HOCHO+H=>H2+CO+OH    6.03E13 -0.35 2.988E3
HOCHO+O=>CO+2OH    1.77E18 -1.9 2.975E3
HOCHO+OH=>H2O+CO2+H    2.62E6 2.06 9.16E2
HOCHO+OH=>H2O+CO+OH    1.85E7 1.51 -9.62E2
HOCHO+CH3=>CH4+CO+OH    3.9E-7 5.8 2.2E3
HOCHO+HO2=>H2O2+CO+OH    1.0E12 0.0 1.192E4
OCHO+OH=HO2CHO    2.0E13 0.0 0.0E0
2CH3(+M)=C2H6(+M)    2.277E15 -0.69 1.749E2
   H2O/5.0/
   CO/2.0/
   CO2/3.0/
   LOW/8.054E31 -3.75E0 9.816E2/
   TROE/0.0E0 5.7E2 1.0E30 1.0E30/
C2H5+H(+M)=C2H6(+M)    5.21E17 -0.99 1.58E3
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/1.99E41 -7.08E0 6.685E3/
   TROE/8.42E-1 1.25E2 2.219E3 6.882E3/
2CH3=H+C2H5    4.74E12 0.105 1.06643E4
   PLOG/1.0E-2 4.74E12 1.05E-1 1.06643E4/
   PLOG/1.0E-1 2.57E13 -9.6E-2 1.14061E4/
   PLOG/1.0E0 3.1E14 -3.62E-1 1.33725E4/
   PLOG/1.0E1 2.15E10 8.85E-1 1.35325E4/
   PLOG/1.0E2 1.032E2 3.23E0 1.12361E4/
C2H6+O2=C2H5+HO2    6.03E13 0.0 5.187E4
C2H6+O=C2H5+OH    3.55E6 2.4 5.83E3
C2H6+H=C2H5+H2    1.15E8 1.9 7.53E3
C2H6+OH=C2H5+H2O    1.48E7 1.9 9.5E2
C2H6+HO2=C2H5+H2O2    3.46E1 3.61 1.692E4
C2H6+CH=C2H5+CH2    1.1E14 0.0 -2.6E2
C2H6+CH2(S)=C2H5+CH3    1.2E14 0.0 0.0E0
C2H6+CH3=C2H5+CH4    5.55E-4 4.72 3.231E3
C2H6+CH3O=C2H5+CH3OH    2.41E11 0.0 7.09E3
C2H6+CH3O2=C2H5+CH3O2H    1.94E1 3.64 1.71E4
C2H4+H(+M)=C2H5(+M)    9.569E8 1.463 1.355E3
   H2/2.0/
   H2O/6.0/
   CH4/2.0/
   CO/1.5/
   CO2/2.0/
   C2H6/3.0/
   AR/0.7/
   LOW/1.419E39 -6.642E0 5.769E3/
   TROE/-5.69E-1 2.99E2 -9.147E3 1.524E2/
C2H5+H=C2H4+H2    2.0E12 0.0 0.0E0
2C2H4=C2H5+C2H3    4.82E14 0.0 7.153E4
C2H5+CH3=CH4+C2H4    1.18E4 2.45 -2.921E3
C2H5+O=CH3CHO+H    1.1E14 0.0 0.0E0
C2H5+O2=C2H4+HO2    2.094E9 0.49 -3.914E2
   PLOG/4.0E-2 2.094E9 4.9E-1 -3.914E2/
   PLOG/1.0E0 1.843E7 1.13E0 -7.206E2/
   PLOG/1.0E1 7.561E14 -1.01E0 4.749E3/
C2H5+O2=CH3CHO+OH    4.908E-6 4.76 2.543E2
   PLOG/4.0E-2 4.908E-6 4.76E0 2.543E2/
   PLOG/1.0E0 6.803E-2 3.57E0 2.643E3/
   PLOG/1.0E1 8.265E2 2.41E0 5.285E3/
C2H3+H(+M)=C2H4(+M)    6.08E12 0.27 2.8E2
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/1.4E30 -3.86E0 3.32E3/
   TROE/7.82E-1 2.075E2 2.663E3 6.095E3/
C2H4+O2=C2H3+HO2    4.22E13 0.0 5.76231E4
C2H4+H=C2H3+H2    5.07E7 1.93 1.295E4
C2H4+OH=C2H3+H2O    2.23E4 2.745 2.2155E3
C2H4+CH3O=C2H3+CH3OH    1.2E11 0.0 6.75E3
C2H4+CH3O2=C2H3+CH3O2H    8.59E0 3.754 2.7132E4
C2H4+CH3=C2H3+CH4    9.76E2 2.947 1.5148E4
   DUP
C2H4+CH3=C2H3+CH4    8.13E-5 4.417 8.8358E3
   DUP
C2H4+O=CH3+HCO    7.453E6 1.88 1.83E2
CH+CH4=C2H4+H    6.0E13 0.0 0.0E0
CH2(S)+CH3=C2H4+H    2.0E13 0.0 0.0E0
C2H4+OH=CH3+CH2O    5.35E0 2.92 -1.7327E3
   PLOG/1.0E-2 5.35E0 2.92E0 -1.7327E3/
   PLOG/2.5E-2 3.19E1 2.71E0 -1.1723E3/
   PLOG/1.0E-1 5.55E2 2.36E0 -1.808E2/
   PLOG/1.0E0 1.78E5 1.68E0 2.0605E3/
   PLOG/1.0E1 2.37E9 5.6E-1 6.0067E3/
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   PLOG/1.0E2 2.76E13 -5.0E-1 1.14551E4/
C2H4+OH=CH3CHO+H    2.37E-7 5.3 -2.0506E3
   PLOG/1.0E-2 2.37E-7 5.3E0 -2.0506E3/
   PLOG/2.5E-2 8.73E-5 4.57E0 -6.18E2/
   PLOG/1.0E-1 4.03E-1 3.54E0 1.8817E3/
   PLOG/1.0E0 2.38E-2 3.91E0 1.7227E3/
   PLOG/1.0E1 8.25E8 1.01E0 1.05073E4/
   PLOG/1.0E2 6.8E9 8.1E-1 1.38673E4/
C2H4+OH=C2H3OH+H    1.04E4 2.6 4.121E3
   PLOG/1.0E-2 1.04E4 2.6E0 4.121E3/
   PLOG/2.5E-2 1.07E4 2.6E0 4.129E3/
   PLOG/1.0E-1 1.52E4 2.56E0 4.2383E3/
   PLOG/1.0E0 3.19E5 2.19E0 5.2556E3/
   PLOG/1.0E1 1.94E8 1.43E0 7.8288E3/
   PLOG/1.0E2 8.55E10 7.5E-1 1.14908E4/
C2H2+H(+M)=C2H3(+M)    1.71E10 1.266 2.709E3
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/6.346E31 -4.664E0 3.78E3/
   TROE/7.88E-1 -1.02E4 1.0E-30/
C2H3+O2=CHCHO+OH    2.84E14 -0.8 7.232E3
   DUP
   PLOG/1.0E-2 3.91E11 -1.1E-1 2.131E3/
   PLOG/1.0E-1 1.13E9 5.5E-1 4.6E1/
   PLOG/3.16E-1 8.46E8 5.6E-1 7.0E-1/
   PLOG/1.0E0 2.75E14 -1.83E0 4.6E0/
   PLOG/3.16E0 2.58E20 -2.84E0 7.53E3/
   PLOG/1.0E1 9.18E14 -2.26E0 -4.0E-1/
   PLOG/3.16E1 6.11E25 -4.21E0 1.305E4/
   PLOG/1.0E2 1.65E30 -5.35E0 1.843E4/
C2H3+O2=CHCHO+OH    2.84E14 -0.8 7.232E3
   DUP
   PLOG/1.0E-2 9.91E11 -6.6E-1 -6.0E-1/
   PLOG/1.0E-1 6.94E14 -1.16E0 4.542E3/
   PLOG/3.16E-1 2.79E13 -7.2E-1 3.479E3/
   PLOG/1.0E0 4.99E11 -1.4E-1 1.995E3/
   PLOG/3.16E0 2.35E10 2.3E-1 1.573E3/
   PLOG/1.0E1 1.7E14 -8.2E-1 4.45E3/
   PLOG/3.16E1 1.42E11 5.0E-2 3.774E3/
   PLOG/1.0E2 3.17E11 -2.0E-2 5.338E3/
C2H3+O2=C2H2+HO2    6.49E6 1.5 5.218E3
   DUP
   PLOG/1.0E-2 1.08E7 1.28E0 3.322E3/
   PLOG/1.0E-1 7.75E6 1.33E0 3.216E3/
   PLOG/3.16E-1 1.21E7 1.27E0 3.311E3/
   PLOG/1.0E0 2.15E7 1.19E0 3.367E3/
   PLOG/3.16E0 1.13E8 1.0E0 3.695E3/
   PLOG/1.0E1 1.31E11 1.2E-1 5.872E3/
   PLOG/3.16E1 1.19E9 8.2E-1 5.617E3/
   PLOG/1.0E2 1.06E17 -1.45E0 1.223E4/
C2H3+O2=C2H2+HO2    6.49E6 1.5 5.218E3
   DUP
   PLOG/1.0E-2 4.76E1 2.75E0 -7.964E2/
   PLOG/1.0E-1 5.16E1 2.73E0 -7.683E2/
   PLOG/3.16E-1 5.55E1 2.73E0 -6.585E2/
   PLOG/1.0E0 4.6E1 2.76E0 -4.928E2/
   PLOG/3.16E0 3.75E0 3.07E0 -6.01E2/
   PLOG/1.0E1 5.48E0 3.07E0 8.57E1/
   PLOG/3.16E1 4.47E8 0.0E0 9.55E2/
   PLOG/1.0E2 2.02E1 2.94E0 1.847E3/
C2H3+O2=CH2CO+OH    1.17E3 2.43 7.074E3
   DUP
   PLOG/1.0E-2 8.66E2 2.41E0 6.061E3/
   PLOG/1.0E-1 8.91E2 2.41E0 6.078E3/
   PLOG/3.16E-1 9.43E2 2.4E0 6.112E3/
   PLOG/1.0E0 1.06E3 2.39E0 6.18E3/
   PLOG/3.16E0 1.09E3 2.38E0 6.179E3/
   PLOG/1.0E1 1.39E3 2.36E0 6.074E3/
   PLOG/3.16E1 2.49E6 1.42E0 8.48E3/
   PLOG/1.0E2 1.66E10 3.6E-1 1.201E4/
C2H3+O2=CH2CO+OH    1.17E3 2.43 7.074E3
   DUP
   PLOG/1.0E-2 1.82E-1 3.12E0 1.331E3/
   PLOG/1.0E-1 2.07E-1 3.11E0 1.383E3/
   PLOG/3.16E-1 2.71E-1 3.08E0 1.496E3/
   PLOG/1.0E0 5.26E-1 3.01E0 1.777E3/
   PLOG/3.16E0 1.37E0 2.9E0 2.225E3/
   PLOG/1.0E1 4.19E-1 2.93E0 2.052E3/
   PLOG/3.16E1 1.19E-4 4.21E0 2.043E3/
   PLOG/1.0E2 1.3E-3 3.97E0 3.414E3/
C2H3+O2=CH2O+HCO    1.16E16 -1.13 3.791E3
   DUP
   PLOG/1.0E-2 2.49E36 -7.6E0 1.264E4/
   PLOG/1.0E-1 2.43E36 -7.6E0 1.261E4/
   PLOG/3.16E-1 1.95E36 -7.57E0 1.249E4/
   PLOG/1.0E0 2.73E35 -7.32E0 1.182E4/
   PLOG/3.16E0 1.43E36 -7.47E0 1.246E4/
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   PLOG/1.0E1 5.18E35 -7.2E0 1.343E4/
   PLOG/3.16E1 3.19E20 -2.57E0 5.578E3/
   PLOG/1.0E2 2.73E33 -6.28E0 1.6E4/
C2H3+O2=CH2O+HCO    1.16E16 -1.13 3.791E3
   DUP
   PLOG/1.0E-2 4.54E15 -1.28E0 5.153E2/
   PLOG/1.0E-1 4.59E15 -1.28E0 5.13E2/
   PLOG/3.16E-1 4.81E15 -1.29E0 5.206E2/
   PLOG/1.0E0 6.08E15 -1.31E0 6.457E2/
   PLOG/3.16E0 9.45E15 -1.36E0 1.066E3/
   PLOG/1.0E1 2.56E15 -1.18E0 1.429E3/
   PLOG/3.16E1 1.03E69 -1.923E1 1.476E4/
   PLOG/1.0E2 4.21E10 1.9E-1 8.306E2/
C2H3+O2=>CH2O+H+CO    1.16E16 -1.13 3.791E3
   DUP
   PLOG/1.0E-2 5.82E36 -7.6E0 1.264E4/
   PLOG/1.0E-1 5.66E36 -7.6E0 1.261E4/
   PLOG/3.16E-1 4.55E36 -7.57E0 1.249E4/
   PLOG/1.0E0 6.36E35 -7.32E0 1.182E4/
   PLOG/3.16E0 3.35E36 -7.47E0 1.246E4/
   PLOG/1.0E1 1.21E36 -7.2E0 1.343E4/
   PLOG/3.16E1 7.43E20 -2.57E0 5.578E3/
   PLOG/1.0E2 6.36E33 -6.28E0 1.6E4/
C2H3+O2=>CH2O+H+CO    1.16E16 -1.13 3.791E3
   DUP
   PLOG/1.0E-2 1.06E16 -1.28E0 5.153E2/
   PLOG/1.0E-1 1.07E16 -1.28E0 5.13E2/
   PLOG/3.16E-1 1.13E16 -1.29E0 5.206E2/
   PLOG/1.0E0 1.42E16 -1.31E0 6.457E2/
   PLOG/3.16E0 2.2E16 -1.36E0 1.066E3/
   PLOG/1.0E1 5.98E15 -1.18E0 1.429E3/
   PLOG/3.16E1 2.39E69 -1.923E1 1.476E4/
   PLOG/1.0E2 9.81E10 1.9E-1 8.306E2/
C2H3+O2=CO+CH3O    3.09E13 -0.89 3.682E3
   DUP
   PLOG/1.0E-2 8.19E18 -2.66E0 3.201E3/
   PLOG/1.0E-1 4.06E14 -1.32E0 8.858E2/
   PLOG/3.16E-1 4.34E14 -1.33E0 9.006E2/
   PLOG/1.0E0 1.03E11 -3.3E-1 -7.478E2/
   PLOG/3.16E0 1.89E12 -3.0E0 -8.995E3/
   PLOG/1.0E1 1.93E24 -5.63E0 1.8E0/
   PLOG/3.16E1 1.1E18 -2.22E0 5.178E3/
   PLOG/1.0E2 5.79E32 -6.45E0 1.681E4/
C2H3+O2=CO+CH3O    3.09E13 -0.89 3.682E3
   DUP
   PLOG/1.0E-2 1.29E9 1.8E-1 -1.717E3/
   PLOG/1.0E-1 5.99E11 -2.93E0 -9.564E3/
   PLOG/3.16E-1 2.91E11 -2.93E0 -1.012E4/
   PLOG/1.0E0 5.77E21 -3.54E0 4.772E3/
   PLOG/3.16E0 4.99E15 -1.62E0 1.849E3/
   PLOG/1.0E1 9.33E16 -1.96E0 3.324E3/
   PLOG/3.16E1 1.02E72 -2.069E1 1.586E4/
   PLOG/1.0E2 1.1E9 3.1E-1 1.024E3/
C2H3+O2=CO2+CH3    6.16E13 -1.05 3.743E3
   DUP
   PLOG/1.0E-2 2.37E35 -7.76E0 1.263E4/
   PLOG/1.0E-1 1.73E35 -7.72E0 1.252E4/
   PLOG/3.16E-1 4.47E34 -7.55E0 1.214E4/
   PLOG/1.0E0 7.25E31 -6.7E0 1.044E4/
   PLOG/3.16E0 3.63E35 -7.75E0 1.283E4/
