THESIS

AUTOIGNTION AND FLAME SPEED OF PREMIXED LIQUEFIED PETROLEUM GAS IN A RAPID COMPRESSION MACHINE: EXPERIMENTAL RESULTS AND REDUCED CHEMICAL KINETIC MECHANISM

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ABSTRACT

AUTOIGNTION AND FLAME SPEED OF PREMIXED LIQUEFIED PETROLEUM GAS IN A RAPID COMPRESSION MACHINE: EXPERIMENTAL RESULTS AND REDUCED CHEMICAL KINETIC MECHANISM

Liquefied petroleum gas (LPG) has many properties that make it an attractive alternative fuel such as lower cost than conventional fuels and an established distribution infrastructure. The development of high efficiency, spark ignited LPG engines is currently limited by engine knock and misfire. The knock and misfire limits are further complicated by the wide range of chemical reactivity in LPG, particularly in international markets. In this study, a rapid compression machine (RCM) was used to characterize the effects of variation in LPG fuel reactivity, equivalence ratio, and exhaust gas recirculation (EGR) on the autoignition and flame speeds of LPG/oxidizer/inert/EGR blends. Experiments were conducted with 100% propane and blends of propane with propene, ethane, isobutane, or n-butane. EGR was simulated with mixtures of Ar, CO_2, CO, and NO at substitution percentages from 0 to 30 mass percent. Equivalence ratio was varied from 0.75 to 1.5. Ignition delay period under homogeneous autoignition conditions was measured at compressed pressures and temperatures of 23 to 25 bar and 701 to 921 K, respectively. Laminar flame speeds and apparent heat release rates (AHRR) at 24 bar with mixture temperatures of 700 K or 867 K were obtained by firing a laser ignition system into the reaction chamber shortly after compression and analyzing the propagating flame with high speed schlieren imaging. Zero-dimensional simulations of published autoignition

experiments were performed using Chemkin-Pro with several detailed chemical kinetic mechanisms to determine their suitability at predicting ignition delay periods. Multiple reduced chemical kinetic mechanisms were created from the NUIGMech1.1 mechanism to determine the optimal balance between accuracy and computational efficiency for future three-dimensional, time-dependent spark-ignited engine simulations. The chosen reduction, ALPINE 153, was used to model ignition delay periods and flame speeds measured in the RCM during this study.

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1. INTRODUCTION

1.1 Motivation

Emission standards for greenhouse gases such as those set by the California Air Resources Board (CARB) and the European Union (Euro 6) will continue to increase in an effort to improve Earth's air quality. While the passenger car industry has slowly been lowering emissions by increasing fuel efficiency through the introduction of electric vehicles and hybrid drivetrains, the heavy trucking industry and transportation sector still mainly relies on compression ignition (CI) diesel fuel engines. Lower carbon chain fuels produce less CO_2 and particulate matter emissions than conventional fuels but have been unable to meet the same thermal efficiency as the standard diesel engines, resulting in lower fuel economy when used. Spark ignited (SI) liquefied petroleum gas (LPG) engines have the potential to provide the same thermal efficiency as a diesel engine while producing less emissions and costing less per volume than diesel fuel. LPG engines would also require less overhead cost and infrastructure investment compared to other low carbon fuels such as compressed natural gas (CNG).

To make the most efficient heavy-duty LPG engine, several strategies must be simulated, analyzed, and implemented. Optimizing these strategies requires a comprehensive understanding and model of the combustion of homogeneous LPG under engine-like conditions with varying fuel compositions, equivalence ratios, and exhaust gas recirculation (EGR) levels. Central to the current high efficiency engine development work is the use of controlled end-gas autoignition (C-EGAI), which uses sophisticated control algorithms to enable a specified fraction of combustion to occur via autoignition

upstream of the propagating flame. Further efficiency gains can be provided by stratified combustion via direct injection (DI), EGR dilution, and optimized combustion chamber design. These design strategies require computational modeling with chemical kinetic mechanisms that are accurate enough to capture the combustion physics of flame propagation and end-gas autoignition, but sufficiently compact (~100 species) to facilitate reasonable computational times. Maximizing the efficiency of LPG engines through this combined experimental/computation approach will result in LPG engines as viable alternatives to current engine offerings, at which point the fuel cost savings will offset any initial price difference when distributed over the product life cycle. In pursuit of this goal, the U.S. Department of Energy has funded a partnership between Colorado State University (CSU), Cummins Inc., and Argonne National Laboratory to develop a heavy duty, 15 L DISI LPG engine for on-road heavy trucking applications that achieves 44% brake thermal efficiency (BTE). The Advanced Liquid Propane Injected Engine (ALPINE) project will convert a Cummins X15 diesel engine into a high-efficiency LPG engine.