   PLOG/1.0E1 2.09E35 -7.53E0 1.405E4/
   PLOG/3.16E1 3.84E18 -2.44E0 5.408E3/
   PLOG/1.0E2 1.21E32 -6.32E0 1.619E4/
C2H3+O2=CO2+CH3    6.16E13 -1.05 3.743E3
   DUP
   PLOG/1.0E-2 6.27E13 -1.16E0 4.063E2/
   PLOG/1.0E-1 6.24E13 -1.16E0 4.014E2/
   PLOG/3.16E-1 6.12E13 -1.16E0 3.97E2/
   PLOG/1.0E0 5.32E13 -1.14E0 4.467E2/
   PLOG/3.16E0 1.45E14 -1.26E0 9.877E2/
   PLOG/1.0E1 5.02E13 -1.11E0 1.409E3/
   PLOG/3.16E1 1.4E70 -2.011E1 1.543E4/
   PLOG/1.0E2 9.21E8 2.5E-1 8.553E2/
C2H3+H=C2H2+H2    1.7E14 0.0 0.0E0
C2H3+OH=C2H2+H2O    3.011E13 0.0 0.0E0
C2H3+CH3=C2H2+CH4    3.92E11 0.0 0.0E0
2C2H3=C2H2+C2H4    9.6E11 0.0 0.0E0
C2H+H(+M)=C2H2(+M)    1.0E17 0.0 0.0E0
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/3.75E33 -4.8E0 1.9E3/
   TROE/6.46E-1 1.32E2 1.315E3 5.566E3/
C2H+H2=H+C2H2    4.9E5 2.5 5.6E2
C2H+O2=CO2+CHV    2.17E10 0.0 0.0E0
C2H+O2=HCO+CO    5.0E13 0.0 1.5E3
C2H+O=CO+CHV    6.2E12 0.0 0.0E0
C2H+O=CO+CH    5.0E13 0.0 0.0E0
```

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C2H+OH=H+HCCO    2.0E13 0.0 0.0E0
C2H2+O=CH2+CO    7.395E8 1.28 2.472E3
C2H2+O=HCCO+H    2.958E9 1.28 2.472E3
C2H2+HO2=CH2CO+OH    6.03E9 0.0 7.949E3
C2H2+CH2=C3H3+H    1.2E13 0.0 6.62E3
C2H2+CH2(S)=C3H3+H    2.0E13 0.0 0.0E0
C2H2+HCO=C2H3+CO    1.0E7 2.0 6.0E3
C2H2+HCCO=C3H3+CO    1.0E11 0.0 3.0E3
C2H2+OH=C2H+H2O    2.632E6 2.14 1.706E4
C2H2+OH=CH2CO+H    1.578E3 2.56 -8.445E2
   PLOG/1.0E-2 1.578E3 2.56E0 -8.445E2/
   PLOG/2.5E-2 1.518E4 2.28E0 -2.921E2/
   PLOG/1.0E-1 3.017E5 1.92E0 5.981E2/
   PLOG/1.0E0 7.528E6 1.55E0 2.106E3/
   PLOG/1.0E1 5.101E6 1.65E0 3.4E3/
   PLOG/1.0E2 1.457E4 2.45E0 4.477E3/
C2H2+OH=CH3+CO    4.757E5 1.68 -3.298E2
   PLOG/1.0E-2 4.757E5 1.68E0 -3.298E2/
   PLOG/2.5E-2 4.372E6 1.4E0 2.265E2/
   PLOG/1.0E-1 7.648E7 1.05E0 1.115E3/
   PLOG/1.0E0 1.277E9 7.3E-1 2.579E3/
   PLOG/1.0E1 4.312E8 9.2E-1 3.736E3/
   PLOG/1.0E2 8.25E5 1.77E0 4.697E3/
CH3CHO(+M)=CH3+HCO(+M)    2.45E22 -1.74 8.6355E4
   LOW/1.03E59 -1.13E1 9.59125E4/
   TROE/2.49E-3 7.181E2 6.089E0 3.78E3/
CH3CHO(+M)=CH4+CO(+M)    2.72E21 -1.74 8.6355E4
   LOW/1.144E58 -1.13E1 9.59125E4/
   TROE/2.49E-3 7.181E2 6.089E0 3.78E3/
CH3CHO+OH=CH3+HOCHO    3.0E15 -1.076 0.0E0
C2H3OH=CH3CHO    7.42E46 -10.56 6.742E4
   PLOG/1.0E-1 7.42E46 -1.056E1 6.742E4/
   PLOG/1.0E0 4.42E42 -9.09E0 6.70692E4/
   PLOG/1.0E2 2.9E27 -4.35E0 6.16129E4/
C2H3OH+HO2=CH3CHO+HO2    1.49E5 1.67 6.81E3
CH2+CO(+M)=CH2CO(+M)    8.1E11 0.0 0.0E0
   H2/2.0/
   H2O/6.0/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   C2H6/3.0/
   HE/0.7/
   LOW/2.69E33 -5.11E0 7.095E3/
   TROE/5.907E-1 2.75E2 1.226E3 5.185E3/
CH2CO+H=HCCO+H2    1.401E15 -0.171 8.7832E3
CH2CO+O=HCCO+OH    1.0E13 0.0 8.0E3
CH2CO+OH=HCCO+H2O    1.0E13 0.0 2.0E3
CH2CO+H=CH3+CO    7.704E13 -0.171 4.1832E3
CH+CH2O=H+CH2CO    9.46E13 0.0 -5.15E2
CH2CO+O=CH2+CO2    1.75E12 0.0 1.35E3
CH2CO+OH=CH2OH+CO    2.0E12 0.0 -1.01E3
CH2CO+CH2(S)=C2H4+CO    1.6E14 0.0 0.0E0
CH2CO+CH3=C2H5+CO    4.769E4 2.312 9.468E3
CH+CO+M=HCCO+M    7.57E22 -1.9 0.0E0
HCCO+OH=>H2+2CO    1.0E14 0.0 0.0E0
HCCO+O=>H+2CO    8.0E13 0.0 0.0E0
HCCO+CH=CO+C2H2    5.0E13 0.0 0.0E0
HCCO+H=CH2(S)+CO    1.0E14 0.0 0.0E0
HCCO+O2=>OH+2CO    1.91E11 -0.02 1.02E3
HCCO+O2=>CO2+CO+H    4.78E12 -0.142 1.15E3
CH3O+HCO=CH3OH+CO    9.0E13 0.0 0.0E0
CH2(S)+C2H4=C2H3+CH3    1.77E19 -1.94 6.79E3
   DUP
   PLOG/1.0E-2 1.77E19 -1.94E0 6.79E3/
   PLOG/1.0E-1 1.68E19 -1.8E0 4.31E3/
   PLOG/1.0E0 4.16E24 -3.19E0 9.76E3/
   PLOG/1.0E1 7.89E24 -3.07E0 1.39E4/
   PLOG/1.0E2 7.36E29 -4.28E0 2.38E4/
CH2(S)+C2H4=C2H3+CH3    1.77E19 -1.94 6.79E3
   DUP
   PLOG/1.0E-2 4.3E12 1.9E-1 -1.1041E2/
   PLOG/1.0E-1 2.26E11 5.4E-1 4.781E1/
   PLOG/1.0E0 4.92E9 1.02E0 5.9977E2/
   PLOG/1.0E1 1.47E8 1.33E0 1.2284E3/
   PLOG/1.0E2 8.11E10 5.5E-1 5.5065E3/
C2H3+CH2O=C2H4+HCO    1.0E11 0.0 0.0E0
   PLOG/1.0E-3 1.11E7 1.09E0 1.8072E3/
   PLOG/1.0E-2 2.47E7 9.93E-1 1.9949E3/
   PLOG/1.0E-1 2.47E8 7.04E-1 2.5962E3/
   PLOG/1.0E0 1.42E10 2.09E-1 3.9342E3/
   PLOG/1.0E1 3.45E13 -7.26E-1 6.9443E3/
   PLOG/1.0E2 3.31E14 -8.66E-1 1.09657E4/
   PLOG/1.0E3 1.65E1 3.17E0 9.3998E3/
C3H3+O=CH2O+C2H    2.0E13 0.0 0.0E0
C3H3+HO2=>OH+CO+C2H3    8.0E11 0.0 0.0E0
C2H5+C2H=C3H3+CH3    1.81E13 0.0 0.0E0
C3H3+O2=CH2CO+HCO    1.7E5 1.7 1.5E3
C3H3+H=C3H2+H2    2.14E5 2.52 7.453E3
C3H3+OH=C3H2+H2O    2.0E13 0.0 8.0E3
C3H3+OH=CH2O+C2H2    2.0E12 0.0 0.0E0
C3H3+OH=C2H3+HCO    1.0E13 0.0 0.0E0
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C3H3+OH=C2H4+CO    1.0E13 0.0 0.0E0
C3H6OH2-1=C2H3OH+CH3    2.689E9 1.319 2.948E4
C2H2+C2H(+M)=C4H3-I(+M)    8.3E10 0.899 -3.63E2
   H2/2.0/
   H2O/6.0/
   CH4/2.0/
   CO/1.5/
   CO2/2.0/
   C2H6/3.0/
   C2H2/2.5/
   C2H4/2.5/
   LOW/1.24E31 -4.718E0 1.871E3/
   TROE/1.0E0 1.0E2 5.613E3 1.339E4/
C3H3+CH=C4H3-I+H    5.0E13 0.0 0.0E0
C4H3-I+O2=HCCO+CH2CO    7.86E16 -1.8 0.0E0
C4H3-I+CH3=C5H6    1.0E12 0.0 0.0E0
!Ignored from donor mechanism
!2O+M=O2+M    6.165E15 -0.5 0.0E0
!    H2/2.5/H2O/12.0/CO/1.9/CO2/3.8/HE/0.83/CH4/2.0/C2H6/3.0/
!Ignored from donor mechanism
!H+OH+M=H2O+M    3.5E22 -2.0 0.0E0
!    H2/0.73/H2O/3.65/CH4/2.0/C2H6/3.0/
!Ignored from donor mechanism
!O+H+M=OH+M    4.714E18 -1.0 0.0E0
!    H2/2.5/H2O/12.0/CO/1.5/CO2/2.0/HE/0.75/CH4/2.0/C2H6/3.0/
!Ignored from donor mechanism
!H+O+M=OHV+M    1.5E13 0.0 5.975E3
!    H2/1.0/H2O/6.5/O2/0.4/N2/0.4/
!Ignored from donor mechanism
!H+O2(+M)=HO2(+M)    4.65E12 0.44 0.0E0
!    H2/1.3/CO/1.9/CO2/3.8/HE/0.64/H2O/10.0/CH4/2.0/C2H6/3.0/
!    LOW/1.737E19 -1.23E0 0.0E0/
!    TROE/6.7E-1 1.0E-30 1.0E30 1.0E30/
!Ignored from donor mechanism
!CO+O(+M)=CO2(+M)    1.362E10 0.0 2.384E3
!    H2/2.0/H2O/12.0/CO/1.75/CO2/3.6/HE/0.7/
!    LOW/1.173E24 -2.79E0 4.191E3/
!Ignored from donor mechanism
!CH3+H(+M)=CH4(+M)    1.27E16 -0.63 3.83E2
!    H2/2.0/H2O/6.0/CO/1.5/CO2/2.0/CH4/2.0/C2H6/3.0/HE/0.7/
!    LOW/2.477E33 -4.76E0 2.44E3/
!    TROE/7.83E-1 7.4E1 2.941E3 6.964E3/
!Ignored from donor mechanism
!CH2+H(+M)=CH3(+M)    2.5E16 -0.8 0.0E0
!    H2/2.0/H2O/6.0/CO/1.5/CO2/2.0/CH4/2.0/C2H6/3.0/HE/0.7/
!    LOW/3.2E27 -3.14E0 1.23E3/
!    TROE/6.8E-1 7.8E1 1.995E3 5.59E3/
!Added from donor mechanism
CH2OH+HO2=HOCH2O+OH    1.0E13 0.0 0.0E0
!Ignored from donor mechanism
!HCO+H(+M)=CH2O(+M)    1.09E12 0.48 -2.6E2
!    H2/2.0/H2O/6.0/CO/1.5/CO2/2.0/CH4/2.0/C2H6/3.0/HE/0.7/
!    LOW/1.35E24 -2.57E0 1.425E3/
!    TROE/7.824E-1 2.71E2 2.755E3 6.57E3/
!Ignored from donor mechanism
!CO+H2(+M)=CH2O(+M)    4.3E7 1.5 7.96E4
!    H2/2.0/H2O/6.0/CO/1.5/CO2/2.0/CH4/2.0/C2H6/3.0/HE/0.7/
!    LOW/5.07E27 -3.42E0 8.4348E4/
!    TROE/9.32E-1 1.97E2 1.54E3 1.03E4/
!Added from donor mechanism
CH2O+OH=HOCH2O    6.32E6 1.63 4.284E3
!Added from donor mechanism
HOCH2O=HOCHO+H    4.403E8 1.363 1.1664E4
   PLOG/1.0E-3 2.042E12 -1.61E0 7.28E3/
   PLOG/4.0E-3 8.065E13 -1.9E0 8.11E3/
   PLOG/1.8E-2 3.55E15 -2.2E0 8.99E3/
   PLOG/7.5E-2 1.56E17 -2.5E0 9.91E3/
   PLOG/3.16E-1 5.389E18 -2.77E0 1.085E4/
   PLOG/1.334E0 8.624E19 -2.93E0 1.173E4/
   PLOG/5.623E0 2.405E20 -2.87E0 1.243E4/
   PLOG/2.3714E1 3.214E19 -2.42E0 1.274E4/
   PLOG/1.0E2 1.032E17 -1.48E0 1.248E4/
!Ignored from donor mechanism
!C2H5+H(+M)=C2H6(+M)    5.21E17 -0.99 1.58E3
!    H2/2.0/H2O/6.0/CO/1.5/CO2/2.0/CH4/2.0/C2H6/3.0/HE/0.7/
!    LOW/1.99E41 -7.08E0 6.685E3/
!    TROE/8.42E-1 1.25E2 2.219E3 6.882E3/
!Added from donor mechanism
C2H6+C2H5O2=C2H5+C2H5O2H    8.6E0 3.76 1.72E4
!Ignored from donor mechanism
!C2H4+H(+M)=C2H5(+M)    9.569E8 1.463 1.355E3
!    H2/2.0/H2O/6.0/CH4/2.0/CO/1.5/CO2/2.0/C2H6/3.0/
!    LOW/1.419E39 -6.642E0 5.769E3/
!    TROE/-5.69E-1 2.99E2 -9.147E3 1.524E2/
!Added from donor mechanism
C2H5+HO2=C2H5O+OH    1.1E13 0.0 0.0E0
!Added from donor mechanism
C2H5+CH3O2=C2H5O+CH3O    8.0E12 0.0 -1.0E3
!Added from donor mechanism
C2H5+O2=C2H5O2    3.398E53 -13.9 9.279E3
   PLOG/4.0E-2 3.398E53 -1.39E1 9.279E3/
   PLOG/1.0E0 9.362E59 -1.528E1 1.424E4/
   PLOG/1.0E1 1.262E60 -1.491E1 1.624E4/
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!Added from donor mechanism
C2H5+O2=C2H4O1-2+OH    1.303E3 1.93 -5.027E2
   PLOG/4.0E-2 1.303E3 1.93E0 -5.027E2/
   PLOG/1.0E0 2.438E2 2.18E0 -6.25E1/
   PLOG/1.0E1 4.621E9 1.5E-1 5.409E3/
!Added from donor mechanism
C2H5O2=CH3CHO+OH    1.237E35 -9.42 3.636E4
   PLOG/4.0E-2 1.237E35 -9.42E0 3.636E4/
   PLOG/1.0E0 1.687E36 -9.22E0 3.87E4/
   PLOG/1.0E1 2.52E41 -1.02E1 4.371E4/
!Added from donor mechanism
C2H5O2=C2H4+HO2    1.782E32 -7.1 3.284E4
   PLOG/4.0E-2 1.782E32 -7.1E0 3.284E4/
   PLOG/1.0E0 2.701E37 -8.47E0 3.584E4/
   PLOG/1.0E1 1.98E38 -8.46E0 3.79E4/
!Added from donor mechanism
C2H5O2=C2H4O1-2+OH    5.778E45 -11.9 4.112E3
   PLOG/4.0E-2 5.778E45 -1.19E1 4.112E3/
   PLOG/1.0E0 1.916E43 -1.075E1 4.24E4/
   PLOG/1.0E1 3.965E43 -1.046E1 4.558E4/
!Added from donor mechanism
C2H5O2+HO2=C2H5O2H+O2    1.75E10 0.0 -3.275E3
!Added from donor mechanism
C2H5O2+CH2O=C2H5O2H+HCO    1.99E12 0.0 1.166E4
!Added from donor mechanism
C2H5O2+CH4=C2H5O2H+CH3    1.81E11 0.0 1.848E4
!Added from donor mechanism
C2H5O2+CH3OH=C2H5O2H+CH2OH    1.81E12 0.0 1.371E4
!Added from donor mechanism
C2H5O2+H2=C2H5O2H+H    1.5E14 0.0 2.603E4
!Added from donor mechanism
C2H5O2H=C2H5O+OH    6.31E14 0.0 4.23E4
!Added from donor mechanism
C2H4O1-2=CH3+HCO    3.63E13 0.0 5.72E4
!Added from donor mechanism
C2H4O1-2=CH3CHO    7.407E12 0.0 5.38E4
!Ignored from donor mechanism
!C2H3+H(+M)=C2H4(+M)    6.08E12 0.27 2.8E2
!    H2/2.0/H2O/6.0/CO/1.5/CO2/2.0/CH4/2.0/C2H6/3.0/HE/0.7/
!    LOW/1.4E30 -3.86E0 3.32E3/
!    TROE/7.82E-1 2.075E2 2.663E3 6.095E3/
!Added from donor mechanism
C2H4(+M)=H2+H2CC(+M)    8.0E12 0.44 8.877E4
   C2H6/3.0/
   H2O/6.0/
   CO2/2.0/
   H2/2.0/
   CO/1.5/
   CH4/2.0/
   LOW/7.0E50 -9.31E0 9.986E4/
   TROE/7.345E-1 1.8E2 1.035E3 5.417E3/
!Added from donor mechanism
C2H4+C2H5O2=C2H3+C2H5O2H    8.59E0 3.754 2.7132E4
!Added from donor mechanism
C2H4+CH3CO3=C2H3+CH3CO3H    1.13E13 0.0 3.043E4
!Added from donor mechanism
C2H4+O=CH2CHO+H    6.098E6 1.88 1.83E2
!Added from donor mechanism
C2H4+HO2=C2H4O1-2+OH    3.345E12 0.0 1.719E4
!Added from donor mechanism
C2H4+CH3O2=C2H4O1-2+CH3O    2.82E12 0.0 1.711E4
!Added from donor mechanism
C2H4+C2H5O2=C2H4O1-2+C2H5O    2.82E12 0.0 1.711E4
!Ignored from donor mechanism
!C2H2+H(+M)=C2H3(+M)    1.71E10 1.266 2.709E3
!    H2/2.0/H2O/6.0/CO/1.5/CO2/2.0/CH4/2.0/C2H6/3.0/HE/0.7/
!    LOW/6.346E31 -4.664E0 3.78E3/
!    TROE/7.88E-1 -1.02E4 1.0E-30/
!Added from donor mechanism
C2H3+O2=C2H3OO    4.07E27 -4.67 5.222E3
   DUP
   PLOG/1.0E-2 1.55E24 -5.45E0 9.662E3/
   PLOG/1.0E-1 3.48E56 -1.501E1 1.916E4/
   PLOG/3.16E-1 1.25E64 -1.697E1 2.129E4/
   PLOG/1.0E0 3.34E61 -1.579E1 2.015E4/
   PLOG/3.16E0 7.34E53 -1.311E1 1.73E4/
   PLOG/1.0E1 4.16E48 -1.121E1 1.6E4/
   PLOG/3.16E1 2.33E43 -9.38E0 1.481E4/
   PLOG/1.0E2 3.41E39 -8.04E0 1.436E4/
!Added from donor mechanism
C2H3+O2=C2H3OO    4.07E27 -4.67 5.222E3
   DUP
   PLOG/1.0E-2 1.78E-9 4.15E0 -4.707E3/
   PLOG/1.0E-1 2.36E22 -4.52E0 2.839E3/
   PLOG/3.16E-1 2.0E26 -5.43E0 2.725E3/
   PLOG/1.0E0 6.13E28 -5.89E0 3.154E3/
   PLOG/3.16E0 2.14E29 -5.8E0 3.52E3/
   PLOG/1.0E1 3.48E28 -5.37E0 3.636E3/
   PLOG/3.16E1 3.32E27 -4.95E0 3.61E3/
   PLOG/1.0E2 1.03E27 -4.72E0 3.68E3/
!Added from donor mechanism
C2H3+O2=CH2CHO+O    1.76E12 0.15 4.205E3
   DUP
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   PLOG/1.0E-2 7.88E20 -2.67E0 6.742E3/
   PLOG/1.0E-1 7.72E20 -2.67E0 6.713E3/
   PLOG/3.16E-1 9.87E20 -2.7E0 6.724E3/
   PLOG/1.0E0 7.1E20 -2.65E0 6.489E3/
   PLOG/3.16E0 4.5E20 -2.53E0 6.406E3/
   PLOG/1.0E1 1.76E23 -3.22E0 8.697E3/
   PLOG/3.16E1 3.14E25 -3.77E0 1.153E4/
   PLOG/1.0E2 1.02E26 -3.8E0 1.391E4/
!Added from donor mechanism
C2H3+O2=CH2CHO+O    1.76E12 0.15 4.205E3
   DUP
   PLOG/1.0E-2 1.36E10 6.2E-1 -2.776E2/
   PLOG/1.0E-1 1.42E10 6.2E-1 -2.477E2/
   PLOG/3.16E-1 1.66E10 6.0E-1 -1.625E2/
   PLOG/1.0E0 2.02E10 5.8E-1 3.84E1/
   PLOG/3.16E0 9.75E9 6.7E-1 2.48E2/
   PLOG/1.0E1 7.34E9 7.2E-1 7.781E2/
   PLOG/3.16E1 1.57E9 9.2E-1 1.219E3/
   PLOG/1.0E2 7.85E7 1.28E0 1.401E3/
!Added from donor mechanism
C2H3OO=CHCHO+OH    5.89E36 -7.1 5.144E4
   DUP
   PLOG/1.0E-2 3.64E49 -1.213E1 6.742E4/
   PLOG/1.0E-1 1.44E36 -9.92E0 4.122E4/
   PLOG/3.16E-1 4.18E40 -1.053E1 4.367E4/
   PLOG/1.0E0 3.79E46 -1.072E1 5.19E4/
   PLOG/3.16E0 1.6E49 -1.124E1 5.415E4/
   PLOG/1.0E1 2.38E51 -1.164E1 5.698E4/
   PLOG/3.16E1 2.0E54 -1.222E1 6.184E4/
   PLOG/1.0E2 9.54E195 -5.227E1 1.635E5/
!Added from donor mechanism
C2H3OO=CHCHO+OH    5.89E36 -7.1 5.144E4
   DUP
   PLOG/1.0E-2 1.17E56 -1.481E1 6.07E4/
   PLOG/1.0E-1 2.32E40 -9.39E0 5.042E4/
   PLOG/3.16E-1 1.61E43 -9.99E0 5.029E4/
   PLOG/1.0E0 2.33E124 -3.677E1 7.01E4/
   PLOG/3.16E0 1.88E103 -2.949E1 6.541E4/
   PLOG/1.0E1 5.96E86 -2.381E1 6.217E4/
   PLOG/3.16E1 1.51E57 -1.394E1 5.539E4/
   PLOG/1.0E2 1.79E34 -6.4E0 5.0E4/
!Added from donor mechanism
C2H3OO=CH2CHO+O    1.22E29 -4.71 4.234E4
   DUP
   PLOG/1.0E-2 2.7E180 -4.819E1 1.693E5/
   PLOG/1.0E-1 3.9E38 -8.69E0 4.277E4/
   PLOG/3.16E-1 4.57E47 -1.121E1 4.705E4/
   PLOG/1.0E0 7.62E81 -2.128E1 6.508E4/
   PLOG/3.16E0 1.86E68 -1.683E1 6.068E4/
   PLOG/1.0E1 2.02E55 -1.269E1 5.584E4/
   PLOG/3.16E1 1.11E53 -1.179E1 5.669E4/
   PLOG/1.0E2 4.3E48 -1.031E1 5.609E4/
!Added from donor mechanism
C2H3OO=CH2CHO+O    1.22E29 -4.71 4.234E4
   DUP
   PLOG/1.0E-2 1.47E30 -6.64E0 4.111E4/
   PLOG/1.0E-1 9.65E-12 5.96E0 2.289E4/
   PLOG/3.16E-1 3.95E22 -3.71E0 3.627E4/
   PLOG/1.0E0 2.39E33 -6.62E0 4.128E4/
   PLOG/3.16E0 6.37E31 -5.96E0 4.126E4/
   PLOG/1.0E1 2.13E29 -5.1E0 4.071E4/
   PLOG/3.16E1 4.66E27 -4.5E0 4.053E4/
   PLOG/1.0E2 5.99E25 -3.85E0 4.012E4/
!Added from donor mechanism
C2H3OO=CH2CO+OH    1.55E24 -3.87 4.985E4
   DUP
   PLOG/1.0E-2 1.15E47 -1.228E1 7.533E4/
   PLOG/1.0E-1 8.43E9 -2.06E0 3.372E4/
   PLOG/3.16E-1 6.06E4 1.7E-1 3.422E4/
   PLOG/1.0E0 1.51E19 -3.61E0 4.306E4/
   PLOG/3.16E0 2.13E33 -7.39E0 5.161E4/
   PLOG/1.0E1 4.44E36 -7.99E0 5.468E4/
   PLOG/3.16E1 1.19E37 -7.8E0 5.646E4/
   PLOG/1.0E2 9.08E35 -7.21E0 5.755E4/
!Added from donor mechanism
C2H3OO=CH2CO+OH    1.55E24 -3.87 4.985E4
   DUP
   PLOG/1.0E-2 2.31E2 -7.3E-1 2.571E4/
   PLOG/1.0E-1 1.83E-23 7.84E0 2.019E4/
   PLOG/3.16E-1 3.82E63 -2.044E1 4.342E4/
   PLOG/1.0E0 3.18E27 -7.76E0 3.723E4/
   PLOG/3.16E0 2.32E-5 3.47E0 3.156E4/
   PLOG/1.0E1 1.06E-1 2.64E0 3.416E4/
   PLOG/3.16E1 5.62E2 1.7E0 3.645E4/
   PLOG/1.0E2 1.11E7 5.2E-1 3.867E4/
!Added from donor mechanism
C2H3OO=CH2O+HCO    1.19E20 -2.29 3.017E4
   DUP
   PLOG/1.0E-2 1.66E174 -5.552E1 6.032E4/
   PLOG/1.0E-1 9.03E66 -1.725E1 4.812E4/
   PLOG/3.16E-1 1.82E43 -9.87E0 3.796E4/
   PLOG/1.0E0 8.64E33 -6.88E0 3.437E4/
   PLOG/3.16E0 7.29E171 -4.353E1 1.919E5/
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   PLOG/1.0E1 1.03E32 -6.06E0 3.55E4/
   PLOG/3.16E1 1.85E34 -6.57E0 3.851E4/
   PLOG/1.0E2 5.7E29 -5.19E0 3.68E4/
!Added from donor mechanism
C2H3OO=CH2O+HCO    1.19E20 -2.29 3.017E4
   DUP
   PLOG/1.0E-2 2.27E35 -7.97E0 3.128E4/
   PLOG/1.0E-1 2.08E26 -4.96E0 2.878E4/
   PLOG/3.16E-1 1.45E20 -3.08E0 2.663E4/
   PLOG/1.0E0 1.06E130 -3.938E1 5.47E4/
   PLOG/3.16E0 2.35E34 -6.87E0 3.57E4/
   PLOG/1.0E1 2.18E175 -5.378E1 6.85E4/
   PLOG/3.16E1 1.07E185 -5.422E1 8.899E4/
   PLOG/1.0E2 4.68E2 1.81E0 1.81E4/
!Added from donor mechanism
C2H3OO=>CH2O+H+CO    1.19E20 -2.29 3.017E4
   DUP
   PLOG/1.0E-2 3.88E174 -5.552E1 6.032E4/
   PLOG/1.0E-1 2.11E67 -1.725E1 4.812E4/
   PLOG/3.16E-1 4.26E43 -9.87E0 3.796E4/
   PLOG/1.0E0 2.02E34 -6.88E0 3.437E4/
   PLOG/3.16E0 1.7E172 -4.353E1 1.919E5/
   PLOG/1.0E1 2.4E32 -6.06E0 3.55E4/
   PLOG/3.16E1 4.32E34 -6.57E0 3.851E4/
   PLOG/1.0E2 1.33E30 -5.19E0 3.68E4/
!Added from donor mechanism
C2H3OO=>CH2O+H+CO    1.19E20 -2.29 3.017E4
   DUP
   PLOG/1.0E-2 5.29E35 -7.97E0 3.128E4/
   PLOG/1.0E-1 4.85E26 -4.96E0 2.878E4/
   PLOG/3.16E-1 3.37E20 -3.08E0 2.663E4/
   PLOG/1.0E0 2.46E130 -3.938E1 5.47E4/
   PLOG/3.16E0 5.49E34 -6.87E0 3.57E4/
   PLOG/1.0E1 5.09E175 -5.378E1 6.85E4/
   PLOG/3.16E1 2.49E185 -5.422E1 8.899E4/
   PLOG/1.0E2 1.09E3 1.81E0 1.81E4/
!Added from donor mechanism
C2H3OO=>CH2O+H+CO    1.19E20 -2.29 3.017E4
   DUP
   PLOG/1.0E-2 5.2E33 -7.92E0 3.132E4/
   PLOG/1.0E-1 1.26E98 -2.709E1 6.406E4/
   PLOG/3.16E-1 1.8E33 -7.27E0 3.376E4/
   PLOG/1.0E0 3.83E33 -7.2E0 3.51E4/
   PLOG/3.16E0 1.28E79 -1.961E1 7.487E4/
   PLOG/1.0E1 4.07E32 -6.62E0 3.721E4/
   PLOG/3.16E1 6.86E44 -1.004E1 4.703E4/
   PLOG/1.0E2 3.25E4 1.694E0 2.33276E4/
!Added from donor mechanism
C2H3OO=>CH2O+H+CO    1.19E20 -2.29 3.017E4
   DUP
   PLOG/1.0E-2 2.31E129 -4.186E1 4.585E4/
   PLOG/1.0E-1 2.42E28 -5.99E0 3.054E4/
   PLOG/3.16E-1 8.69E-50 1.663E1 -3.9E3/
   PLOG/1.0E0 1.19E-39 1.361E1 -1.317E3/
   PLOG/3.16E0 8.8E86 -2.308E1 6.101E4/
   PLOG/1.0E1 1.27E3 1.44E0 1.866E4/
   PLOG/3.16E1 1.97E17 -2.23E0 2.859E4/
   PLOG/1.0E2 1.0E-99 0.0E0 0.0E0/
!Added from donor mechanism
C2H3+H=H2CC+H2    6.0E13 0.0 0.0E0
!Ignored from donor mechanism
!C2H+H(+M)=C2H2(+M)    1.0E17 0.0 0.0E0
!    H2/2.0/H2O/6.0/CO/1.5/CO2/2.0/CH4/2.0/C2H6/3.0/HE/0.7/
!    LOW/3.75E33 -4.8E0 1.9E3/
!    TROE/6.46E-1 1.32E2 1.315E3 5.566E3/
!Added from donor mechanism
C2H2(+M)=H2CC(+M)    8.0E14 -0.52 5.075E4
   C2H6/3.0/
   H2O/6.0/
   C2H4/2.5/
   C2H2/2.5/
   CO2/2.0/
   H2/2.0/
   CO/1.5/
   CH4/2.0/
   LOW/2.45E15 -6.4E-1 4.97E4/
!Added from donor mechanism
H2CC+OH=CH2CO+H    2.0E13 0.0 0.0E0
!Added from donor mechanism
H2CC+O2=2HCO    1.0E13 0.0 0.0E0
!Added from donor mechanism
H2CC+H=C2H2+H    1.0E14 0.0 0.0E0
!Added from donor mechanism
CH3CHO+O2=CH3CO+HO2    3.01E13 0.0 3.915E4
!Added from donor mechanism
CH3CHO+O=CH3CO+OH    5.94E12 0.0 1.868E3
!Added from donor mechanism
CH3CHO+H=CH3CO+H2    1.31E5 2.58 1.22E3
!Added from donor mechanism
CH3CHO+OH=CH3CO+H2O    3.37E12 0.0 -6.19E2
!Added from donor mechanism
CH3CHO+HO2=CH3CO+H2O2    3.01E12 0.0 1.192E4
!Added from donor mechanism
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CH3CHO+CH3=CH3CO+CH4    7.08E-4 4.58 1.966E3
!Added from donor mechanism
CH3CHO+C2H3=CH3CO+C2H4    1.65E1 3.17 9.3998E3
!Added from donor mechanism
CH3CHO+CH3O2=CH3CO+CH3O2H    3.01E12 0.0 1.192E4
!Added from donor mechanism
CH3CHO+CH3CO3=CH3CO+CH3CO3H    3.01E12 0.0 1.192E4
!Added from donor mechanism
CH3CHO+H=CH2CHO+H2    2.72E3 3.1 5.21E3
!Added from donor mechanism
CH3CHO+OH=CH2CHO+H2O    1.72E5 2.4 8.15E2
!Added from donor mechanism
CH3CO(+M)=CH3+CO(+M)    1.07E12 0.63 1.69E4
   LOW/5.65E18 -9.7E-1 1.46E4/
   TROE/6.29E-1 8.73E9 5.52E0 7.6E7/
!Added from donor mechanism
CH3CO(+M)=CH2CO+H(+M)    9.413E7 1.917 4.49872E4
   LOW/1.516E51 -1.027E1 5.539E4/
   TROE/6.009E-1 8.103E9 6.677E2 5.0E9/
!Added from donor mechanism
CH3CO+H=CH2CO+H2    2.0E13 0.0 0.0E0
!Added from donor mechanism
CH3CO+O=CH2CO+OH    2.0E13 0.0 0.0E0
!Added from donor mechanism
CH3CO+CH3=CH2CO+CH4    5.0E13 0.0 0.0E0
!Added from donor mechanism
CH3CO+O2=CH3CO3    1.2E11 0.0 -1.1E3
!Added from donor mechanism
C2H3OH+O2=CH2CHO+HO2    5.31E11 0.21 3.983E4
!Added from donor mechanism
C2H3OH+O=CH2CHO+OH    1.875E6 1.9 -8.6E2
!Added from donor mechanism
C2H3OH+H=CH2CHO+H2    1.48E3 3.077 7.22E3
!Added from donor mechanism
C2H3OH+OH=CH2CHO+H2O    3.33E9 1.1 5.405E2
!Added from donor mechanism
C2H3OH+CH3=CH2CHO+CH4    2.03E-8 5.9 1.052E3
!Added from donor mechanism
C2H3OH+CH3O2=CH2CHO+CH3O2H    3.4E3 2.5 8.922E3
!Added from donor mechanism
CH2CHO(+M)=CH2CO+H(+M)    1.43E15 -0.15 4.56E4
   LOW/6.0E29 -3.8E0 4.34239E4/
   TROE/9.85E-1 3.93E2 9.8E9 5.0E9/
!Added from donor mechanism
CH2CHO(+M)=CH3+CO(+M)    2.93E12 0.29 4.03E4
   LOW/9.52E33 -5.07E0 4.13E4/
   TROE/7.13E-17 1.15E3 4.99E9 1.79E9/
!Added from donor mechanism
CH3CO3H=CH3CO2+OH    5.01E14 0.0 4.015E4
!Added from donor mechanism
CH3CO3+CH2O=CH3CO3H+HCO    1.99E12 0.0 1.166E4
!Added from donor mechanism
CH3CO3+C2H6=CH3CO3H+C2H5    1.7E13 0.0 2.046E4
!Added from donor mechanism
CH3CO3+HO2=CH3CO3H+O2    1.75E10 0.0 -3.275E3
!Added from donor mechanism
CH3CO3+H2O2=CH3CO3H+HO2    2.41E12 0.0 9.936E3
!Added from donor mechanism
CH3CO3+CH4=CH3CO3H+CH3    1.81E11 0.0 1.848E4
!Added from donor mechanism
CH3CO2+M=CH3+CO2+M    4.4E15 0.0 1.05E4
!Added from donor mechanism
CH2CHO+O2=CH2CO+HO2    1.88E5 2.37 2.373E4
   PLOG/1.0E-2 1.88E5 2.37E0 2.373E4/
   PLOG/1.0E-1 1.88E5 2.37E0 2.737E4/
   PLOG/1.0E0 2.51E5 2.33E0 2.38E4/
   PLOG/1.0E1 7.05E7 1.63E0 2.529E4/
!Added from donor mechanism
CH2CHO+O2=>CH2O+CO+OH    2.68E17 -1.84 6.53E3
   PLOG/1.0E-2 2.68E17 -1.84E0 6.53E3/
   PLOG/1.0E-1 1.52E20 -2.58E0 8.98E3/
   PLOG/1.0E0 1.65E19 -2.22E0 1.034E4/
   PLOG/1.0E1 8.953E13 -6.0E-1 1.012E4/
!Ignored from donor mechanism
!CH2+CO(+M)=CH2CO(+M)    8.1E11 0.0 0.0E0
!    H2/2.0/H2O/6.0/CO/1.5/CO2/2.0/CH4/2.0/C2H6/3.0/HE/0.7/
!    LOW/2.69E33 -5.11E0 7.095E3/
!    TROE/5.907E-1 2.75E2 1.226E3 5.185E3/
!Added from donor mechanism
SC2H4OH=CH3CHO+H    5.69E52 -13.38 4.5049E4
   PLOG/1.0E-3 5.69E52 -1.338E1 4.5049E4/
   PLOG/1.0E-2 3.29E56 -1.412E1 4.8129E4/
   PLOG/1.0E-1 8.58E57 -1.416E1 5.0743E4/
   PLOG/1.0E0 5.36E55 -1.315E1 5.1886E4/
   PLOG/1.0E1 1.66E48 -1.064E1 5.0297E4/
   PLOG/2.0E1 8.26E44 -9.59E0 4.9218E4/
   PLOG/5.0E1 1.01E40 -8.06E0 4.7439E4/
   PLOG/1.0E2 1.1E36 -6.84E0 4.5899E4/
!Added from donor mechanism
SC2H4OH=C2H3OH+H    5.4E46 -11.63 4.4323E4
   PLOG/1.0E-3 5.4E46 -1.163E1 4.4323E4/
   PLOG/1.0E-2 1.21E51 -1.255E1 4.724E4/
   PLOG/1.0E-1 2.87E54 -1.315E1 5.0702E4/
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   PLOG/1.0E0 3.79E53 -1.251E1 5.256E4/
   PLOG/1.0E1 6.33E46 -1.02E1 5.1441E4/
   PLOG/2.0E1 3.87E43 -9.17E0 5.044E4/
   PLOG/5.0E1 5.08E38 -7.65E0 4.8713E4/
   PLOG/1.0E2 5.12E34 -6.41E0 4.7182E4/
!Added from donor mechanism
SC2H4OH=C2H5O    5.48E45 -11.63 4.4328E4
   PLOG/1.0E-3 5.48E45 -1.163E1 4.4328E4/
   PLOG/1.0E-2 2.54E49 -1.237E1 4.6445E4/
   PLOG/1.0E-1 1.65E54 -1.34E1 5.033E4/
   PLOG/1.0E0 1.81E55 -1.331E1 5.3132E4/
   PLOG/1.0E1 4.58E49 -1.132E1 5.2714E4/
   PLOG/2.0E1 4.11E46 -1.033E1 5.1834E4/
   PLOG/5.0E1 6.68E41 -8.83E0 5.0202E4/
   PLOG/1.0E2 6.54E37 -7.58E0 4.8697E4/
!Added from donor mechanism
CH3+CH2O=C2H5O    3.0E11 0.0 6.336E3
!Added from donor mechanism
CH3CHO+H=C2H5O    4.61E7 1.71 7.09E3
!Added from donor mechanism
C2H5O+O2=CH3CHO+HO2    4.28E10 0.0 1.097E3
!Added from donor mechanism
SC2H4OH+O2=CH3CHO+HO2    5.26E17 -1.638 8.69E2
!Added from donor mechanism
SC2H4OH+O2=C2H3OH+HO2    5.512E3 2.495 -4.14E2
   PLOG/1.0E-2 5.12E2 2.496E0 -4.14E2/
   PLOG/1.0E-1 5.33E2 2.49E0 -4.02E2/
   PLOG/1.0E0 7.62E2 2.446E0 -2.96E2/
   PLOG/1.0E1 8.92E3 2.146E0 4.7E2/
   PLOG/1.0E2 4.38E5 1.699E0 2.33E3/
!Added from donor mechanism
O2C2H4OH=>OH+2CH2O    1.25E11 0.0 1.89E4
   PLOG/1.0E-2 5.26E17 -1.637E0 8.38E2/
   PLOG/1.0E-1 5.26E17 -1.637E0 8.38E2/
   PLOG/1.0E0 5.28E17 -1.638E0 8.39E2/
   PLOG/1.0E1 1.54E18 -1.771E0 1.12E3/
   PLOG/1.0E2 3.78E20 -2.429E0 3.09E3/
!Added from donor mechanism
C3H8(+M)=CH3+C2H5(+M)    1.29E37 -5.84 9.738E4
   C2H6/3.0/
   H2O/6.0/
   CO2/2.0/
   H2/2.0/
   CO/1.5/
   HE/0.7/
   CH4/2.0/
   LOW/5.64E74 -1.574E1 9.8714E4/
   TROE/3.1E-1 5.0E1 3.0E3 9.0E3/
!Added from donor mechanism
C3H6OOH2-1=HO2+C3H6    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 1.27E-80 2.78E1 -1.57525E4/
   PLOG/1.0E-1 3.07E-68 2.41E1 -1.36247E4/
   PLOG/1.0E0 7.16E-48 1.81E1 -6.62037E3/
   PLOG/1.0E1 5.04E-23 1.05E1 2.46501E3/
   PLOG/1.0E2 1.04E23 -3.25E0 2.02479E4/
!Added from donor mechanism
C3H6OOH2-1=OH+C3H6O1-2    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 2.31E-6 4.58E0 2.7747E3/
   PLOG/1.0E-1 3.37E0 2.89E0 5.13002E3/
   PLOG/1.0E0 1.15E9 5.21E-1 9.00753E3/
   PLOG/1.0E1 5.4E16 -1.64E0 1.26945E4/
   PLOG/1.0E2 2.98E18 -2.0E0 1.42508E4/
!Added from donor mechanism
O2+C3H6OOH2-1=C3H6OOH2-1O2    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 1.15E19 -3.42E0 -4.03727E3/
   PLOG/1.0E-1 1.5E27 -5.55E0 5.17703E2/
   PLOG/1.0E0 4.1E33 -7.19E0 4.5434E3/
   PLOG/1.0E1 5.85E33 -6.97E0 6.01835E3/
   PLOG/1.0E2 6.87E25 -4.35E0 4.01975E3/
!Added from donor mechanism
C3H6O1-2=C2H4+CH2O    6.0E14 0.0 6.0E4
!Added from donor mechanism
C3H6O1-2+OH=>CH2O+C2H3+H2O    5.0E12 0.0 0.0E0
!Added from donor mechanism
C3H6O1-2+H=>CH2O+C2H3+H2    2.63E7 2.0 5.0E3
!Added from donor mechanism
C3H6O1-2+O=>CH2O+C2H3+OH    8.43E13 0.0 5.2E3
!Added from donor mechanism
C3H6O1-2+HO2=>CH2O+C2H3+H2O2    1.0E13 0.0 1.5E4
!Added from donor mechanism
C3H6O1-2+CH3O2=>CH2O+C2H3+CH3O2H    1.0E13 0.0 1.9E4
!Added from donor mechanism
C3H6O1-2+CH3=>CH2O+C2H3+CH4    2.0E11 0.0 1.0E4
!Added from donor mechanism
CH2(S)+C2H4=C3H6    4.82E57 -14.3 1.71E4
   DUP
   PLOG/1.0E-2 4.82E57 -1.43E1 1.71E4/
   PLOG/1.0E-1 3.84E59 -1.44E1 1.84E4/
   PLOG/1.0E0 2.13E58 -1.35E1 2.04E4/
   PLOG/1.0E1 8.48E52 -1.16E1 2.07E4/
   PLOG/1.0E2 6.07E47 -9.85E0 2.21E4/
!Added from donor mechanism
CH2(S)+C2H4=C3H6    4.82E57 -14.3 1.71E4
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   DUP
   PLOG/1.0E-2 1.15E45 -1.11E1 6.1452E3/
   PLOG/1.0E-1 1.83E45 -1.07E1 6.6385E3/
   PLOG/1.0E0 1.3E40 -8.77E0 5.8638E3/
   PLOG/1.0E1 2.27E32 -6.14E0 4.3179E3/
   PLOG/1.0E2 1.28E24 -3.49E0 2.5299E3/
!Added from donor mechanism
CH2(S)+C2H4=C3H5-A+H    8.2E19 -2.06 1.15E3
   DUP
   PLOG/1.0E-2 8.2E19 -2.06E0 1.15E3/
   PLOG/1.0E-1 2.27E21 -2.44E0 2.65E3/
   PLOG/1.0E0 4.44E35 -6.55E0 1.39E4/
   PLOG/1.0E1 1.18E28 -4.09E0 1.4E4/
   PLOG/1.0E2 6.51E26 -3.58E0 1.89E4/
!Added from donor mechanism
CH2(S)+C2H4=C3H5-A+H    8.2E19 -2.06 1.15E3
   DUP
   PLOG/1.0E-2 1.08E7 1.62E0 -3.1746E3/
   PLOG/1.0E-1 1.37E5 2.15E0 -3.7992E3/
   PLOG/1.0E0 3.89E14 -4.2E-1 1.2376E3/
   PLOG/1.0E1 2.45E10 6.7E-1 7.5093E2/
   PLOG/1.0E2 1.81E2 2.97E0 -7.4603E2/
!Added from donor mechanism
C2H3+CH3=C3H5-A+H    4.12E29 -4.95 8.0E3
   DUP
   PLOG/1.0E-2 4.12E29 -4.95E0 8.0E3/
   PLOG/1.0E-1 4.86E30 -5.03E0 1.13E4/
   PLOG/1.0E0 5.3E29 -4.57E0 1.44E4/
   PLOG/1.0E1 1.32E30 -4.54E0 1.93E4/
   PLOG/1.0E2 5.16E28 -4.03E0 2.38E4/
!Added from donor mechanism
C2H3+CH3=C3H5-A+H    4.12E29 -4.95 8.0E3
   DUP
   PLOG/1.0E-2 5.73E15 -7.7E-1 1.1959E3/
   PLOG/1.0E-1 2.06E13 -7.4E-2 1.4287E3/
   PLOG/1.0E0 4.48E10 6.0E-1 1.4216E3/
   PLOG/1.0E1 4.1E6 1.71E0 1.0569E3/
   PLOG/1.0E2 1.37E-1 3.91E0 -3.5355E2/
!Added from donor mechanism
C3H6=C2H3+CH3    1.88E78 -18.7 1.3E5
   DUP
   PLOG/1.0E-2 1.88E78 -1.87E1 1.3E5/
   PLOG/1.0E-1 8.73E76 -1.79E1 1.32E5/
   PLOG/1.0E0 5.8E75 -1.72E1 1.34E5/
   PLOG/1.0E1 8.12E71 -1.58E1 1.36E5/
   PLOG/1.0E2 2.15E64 -1.34E1 1.35E5/
!Added from donor mechanism
C3H6=C2H3+CH3    1.88E78 -18.7 1.3E5
   DUP
   PLOG/1.0E-2 1.69E59 -1.36E1 1.1329E5/
   PLOG/1.0E-1 2.0E60 -1.37E1 1.1489E5/
   PLOG/1.0E0 6.7E54 -1.18E1 1.1384E5/
   PLOG/1.0E1 1.06E47 -9.27E0 1.1151E5/
   PLOG/1.0E2 7.29E38 -6.7E0 1.0874E5/
!Added from donor mechanism
C3H6=C3H5-A+H    9.16E74 -17.6 1.2E5
   DUP
   PLOG/1.0E-2 9.16E74 -1.76E1 1.2E5/
   PLOG/1.0E-1 1.73E70 -1.6E1 1.2E5/
   PLOG/1.0E0 1.08E71 -1.59E1 1.2486E5/
   PLOG/1.0E1 6.4E65 -1.42E1 1.25E5/
   PLOG/1.0E2 8.05E56 -1.15E1 1.22E5/
!Added from donor mechanism
C3H6=C3H5-A+H    9.16E74 -17.6 1.2E5
   DUP
   PLOG/1.0E-2 2.98E54 -1.23E1 1.012E5/
   PLOG/1.0E-1 1.37E43 -8.87E0 9.6365E4/
   PLOG/1.0E0 6.28E42 -8.51E0 9.8004E4/
   PLOG/1.0E1 4.73E35 -6.26E0 9.5644E4/
   PLOG/1.0E2 4.34E28 -4.06E0 9.3114E4/
!Added from donor mechanism
C3H6+H=C3H5-A+H2    3.644E5 2.455 4.3612E3
!Added from donor mechanism
C3H6+O2=C3H5-A+HO2    5.96E19 -1.67 4.61921E4
!Added from donor mechanism
C3H6+O=C3H5-A+OH    5.24E11 0.7 5.884E3
!Added from donor mechanism
C3H6+OH=C3H5-A+H2O    4.46E6 2.072 1.0508E3
!Added from donor mechanism
C3H6+HO2=C3H5-A+H2O2    3.07E-2 4.403 1.35472E4
!Added from donor mechanism
C3H6+CH3=C3H5-A+CH4    2.21E0 3.5 5.675E3
!Added from donor mechanism
C3H6+CH3O=C3H5-A+CH3OH    8.4E10 0.0 2.6E3
!Added from donor mechanism
C3H6+CH3O2=C3H5-A+CH3O2H    7.68E-2 4.403 1.35472E4
!Added from donor mechanism
C3H6+C2H5=C3H5-A+C2H6    1.0E11 0.0 9.8E3
!Added from donor mechanism
C3H6+C2H5O2=C3H5-A+C2H5O2H    7.68E-2 4.403 1.35472E4
!Added from donor mechanism
C3H6+CH3CO3=C3H5-A+CH3CO3H    7.68E-2 4.403 1.35472E4
!Added from donor mechanism
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C3H6+O=C2H4+CH2O    2.11E12 0.36357832 3.6251147E3
   PLOG/1.0E-1 3.239515E10 8.6277366E-1 2.1012156E3/
   PLOG/1.0E0 3.7102143E10 8.4675413E-1 2.152084E3/
   PLOG/1.0E1 6.4621495E10 7.7988106E-1 2.3372114E3/
   PLOG/3.0E1 1.79581E11 6.5836787E-1 2.7279312E3/
   PLOG/1.0E2 2.11E12 3.6357832E-1 3.6251147E3/
!Added from donor mechanism
C3H6+O=C2H5+HCO    4.5392427E9 0.46990082 3.3909714E3
   PLOG/1.0E-1 3.81938E20 -2.8445151E0 2.2008093E3/
   PLOG/1.0E0 6.782E23 -3.7431204E0 5.0411938E3/
   PLOG/1.0E1 5.78554E21 -3.0582581E0 6.6882314E3/
   PLOG/3.0E1 4.41563E16 -1.5513902E0 5.3826196E3/
   PLOG/1.0E2 4.5392427E9 4.6990082E-1 3.3909714E3/
!Added from donor mechanism
C3H6+O=CH3+CH2CHO    6.118106E10 0.72471172 1.7372183E3
   PLOG/1.0E-1 7.1169661E8 1.2452729E0 -2.2913843E2/
   PLOG/1.0E0 2.7972334E9 1.0825886E0 2.8259222E2/
   PLOG/1.0E1 1.8003295E10 8.6375535E-1 1.0689554E3/
   PLOG/3.0E1 3.3952128E10 7.9012293E-1 1.3842371E3/
   PLOG/1.0E2 6.118106E10 7.2471172E-1 1.7372183E3/
!Added from donor mechanism
C3H6+O=H2+CH3CHCO    2.92162E11 -0.46592912 -7.2082123E2
   PLOG/1.0E-1 4.34829E14 -1.3823626E0 3.2638251E2/
   PLOG/1.0E0 5.03596E17 -2.2524612E0 2.2980547E3/
   PLOG/1.0E1 1.88555E14 -1.2406751E0 9.8652802E2/
   PLOG/3.0E1 1.45046E14 -1.2325199E0 8.0590204E2/
   PLOG/1.0E2 2.92162E11 -4.6592912E-1 -7.2082123E2/
!Added from donor mechanism
C3H6+O=CO+C2H6    2.8063963E10 -0.15197791 8.5133477E3
   PLOG/1.0E-1 3.30559E19 -3.0550032E0 4.0607322E3/
   PLOG/1.0E0 4.47648E13 -1.2992022E0 2.5097214E3/
   PLOG/1.0E1 7.29311E16 -2.0833492E0 7.7710391E3/
   PLOG/3.0E1 2.2306699E1 2.136199E0 -3.9348716E3/
   PLOG/1.0E2 2.8063963E10 -1.5197791E-1 8.5133477E3/
!Added from donor mechanism
C3H6+O=H2+C2H4+CO    1.9064245E5 1.4148871 1.8470398E3
   PLOG/1.0E-1 1.40605E19 -2.7684405E0 1.5882145E3/
   PLOG/1.0E0 1.42188E22 -3.5758173E0 4.455772E3/
   PLOG/1.0E1 4.5976E19 -2.7595153E0 6.0180806E3/
   PLOG/3.0E1 5.57149E13 -1.0280579E0 4.2239531E3/
   PLOG/1.0E2 1.9064245E5 1.4148871E0 1.8470398E3/
!Added from donor mechanism
C3H6+O=C3H6O1-2    2.97752E43 -9.6417131 1.2220968E4
   PLOG/1.0E-1 2.6792738E5 5.4898018E-1 -7.0526631E3/
   PLOG/1.0E0 4.51272E27 -5.6762934E0 1.4874851E3/
   PLOG/1.0E1 2.31657E51 -1.2235144E1 1.4682028E4/
   PLOG/3.0E1 2.02009E48 -1.1172639E1 1.4083267E4/
   PLOG/1.0E2 2.97752E43 -9.6417131E0 1.2220968E4/
!Added from donor mechanism
C3H6+O=C2H5CHO    8.41666E38 -8.3907213 1.0066773E4
   PLOG/1.0E-1 4.71689E24 -5.1135931E0 7.6513763E1/
   PLOG/1.0E0 1.04304E54 -1.3354402E1 1.4363056E4/
   PLOG/1.0E1 4.4714E47 -1.1098352E1 1.3584807E4/
   PLOG/3.0E1 8.32695E45 -1.0515912E1 1.3147347E4/
   PLOG/1.0E2 8.41666E38 -8.3907213E0 1.0066773E4/
!Added from donor mechanism
C3H6+H=C2H4+CH3    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.3E-3 1.54E9 1.35E0 2.542E3/
   PLOG/4.0E-2 7.88E10 8.7E-1 3.5996E3/
   PLOG/1.0E0 2.67E12 4.7E-1 5.4311E3/
   PLOG/1.0E1 9.25E22 -2.6E0 1.2898E4/
   PLOG/1.0E2 1.32E23 -2.42E0 1.65E4/
!Added from donor mechanism
C3H6+H=C2H4+CH3    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.3E-3 1.0E-10 0.0E0 0.0E0/
   PLOG/4.0E-2 1.0E-10 0.0E0 0.0E0/
   PLOG/1.0E0 1.0E-10 0.0E0 0.0E0/
   PLOG/1.0E1 1.24E5 2.52E0 3.6791E3/
   PLOG/1.0E2 2.51E3 2.91E0 3.9809E3/
!Added from donor mechanism
C3H6+HO2=C3H6O1-2+OH    1.13E19 -1.68 2.3587E4
   PLOG/1.3E-2 3.73E3 2.64E0 1.1173E4/
   PLOG/9.869E-1 1.78E12 1.1E-1 1.6137E4/
   PLOG/9.87E0 3.9E17 -1.4E0 2.0077E4/
   PLOG/9.869E1 1.13E19 -1.68E0 2.3587E4/
!Added from donor mechanism
C3H5-A+C2H5=C2H4+C3H6    4.0E11 0.0 0.0E0
!Added from donor mechanism
C3H5-A+HCO=C3H6+CO    6.0E13 0.0 0.0E0
!Added from donor mechanism
C3H5-A+O=C2H3CHO+H    6.0E13 0.0 0.0E0
!Added from donor mechanism
C3H5-A+OH=>C2H3CHO+2H    5.3E37 -6.71 2.9306E4
   PLOG/1.0E-1 5.3E37 -6.71E0 2.9306E4/
   PLOG/1.0E0 4.2E32 -5.16E0 3.0126E4/
   PLOG/1.0E1 1.6E20 -1.56E0 2.633E4/
!Added from donor mechanism
C3H5-A+O2=CH3CO+CH2O    1.19E15 -1.01 2.0128E4
   PLOG/1.0E0 1.19E15 -1.01E0 2.0128E4/
   PLOG/1.0E1 7.14E15 -1.21E0 2.1046E4/
!Added from donor mechanism
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C3H5-A+O2=C2H3CHO+OH    1.82E13 -0.41 2.2859E4
   PLOG/1.0E0 1.82E13 -4.1E-1 2.2859E4/
   PLOG/1.0E1 2.47E13 -4.5E-1 2.3017E4/
!Added from donor mechanism
C3H5-A+HO2=C2H3CHO+H2O    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 1.09E0 3.01E0 -3.4211E3/
   PLOG/1.0E-1 6.35E1 2.5E0 -2.3414E3/
   PLOG/1.0E0 6.05E5 1.39E0 5.951E2/
   PLOG/1.0E1 3.1E5 1.59E0 2.6776E3/
   PLOG/1.0E2 5.07E-5 4.59E0 9.275E2/
!Added from donor mechanism
C2H3+CH2O=C2H3CHO+H    1.0E11 0.0 0.0E0
   PLOG/1.0E-3 2.6E4 2.26E0 1.5103E3/
   PLOG/1.0E-2 5.13E4 2.17E0 1.6755E3/
   PLOG/1.0E-1 3.99E5 1.91E0 2.2183E3/
   PLOG/1.0E0 1.75E7 1.45E0 3.428E3/
   PLOG/1.0E1 1.35E9 9.33E-1 5.173E3/
   PLOG/1.0E2 2.24E11 3.57E-1 8.0013E3/
   PLOG/1.0E3 6.01E5 2.09E0 7.8956E3/
!Added from donor mechanism
C3H6+OH=C2H3OH+CH3    1.29E6 1.65 1.233E3
   PLOG/1.3E-3 1.29E6 1.65E0 1.233E3/
   PLOG/1.0E-2 1.82E4 2.1E0 1.162E3/
   PLOG/1.3E-2 2.04E3 2.48E0 1.128E3/
   PLOG/2.5E-2 2.88E2 2.8E0 1.152E3/
   PLOG/1.0E-1 1.4E1 3.21E0 1.208E3/
   PLOG/1.315E-1 7.71E0 3.29E0 1.216E3/
   PLOG/1.0E0 1.13E4 2.5E0 3.238E3/
   PLOG/1.0E1 2.41E19 -1.74E0 1.3107E4/
   PLOG/1.0E2 3.3E-1 3.7E0 3.665E3/
!Added from donor mechanism
C3H6+OH=SC3H5OH+H    2.87E0 2.92 6.25E2
   PLOG/1.3E-3 3.47E6 1.53E0 4.288E3/
   PLOG/1.0E-2 1.08E7 1.34E0 4.576E3/
   PLOG/1.3E-2 9.76E6 1.33E0 4.589E3/
   PLOG/2.5E-2 5.14E6 1.36E0 4.594E3/
   PLOG/1.0E-1 3.13E5 1.69E0 4.603E3/
   PLOG/1.315E-1 1.39E5 1.8E0 4.603E3/
   PLOG/1.0E0 1.03E2 2.83E0 4.53E3/
   PLOG/1.0E1 3.4E-2 3.89E0 4.39E3/
   PLOG/1.0E2 4.46E-6 5.03E0 4.132E3/
!Added from donor mechanism
C3H6+OH=CH3CHO+CH3    6.93E5 1.49 -5.36E2
   PLOG/1.3E-3 6.93E5 1.49E0 -5.36E2/
   PLOG/1.0E-2 5.94E3 2.01E0 -5.6E2/
   PLOG/1.3E-2 1.1E3 2.22E0 -6.8E2/
   PLOG/2.5E-2 1.07E2 2.5E0 -7.59E2/
   PLOG/1.0E-1 7.83E-1 3.1E0 -9.19E2/
   PLOG/1.315E-1 3.07E-1 3.22E0 -9.46E2/
   PLOG/1.0E0 3.16E-4 4.05E0 -1.144E3/
   PLOG/1.0E1 7.59E-6 4.49E0 -6.8E2/
   PLOG/1.0E2 5.45E-5 4.22E0 1.141E3/
!Added from donor mechanism
C3H5-A+C2H3=>C5H6+2H    1.6E35 -14.0 6.11377E4
!Added from donor mechanism
C2H2+CH3=C3H5-A    8.2E53 -13.32 3.32E4
   PLOG/1.0E-1 8.2E53 -1.332E1 3.32E4/
   PLOG/1.0E0 2.68E53 -1.282E1 3.573E4/
   PLOG/2.0E0 3.64E52 -1.246E1 3.6127E4/
   PLOG/5.0E0 1.04E51 -1.189E1 3.6476E4/
   PLOG/1.0E1 4.4E49 -1.14E1 3.67E4/
   PLOG/1.0E2 3.8E44 -9.63E0 3.76E4/
!Added from donor mechanism
CH3CHCO+OH=C2H5+CO2    1.73E12 0.0 -1.01E3
!Added from donor mechanism
CH3CHCO+OH=SC2H4OH+CO    2.0E12 0.0 -1.01E3
!Added from donor mechanism
CH3CHCO+H=C2H5+CO    4.4E12 0.0 1.459E3
!Added from donor mechanism
CH3CHCO+O=CH3CHO+CO    3.2E12 0.0 -4.37E2
!Added from donor mechanism
SC3H5OH=C2H5CHO    8.59E11 0.318 5.59E4
!Added from donor mechanism
SC3H5OH+O2=>C2H3CHO+H+HO2    3.0E13 0.0 3.91E4
!Added from donor mechanism
SC3H5OH+OH=>C2H3CHO+H+H2O    3.1E6 2.0 -2.98E2
!Added from donor mechanism
SC3H5OH+H=>C2H3CHO+H+H2    1.73E5 2.5 2.492E3
!Added from donor mechanism
SC3H5OH+O=>C2H3CHO+H+OH    1.75E12 0.7 5.884E3
!Added from donor mechanism
SC3H5OH+HO2=>C2H3CHO+H+H2O2    9.6E3 2.6 1.39E4
!Added from donor mechanism
SC3H5OH+CH3=>C2H3CHO+H+CH4    2.21E0 3.5 5.675E3
!Added from donor mechanism
SC3H5OH+CH3O2=>C2H3CHO+H+CH3O2H    9.6E3 2.6 1.39E4
!Added from donor mechanism
SC3H5OH+CH3O=>C2H3CHO+H+CH3OH    8.3E10 0.0 2.6E3
!Added from donor mechanism
SC3H5OH+HO2=C2H5CHO+HO2    1.49E5 1.67 6.81E3
!Added from donor mechanism
SC3H5OH+HOCHO=C2H5CHO+HOCHO    2.81E-2 3.286 -4.509E3
!Added from donor mechanism
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C2H3+HCO=C2H3CHO    1.81E13 0.0 0.0E0
!Added from donor mechanism
C2H5+HCO=C2H5CHO    1.81E13 0.0 0.0E0
!Added from donor mechanism
C4H10(+M)=2C2H5(+M)    1.355E37 -6.036 9.2929E4
   LOW/4.72E18 0.0E0 4.9578E4/
   TROE/7.998E-2 1.0E-20 3.243E4 4.858E3/
!Added from donor mechanism
C3H5-A+CH3(+M)=C4H8-1(+M)    1.0E14 -0.32 -2.623E2
   C2H6/3.0/
   H2O/6.0/
   CO2/2.0/
   H2/2.0/
   CO/1.5/
   CH4/2.0/
   LOW/3.91E60 -1.281E1 6.25E3/
   TROE/1.04E-1 1.606E3 6.0E4 6.1184E3/
!Added from donor mechanism
C2H5+C2H3(+M)=C4H8-1(+M)    1.5E13 0.0 0.0E0
   C2H6/3.0/
   H2O/6.0/
   CO2/2.0/
   H2/2.0/
   CO/1.5/
   CH4/2.0/
   LOW/1.55E56 -1.179E1 8.9845E3/
   TROE/1.98E-1 2.2779E3 6.0E4 5.7232E3/
!Added from donor mechanism
C4H8-1+OH=C4H71-2+H2O    3.0E6 1.97 2.84766E3
!Added from donor mechanism
C4H8-1+HO2=C4H71-2+H2O2    1.56E4 2.82 2.44279E4
!Added from donor mechanism
C4H8-1+H=C4H71-2+H2    2.37E4 2.85 8.917E3
!Added from donor mechanism
C4H8-1+O=C4H71-2+OH    6.03E10 0.7 7.632E3
!Added from donor mechanism
C4H8-1+O2=C4H71-2+HO2    1.0E13 0.0 5.877E4
!Added from donor mechanism
C4H8-1+CH3=C4H71-2+CH4    8.4E-1 3.5 1.166E4
!Added from donor mechanism
C4H8-1+H=C2H4+C2H5    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.0E-3 2.55E6 1.93E0 5.564E3/
   PLOG/1.0E-2 5.56E6 1.83E0 5.802E3/
   PLOG/1.0E-1 1.21E9 1.18E0 7.472E3/
   PLOG/1.0E0 9.47E16 -1.03E0 1.3413E4/
   PLOG/1.0E1 4.5E28 -4.24E0 2.3618E4/
   PLOG/1.0E2 7.02E32 -5.22E0 3.1754E4/
!Added from donor mechanism
C4H8-1+H=C2H4+C2H5    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.0E-3 3.45E7 1.81E0 2.263E3/
   PLOG/1.0E-2 8.06E7 1.71E0 2.522E3/
   PLOG/1.0E-1 1.18E10 1.1E0 4.077E3/
   PLOG/1.0E0 6.02E15 -4.9E-1 8.452E3/
   PLOG/1.0E1 7.58E21 -2.14E0 1.4245E4/
   PLOG/1.0E2 2.29E21 -1.87E0 1.7243E4/
!Added from donor mechanism
C4H8-1+H=C3H6+CH3    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.0E-3 7.83E9 1.17E0 1.442E3/
   PLOG/1.0E-2 3.39E10 1.0E0 1.895E3/
   PLOG/1.0E-1 3.7E13 1.4E-1 4.127E3/
   PLOG/1.0E0 4.57E19 -1.54E0 9.061E3/
   PLOG/1.0E1 8.57E23 -2.66E0 1.414E4/
   PLOG/1.0E2 1.32E20 -1.46E0 1.5383E4/
!Added from donor mechanism
C4H8-1+H=C3H6+CH3    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.0E-3 1.8E6 1.76E0 5.9E3/
   PLOG/1.0E-2 3.46E6 1.68E0 6.1E3/
   PLOG/1.0E-1 4.02E8 1.1E0 7.574E3/
   PLOG/1.0E0 1.21E16 -9.9E-1 1.3175E4/
   PLOG/1.0E1 7.14E27 -4.23E0 2.3319E4/
   PLOG/1.0E2 1.0E33 -5.49E0 3.1922E4/
!Added from donor mechanism
C4H8-1+O=>CH2CO+C2H5+H    3.05E6 1.88 1.83E2
!Added from donor mechanism
C4H3-I+H=C2H2+H2CC    2.8E23 -2.55 1.078E4
!Added from donor mechanism
C5H81-3+OH=C2H3CHO+C2H5    1.0E12 0.0 0.0E0
!Added from donor mechanism
C5H6+H=C2H2+C3H5-A    1.548E37 -6.18 3.289E4
!Ignored from donor mechanism
!C3H8(+M)=CH3+C2H5(+M)    1.29E37 -5.84 9.738E4
!    H2/2.0/H2O/6.0/AR/0.7/CO/1.5/CO2/2.0/CH4/2.0/C2H6/3.0/HE/0.7/
!    LOW/5.64E74 -1.574E1 9.8714E4/
!    TROE/3.1E-1 5.0E1 3.0E3 9.0E3/
!Added from donor mechanism
NC3H7+H=C3H8    1.0E14 0.0 0.0E0
!Added from donor mechanism
IC3H7+H=C3H8    1.0E14 0.0 0.0E0
!Added from donor mechanism
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C3H8+IC3H7=NC3H7+C3H8    3.0E10 0.0 1.29E4
!Added from donor mechanism
C3H8+O2=NC3H7+HO2    6.0E13 0.0 5.229E4
!Added from donor mechanism
C3H8+H=NC3H7+H2    3.49E5 2.69 6.45E3
!Added from donor mechanism
C3H8+O=NC3H7+OH    3.71E6 2.4 5.505E3
!Added from donor mechanism
C3H8+OH=NC3H7+H2O    2.732E7 1.811 8.684E2
!Added from donor mechanism
C3H8+HO2=NC3H7+H2O2    4.08E1 3.59 1.716E4
!Added from donor mechanism
C3H8+CH3=NC3H7+CH4    9.04E-1 3.65 7.154E3
!Added from donor mechanism
C3H8+C2H3=NC3H7+C2H4    1.0E11 0.0 1.04E4
!Added from donor mechanism
C3H8+C2H5=NC3H7+C2H6    1.0E11 0.0 1.04E4
!Added from donor mechanism
C3H8+C3H5-A=NC3H7+C3H6    7.94E11 0.0 2.05E4
!Added from donor mechanism
C3H8+IC3H7O2=NC3H7+IC3H7O2H    1.7E13 0.0 2.046E4
!Added from donor mechanism
C3H8+O2CHO=NC3H7+HO2CHO    5.52E4 2.55 1.648E4
!Added from donor mechanism
C3H8+O2=IC3H7+HO2    2.0E13 0.0 4.964E4
!Added from donor mechanism
C3H8+H=IC3H7+H2    1.3E6 2.4 4.471E3
!Added from donor mechanism
C3H8+O=IC3H7+OH    5.49E5 2.5 3.14E3
!Added from donor mechanism
C3H8+OH=IC3H7+H2O    9.1715E9 0.935 5.047E2
!Added from donor mechanism
C3H8+HO2=IC3H7+H2O2    6.32E1 3.37 1.372E4
!Added from donor mechanism
C3H8+CH3=IC3H7+CH4    6.4E4 2.17 7.52E3
!Added from donor mechanism
C3H8+C2H3=IC3H7+C2H4    1.0E11 0.0 1.04E4
!Added from donor mechanism
C3H8+C2H5=IC3H7+C2H6    1.0E11 0.0 1.04E4
!Added from donor mechanism
C3H8+C3H5-A=IC3H7+C3H6    7.94E11 0.0 1.62E4
!Added from donor mechanism
C3H8+O2CHO=IC3H7+HO2CHO    1.475E4 2.6 1.391E4
!Added from donor mechanism
C3H8+IC3H7O2=IC3H7+IC3H7O2H    2.0E12 0.0 1.7E4
!Added from donor mechanism
IC3H7+H=C2H5+CH3    2.0E13 0.0 0.0E0
!Added from donor mechanism
IC3H7+OH=C3H6+H2O    2.41E13 0.0 0.0E0
!Added from donor mechanism
IC3H7+O=CH3CHO+CH3    4.818E13 0.0 0.0E0
!Added from donor mechanism
IC3H7+HO2=IC3H7O+OH    7.0E12 0.0 -1.0E3
!Added from donor mechanism
IC3H7+CH3O2=IC3H7O+CH3O    7.0E12 0.0 -1.0E3
!Added from donor mechanism
O2+NC3H7=HO2+C3H6    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 5.05E10 2.06E-2 5.01905E2/
   PLOG/1.0E-1 7.47E15 -1.45E0 4.1129E3/
   PLOG/1.0E0 1.18E19 -2.35E0 7.29953E3/
   PLOG/1.0E1 2.63E0 3.46E0 2.48117E3/
   PLOG/1.0E2 7.37E2 2.71E0 5.49647E3/
!Added from donor mechanism
O2+IC3H7=HO2+C3H6    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 5.91E9 4.28E-1 -1.43857E3/
   PLOG/1.0E-1 1.6E14 -8.45E-1 1.42377E3/
   PLOG/1.0E0 4.05E18 -2.07E0 4.97147E3/
   PLOG/1.0E1 4.91E17 -1.66E0 6.96404E3/
   PLOG/1.0E2 9.84E7 1.34E0 5.37912E3/
!Added from donor mechanism
O2+NC3H7=C3H6OOH1-2    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 2.97E15 -2.84E0 3.56751E3/
   PLOG/1.0E-1 2.64E12 -1.58E0 3.36232E3/
   PLOG/1.0E0 2.78E2 1.63E0 -4.92364E2/
   PLOG/1.0E1 1.3E14 -1.73E0 5.16366E3/
   PLOG/1.0E2 7.63E16 -2.3E0 9.03614E3/
!Added from donor mechanism
O2+NC3H7=C3H6OOH1-3    1.0E11 0.0 0.0E0
   DUP
   PLOG/1.0E-2 3.09E146 -4.59E1 3.12822E4/
   PLOG/1.0E-1 1.26E47 -1.24E1 8.20313E3/
   PLOG/1.0E0 1.3E23 -4.03E0 5.08867E3/
   PLOG/1.0E1 3.94E-18 8.88E0 -6.1997E3/
   PLOG/1.0E2 6.58E-15 7.8E0 -3.43101E3/
!Added from donor mechanism
O2+NC3H7=C3H6OOH1-3    1.0E11 0.0 0.0E0
   DUP
   PLOG/1.0E-2 6.19E8 8.78E-1 1.11866E4/
   PLOG/1.0E-1 1.12E14 -5.31E-1 1.38975E4/
   PLOG/1.0E0 2.07E14 -4.0E-1 1.51581E4/
   PLOG/1.0E1 1.02E21 -2.26E0 1.8554E4/
   PLOG/1.0E2 1.05E15 -4.86E-1 1.58767E4/
!Added from donor mechanism
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O2+IC3H7=C3H6OOH2-1    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 4.86E10 -1.56E0 -7.08183E2/
   PLOG/1.0E-1 3.76E11 -1.48E0 4.70031E2/
   PLOG/1.0E0 4.08E12 -1.45E0 2.16878E3/
   PLOG/1.0E1 1.13E14 -1.5E0 5.25342E3/
   PLOG/1.0E2 3.56E10 -1.16E-1 7.05645E3/
!Added from donor mechanism
O2+NC3H7=NC3H7O2    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 9.2E8 4.05E-1 -4.39865E3/
   PLOG/1.0E-1 1.45001E14 -9.84E-1 -1.7108E3/
   PLOG/1.0E0 2.09001E13 -4.99E-1 -9.38423E2/
   PLOG/1.0E1 1.15001E20 -2.42E0 2.45126E3/
   PLOG/1.0E2 2.07001E16 -1.3E0 8.03419E2/
!Added from donor mechanism
O2+IC3H7=IC3H7O2    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 7.33E5 1.33E0 -6.34564E3/
   PLOG/1.0E-1 2.24E11 -1.05E-1 -3.69787E3/
   PLOG/1.0E0 1.54E18 -2.02E0 -4.98567E2/
   PLOG/1.0E1 6.74E27 -4.85E0 3.77982E3/
   PLOG/1.0E2 1.67E29 -5.15E0 5.03645E3/
!Added from donor mechanism
NC3H7O2=HO2+C3H6    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 4.3E53 -1.4E1 3.9526E4/
   PLOG/1.0E-1 9.52E57 -1.5E1 4.26843E4/
   PLOG/1.0E0 6.9E33 -7.03E0 3.65435E4/
   PLOG/1.0E1 2.55E16 -1.22E0 3.24803E4/
   PLOG/1.0E2 2.26E32 -6.22E0 3.79482E4/
!Added from donor mechanism
IC3H7O2=C3H6+HO2    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 1.61E75 -2.06E1 4.6203E4/
   PLOG/1.0E-1 1.72E66 -1.73E1 4.54589E4/
   PLOG/1.0E0 4.03E56 -1.4E1 4.40102E4/
   PLOG/1.0E1 1.29E40 -8.58E0 3.94186E4/
   PLOG/1.0E2 6.4E25 -4.02E0 3.49139E4/
!Added from donor mechanism
NC3H7O2=C3H6OOH1-2    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 9.48E20 -5.14E0 2.37097E4/
   PLOG/1.0E-1 1.24E22 -4.93E0 2.64778E4/
   PLOG/1.0E0 1.99E20 -3.92E0 2.76341E4/
   PLOG/1.0E1 2.58E42 -1.03E1 3.76702E4/
   PLOG/1.0E2 2.79E42 -1.01E1 3.91082E4/
!Added from donor mechanism
NC3H7O2=C3H6OOH1-3    1.0E11 0.0 0.0E0
   DUP
   PLOG/1.0E-2 1.69E4 1.56E0 1.85703E4/
   PLOG/1.0E-1 5.85E4 1.66E0 1.9612E4/
   PLOG/1.0E0 1.5E3 2.32E0 1.97537E4/
   PLOG/1.0E1 1.01E0 3.38E0 1.89948E4/
   PLOG/1.0E2 3.39E0 3.23E0 1.92093E4/
!Added from donor mechanism
NC3H7O2=C3H6OOH1-3    1.0E11 0.0 0.0E0
   DUP
   PLOG/1.0E-2 7.72E17 5.57E-4 4.03931E4/
   PLOG/1.0E-1 7.02E18 -1.18E-3 4.69318E4/
   PLOG/1.0E0 1.19E20 -7.68E-3 5.52238E4/
   PLOG/1.0E1 1.26E23 -3.15E-2 7.54407E4/
   PLOG/1.0E2 4.06E26 -3.66E-2 9.94007E4/
!Added from donor mechanism
IC3H7O2=C3H6OOH2-1    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 6.0E33 -8.94E0 3.04423E4/
   PLOG/1.0E-1 2.48E34 -8.62E0 3.29047E4/
   PLOG/1.0E0 2.01E33 -7.75E0 3.48901E4/
   PLOG/1.0E1 4.62E27 -5.55E0 3.50367E4/
   PLOG/1.0E2 2.22E18 -2.35E0 3.32447E4/
!Added from donor mechanism
C3H6OOH1-2=C3H6OOH1-3    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 6.24E-135 4.57E1 -1.94619E4/
   PLOG/1.0E-1 3.0E-176 5.79E1 -4.04217E4/
   PLOG/1.0E0 1.0E-15 1.02E1 2.85937E4/
   PLOG/1.0E1 5.36E-85 3.1E1 5.35821E2/
   PLOG/1.0E2 1.58E-133 4.51E1 -2.11265E4/
!Added from donor mechanism
C3H6OOH1-2=HO2+C3H6    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 1.49E-15 9.24E0 1.89606E4/
   PLOG/1.0E-1 2.9E-44 1.76E1 1.8887E3/
   PLOG/1.0E0 1.08E31 -4.56E0 3.21226E4/
   PLOG/1.0E1 1.16E-9 7.46E0 1.47457E4/
   PLOG/1.0E2 1.27E-15 8.78E0 9.26654E3/
!Added from donor mechanism
C3H6OOH1-3=HO2+C3H6    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 3.55E-90 2.75E1 -3.5057E4/
   PLOG/1.0E-1 3.21E4 -3.42E-1 4.33923E3/
   PLOG/1.0E0 1.97E26 -5.97E0 1.87428E4/
   PLOG/1.0E1 1.6E10 -4.44E-1 1.75318E4/
   PLOG/1.0E2 3.45E17 -2.82E0 2.15791E4/
!Added from donor mechanism
O2+C3H6OOH1-3=C3H6OOH1-3O2    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 2.95E42 -1.02E1 5.86236E3/
   PLOG/1.0E-1 4.3E42 -9.88E0 7.52686E3/
   PLOG/1.0E0 7.47E36 -7.85E0 6.72435E3/
   PLOG/1.0E1 2.18E27 -4.75E0 4.02617E3/
   PLOG/1.0E2 1.46E18 -1.85E0 1.00584E3/
!Added from donor mechanism
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O2+C3H6OOH1-3=OH+C3KET13    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 6.2E30 -6.23E0 5.24155E3/
   PLOG/1.0E-1 2.42E32 -6.58E0 8.14472E3/
   PLOG/1.0E0 3.7E27 -5.03E0 8.65443E3/
   PLOG/1.0E1 3.58E15 -1.36E0 5.98573E3/
   PLOG/1.0E2 6.32E0 3.02E0 1.62507E3/
!Added from donor mechanism
O2+C3H6OOH1-3=HO2+AC3H5OOH    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 1.46E15 -1.27E0 3.27888E3/
   PLOG/1.0E-1 2.53E20 -2.73E0 7.33277E3/
   PLOG/1.0E0 2.77E20 -2.61E0 9.79694E3/
   PLOG/1.0E1 3.08E11 1.79E-1 8.56997E3/
   PLOG/1.0E2 6.76E-4 4.57E0 4.46375E3/
!Added from donor mechanism
O2+C3H6OOH1-2=HO2+AC3H5OOH    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 6.32E10 1.66E-3 8.74545E2/
   PLOG/1.0E-1 5.12E16 -1.68E0 4.87214E3/
   PLOG/1.0E0 1.51E20 -2.59E0 8.51258E3/
   PLOG/1.0E1 1.51E16 -1.27E0 9.3915E3/
   PLOG/1.0E2 4.35E3 2.55E0 6.47735E3/
!Added from donor mechanism
O2+C3H6OOH1-2=O2+C3H6OOH2-1    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 1.68E33 -7.31E0 8.13443E3/
   PLOG/1.0E-1 4.31E38 -8.76E0 1.33994E4/
   PLOG/1.0E0 8.96E39 -8.95E0 1.7948E4/
   PLOG/1.0E1 3.58E31 -6.24E0 1.90919E4/
   PLOG/1.0E2 1.02E10 3.04E-1 1.44948E4/
!Added from donor mechanism
O2+C3H6OOH2-1=HO2+AC3H5OOH    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 1.83E15 -1.76E0 4.65656E3/
   PLOG/1.0E-1 4.68E15 -1.86E0 6.59916E3/
   PLOG/1.0E0 1.81E22 -3.78E0 1.18049E4/
   PLOG/1.0E1 8.68E20 -3.2E0 1.53524E4/
   PLOG/1.0E2 2.23E4 1.94E0 1.30748E4/
!Added from donor mechanism
C3H6OOH1-3O2=C3KET13+OH    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 4.08E29 -6.39E0 2.34402E4/
   PLOG/1.0E-1 2.49E25 -4.95E0 2.26125E4/
   PLOG/1.0E0 1.01E19 -2.88E0 2.08036E4/
   PLOG/1.0E1 4.46E11 -5.38E-1 1.84411E4/
   PLOG/1.0E2 1.67E5 1.48E0 1.62379E4/
!Added from donor mechanism
C3H6OOH1-3O2=HO2+AC3H5OOH    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 3.85E46 -1.14E1 3.78724E4/
   PLOG/1.0E-1 5.56E44 -1.05E1 3.88355E4/
   PLOG/1.0E0 3.87E37 -8.08E0 3.75223E4/
   PLOG/1.0E1 6.42E26 -4.59E0 3.43972E4/
   PLOG/1.0E2 1.96E16 -1.27E0 3.09174E4/
!Added from donor mechanism
C3KET13=>CH2O+CH2CHO+OH    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 3.41E64 -1.59E1 5.57614E4/
   PLOG/1.0E-1 1.97E61 -1.46E1 5.60115E4/
   PLOG/1.0E0 1.07E54 -1.21E1 5.45628E4/
   PLOG/1.0E1 5.29E43 -8.74E0 5.15685E4/
   PLOG/1.0E2 4.06E33 -5.54E0 4.82254E4/
!Added from donor mechanism
IC3H7O+OH=IC3H7O2H    1.0E15 -0.8 0.0E0
!Added from donor mechanism
IC3H7O2+H2=IC3H7O2H+H    3.01E13 0.0 2.603E4
!Added from donor mechanism
IC3H7O2+HO2=IC3H7O2H+O2    1.75E10 0.0 -3.275E3
!Added from donor mechanism
IC3H7O2+CH2O=IC3H7O2H+HCO    5.6E12 0.0 1.36E4
!Added from donor mechanism
IC3H7O2+CH4=IC3H7O2H+CH3    1.12E13 0.0 2.464E4
!Added from donor mechanism
IC3H7O2+C2H4=IC3H7O2H+C2H3    1.13E13 0.0 3.043E4
!Added from donor mechanism
IC3H7O2+C2H6=IC3H7O2H+C2H5    1.7E13 0.0 2.046E4
!Added from donor mechanism
IC3H7O2+CH3O2=>IC3H7O+CH3O+O2    1.4E16 -1.61 1.86E3
!Added from donor mechanism
2IC3H7O2=>2IC3H7O+O2    1.4E16 -1.61 1.86E3
!Added from donor mechanism
IC3H7O2+CH3=IC3H7O+CH3O    7.0E12 0.0 -1.0E3
!Added from donor mechanism
IC3H7O2+IC3H7=2IC3H7O    7.0E12 0.0 -1.0E3
!Added from donor mechanism
IC3H7O2+C3H5-A=IC3H7O+C3H5O    7.0E12 0.0 -1.0E3
!Added from donor mechanism
C3H6+IC3H7O2=C3H5-A+IC3H7O2H    7.68E-2 4.403 1.35472E4
!Added from donor mechanism
C3H6+O=H+CH3CHCHO    6.28E12 -0.081882 2.36E3
   PLOG/1.0E-1 1.52E11 3.61E-1 9.82E2/
   PLOG/1.0E0 1.92E11 3.29E-1 1.0E3/
   PLOG/1.0E1 1.97E11 3.3E-1 1.08E3/
   PLOG/3.0E1 6.7E11 1.81E-1 1.49E3/
   PLOG/1.0E2 6.28E12 -8.1882E-2 2.36E3/
!Added from donor mechanism
C3H6+H=NC3H7    1.0E0 1.0 0.0E0
   DUP
   PLOG/1.3E-3 7.99E81 -2.3161E1 2.2239E4/
   PLOG/4.0E-2 4.24E68 -1.8427E1 1.9665E4/
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   PLOG/1.0E0 1.04E49 -1.15E1 1.5359E4/
   PLOG/1.0E1 6.2E41 -8.892E0 1.4637E4/
   PLOG/1.0E2 4.22E27 -4.39E0 9.3458E3/
!Added from donor mechanism
C3H6+H=NC3H7    1.0E0 1.0 0.0E0
   DUP
   PLOG/1.3E-3 1.85E26 -5.83E0 3.8658E3/
   PLOG/4.0E-2 2.82E30 -6.49E0 5.4708E3/
   PLOG/1.0E0 3.78E28 -5.57E0 5.6251E3/
   PLOG/1.0E1 1.46E25 -4.28E0 5.2478E3/
   PLOG/1.0E2 1.0E-10 0.0E0 0.0E0/
!Added from donor mechanism
C3H6+H=IC3H7    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.3E-3 1.35E44 -1.068E1 8.1964E3/
   PLOG/4.0E-2 2.11E57 -1.423E1 1.5147E4/
   PLOG/1.0E0 3.26E61 -1.494E1 2.0161E4/
   PLOG/1.0E1 5.3E56 -1.312E1 2.0667E4/
   PLOG/1.0E2 1.11E50 -1.08E1 2.0202E4/
!Added from donor mechanism
C3H6+H=IC3H7    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.3E-3 2.17E130 -3.258E1 1.3614E5/
   PLOG/4.0E-2 2.25E29 -5.84E0 4.2419E3/
   PLOG/1.0E0 1.06E30 -5.63E0 5.6134E3/
   PLOG/1.0E1 6.11E26 -4.44E0 5.1823E3/
   PLOG/1.0E2 2.73E23 -3.26E0 4.597E3/
!Added from donor mechanism
C2H4+CH3=NC3H7    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.3E-3 8.67E48 -1.254E1 1.8206E4/
   PLOG/4.0E-2 1.06E49 -1.204E1 2.0001E4/
   PLOG/1.0E0 7.67E47 -1.117E1 2.2366E4/
   PLOG/1.0E1 1.81E45 -1.003E1 2.3769E4/
   PLOG/1.0E2 2.04E40 -8.25E0 2.4214E4/
!Added from donor mechanism
C2H4+CH3=NC3H7    1.0E0 1.0 1.0E0
   DUP
   PLOG/1.3E-3 1.12E43 -1.13E1 1.308E4/
   PLOG/4.0E-2 7.28E39 -9.88E0 1.3164E4/
   PLOG/1.0E0 2.6E33 -7.46E0 1.2416E4/
   PLOG/1.0E1 3.85E27 -5.38E0 1.1455E4/
   PLOG/1.0E2 1.66E21 -3.17E0 1.0241E4/
!Added from donor mechanism
C3H5-A+HO2=C3H5O+OH    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 1.02E13 -1.58E-1 -1.417E3/
   PLOG/1.0E-1 4.98E14 -6.42E-1 -3.491E2/
   PLOG/1.0E0 7.77E17 -1.52E0 2.3792E3/
   PLOG/1.0E1 2.93E15 -6.84E-1 3.6153E3/
   PLOG/1.0E2 1.64E4 2.74E0 1.1444E3/
!Added from donor mechanism
C3H5-A+HO2=AC3H5OOH    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 1.91E31 -7.23E0 1.3362E3/
   PLOG/1.0E-1 6.31E42 -1.03E1 5.5689E3/
   PLOG/1.0E0 1.03E45 -1.06E1 7.8515E3/
   PLOG/1.0E1 2.79E37 -7.92E0 6.4979E3/
   PLOG/1.0E2 1.44E32 -6.01E0 6.0536E3/
!Added from donor mechanism
AC3H5OOH=C2H3CHO+H2O    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 1.99E50 -1.27E1 5.35319E4/
   PLOG/1.0E-1 4.72E47 -1.15E1 5.43609E4/
   PLOG/1.0E0 1.5E40 -8.84E0 5.31792E4/
   PLOG/1.0E1 2.54E28 -5.0E0 4.99194E4/
   PLOG/1.0E2 1.48E16 -1.12E0 4.59493E4/
!Added from donor mechanism
AC3H5OOH=C3H5O+OH    1.0E11 0.0 0.0E0
   PLOG/1.0E-2 1.49E58 -1.39E1 5.42669E4/
   PLOG/1.0E-1 1.8E54 -1.24E1 5.41938E4/
   PLOG/1.0E0 3.36E46 -9.81E0 5.24685E4/
   PLOG/1.0E1 2.39E36 -6.54E0 4.9429E4/
   PLOG/1.0E2 1.28E27 -3.61E0 4.63331E4/
!Added from donor mechanism
C3H5O=C2H3+CH2O    1.0E11 0.0 0.0E0
   PLOG/1.0E-3 7.26E6 1.82E-1 1.78155E4/
   PLOG/1.0E-2 6.97E16 -2.5E0 2.08787E4/
   PLOG/1.0E-1 6.64E23 -4.23E0 2.3565E4/
   PLOG/1.0E0 1.07E26 -4.56E0 2.46229E4/
   PLOG/1.0E1 6.5E29 -5.37E0 2.6645E4/
   PLOG/1.0E2 4.63E31 -5.59E0 2.89153E4/
   PLOG/1.0E3 8.52E25 -3.61E0 2.78634E4/
!Added from donor mechanism
C3H5O=CH2CH2CHO    1.0E11 0.0 0.0E0
   PLOG/1.0E-3 5.25E-49 1.55E1 -1.56399E4/
   PLOG/1.0E-2 1.46E-88 2.76E1 -3.5995E4/
   PLOG/1.0E-1 4.44E-22 8.38E0 -3.819E3/
   PLOG/1.0E0 6.23E12 -1.44E0 1.08292E4/
   PLOG/1.0E1 3.48E42 -9.91E0 2.52979E4/
   PLOG/1.0E2 1.88E38 -8.16E0 2.59745E4/
   PLOG/1.0E3 1.67E21 -2.74E0 2.03377E4/
!Added from donor mechanism
C3H5O=C2H3CHO+H    1.0E11 0.0 0.0E0
   PLOG/1.0E-3 3.0E15 -2.31E0 1.46679E4/
   PLOG/1.0E-2 1.5E22 -3.96E0 1.8283E4/
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    PLOG/1.0E-1 1.95E23 -3.99E0 1.91433E4/
    PLOG/1.0E0 1.15E25 -4.24E0 2.03112E4/
    PLOG/1.0E1 1.76E28 -4.89E0 2.27652E4/
    PLOG/1.0E2 1.41E27 -4.28E0 2.37706E4/
    PLOG/1.0E3 2.57E20 -2.06E0 2.20401E4/
!Added from donor mechanism
C3H5O=C2H4+HCO    1.0E11 0.0 0.0E0
    PLOG/1.0E-3 6.62E16 -2.84E0 1.3197E4/
    PLOG/1.0E-2 1.26E20 -3.53E0 1.54692E4/
    PLOG/1.0E-1 2.13E21 -3.64E0 1.65845E4/
    PLOG/1.0E0 1.07E24 -4.16E0 1.8985E4/
    PLOG/1.0E1 8.42E25 -4.4E0 2.23826E4/
    PLOG/1.0E2 1.86E21 -2.73E0 2.36588E4/
    PLOG/1.0E3 4.75E8 1.14E0 2.09225E4/
!Added from donor mechanism
CH2CH2CHO=C2H3+CH2O    1.0E11 0.0 0.0E0
    PLOG/1.0E-3 6.89E-69 2.15E1 2.638E3/
    PLOG/1.0E-2 5.34E-33 1.11E1 1.67491E4/
    PLOG/1.0E-1 6.11E26 -6.01E0 4.41167E4/
    PLOG/1.0E0 8.04E35 -8.31E0 4.69197E4/
    PLOG/1.0E1 5.52E40 -9.19E0 5.05087E4/
    PLOG/1.0E2 5.85E35 -7.18E0 5.20384E4/
    PLOG/1.0E3 1.93E19 -1.94E0 4.844E4/
!Added from donor mechanism
CH2CH2CHO=C2H3CHO+H    1.0E11 0.0 0.0E0
    PLOG/1.0E-3 1.61E10 -1.24E0 3.23713E4/
    PLOG/1.0E-2 5.84E15 -2.61E0 3.28784E4/
    PLOG/1.0E-1 3.64E23 -4.6E0 3.42753E4/
    PLOG/1.0E0 7.58E31 -6.63E0 3.78954E4/
    PLOG/1.0E1 2.86E32 -6.3E0 3.99907E4/
    PLOG/1.0E2 1.57E23 -3.14E0 3.80117E4/
    PLOG/1.0E3 4.52E12 2.14E-1 3.45705E4/
!Added from donor mechanism
CH2CH2CHO=C2H4+HCO    1.0E11 0.0 0.0E0
    PLOG/1.0E-3 2.9E32 -7.24E0 2.56875E4/
    PLOG/1.0E-2 5.3E33 -7.28E0 2.71006E4/
    PLOG/1.0E-1 2.0E35 -7.41E0 2.90273E4/
    PLOG/1.0E0 1.01E34 -6.7E0 3.00181E4/
    PLOG/1.0E1 9.76E27 -4.63E0 2.89239E4/
    PLOG/1.0E2 2.11E19 -1.85E0 2.62398E4/
    PLOG/1.0E3 1.59E13 6.3E-2 2.40863E4/
!Added from donor mechanism
C3H5-A+CH3O2=C3H5O+CH3O    1.0E11 0.0 0.0E0
    PLOG/1.0E-2 3.33E12 -1.58E-1 -1.417E3/
    PLOG/1.0E-1 1.66E14 -6.42E-1 -3.491E2/
    PLOG/1.0E0 2.595E17 -1.52E0 2.3792E3/
    PLOG/1.0E1 9.78E14 -6.84E-1 3.6153E3/
    PLOG/1.0E2 5.47E3 2.74E0 1.1444E3/
!Added from donor mechanism
CH3CHCHO=C2H3CHO+H    1.0E0 1.0 1.0E0
    PLOG/1.0E-2 1.74E50 -1.173E1 5.287E4/
    PLOG/1.0E-1 1.13E47 -1.057E1 5.0479E4/
    PLOG/1.0E0 2.94E43 -9.29E0 4.881E4/
    PLOG/2.5E0 1.16E42 -8.78E0 4.8382E4/
    PLOG/5.0E0 9.48E40 -8.4E0 4.8095E4/
    PLOG/1.0E1 7.19E39 -8.01E0 4.7818E4/
    PLOG/2.5E1 2.13E38 -7.49E0 4.7438E4/
    PLOG/5.0E1 1.42E37 -7.09E0 4.7128E4/
!Added from donor mechanism
CH3CHCHO=CH3CHCO+H    8.328E12 -0.02 3.241E4
!Added from donor mechanism
C3H5O+O2=C2H3CHO+HO2    1.0E12 0.0 6.0E3
!Added from donor mechanism
CH3+CH3CHO=IC3H7O    1.0E11 0.0 9.256E3
!Ignored from donor mechanism
!C3H5-A+CH3(+M)=C4H8-1(+M)    1.0E14 -0.32 -2.623E2
!    H2/2.0/H2O/6.0/CH4/2.0/CO/1.5/CO2/2.0/C2H6/3.0/AR/0.7/
!    LOW/3.91E60 -1.281E1 6.25E3/
!    TROE/1.04E-1 1.606E3 6.0E4 6.1184E3/
!Ignored from donor mechanism
!C2H5+C2H3(+M)=C4H8-1(+M)    1.5E13 0.0 0.0E0
!    H2/2.0/H2O/6.0/CH4/2.0/CO/1.5/CO2/2.0/C2H6/3.0/AR/0.7/
!    LOW/1.55E56 -1.179E1 8.9845E3/
!    TROE/1.98E-1 2.2779E3 6.0E4 5.7232E3/
!Added from donor mechanism
C4H8-1+O=NC3H7+HCO    7.45E6 1.88 1.83E2
!Added from donor mechanism
C4H8-1+O=>C2H5CHCO+2H    3.05E6 1.88 1.83E2
!Added from donor mechanism
C2H5CHCO+OH=NC3H7+CO2    3.73E12 0.0 -1.01E3
!Added from donor mechanism
C2H5CHCO+H=NC3H7+CO    4.4E12 0.0 1.459E3
!Added from donor mechanism
C2H5CHCO+O=C3H6+CO2    3.2E12 0.0 -4.37E2
END
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