1.2 Liquefied Petroleum Gas

LPG is primarily a mixture of propane (C_3H_8), propene (C_3H_6) and butane (C_4H_{10}) and is produced during the extraction of natural gas or during petroleum refining. In the United States, the standard LPG mixture used as automotive fuel is HD-5. HD-5 is a more stringent standard than commercial propane, which enables it to be used for internal combustion engines. Based on the standard, HD-5 must consist of at least 90% propane by volume, with a maximum of 5% propene and 5% other gases such as butane and ethane (C_2H_6) [1]. Sampling from around the United States shows that the mean composition of HD-5 is 96.06% propane, 2.48% ethane, 0.96% isobutane (i-C_4H_{10}),

0.29% propene, and 0.18% n-butane (n- C_4H_{10}) by volume but samples have exhibited levels of ethane as high as 6% and n-butane/isobutane as high as 7% [2]. LPG used for automotive fuel in the rest of the world is commonly referred to as Autogas. The use of LPG as automotive fuel has steadily increased over the last twenty years, with the largest consumers being Europe and Korea as seen below in Figure 1.

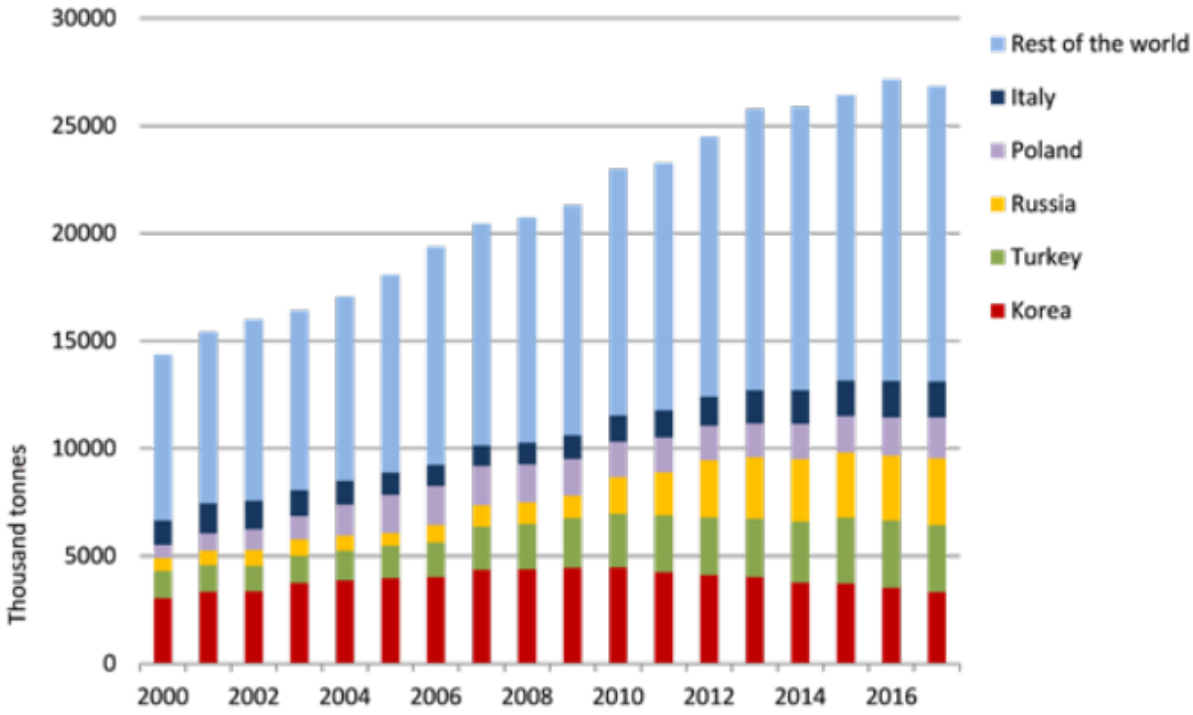

Figure 1: Worldwide consumption of LPG as automotive fuel by country [3].

In Europe, the composition of LPG varies by country and by season. For example, in Italy the LPG mixture during the winter months is 90% propane/10% butane, but in the summer, it is 20%/80% [4]. The drastic changes in composition are due to seasonal changes in temperature and because the evaporation temperature of butane is much higher than propane. If a high butane mixture was used in very cold weather, it is possible that the fuel would not evaporate to properly mix with air for combustion. Korea uses a similar seasonal blend with 10% propane/85% butane in the summer but 35%

propane/60% butane in the winter [5]. This variation makes it difficult to optimize an LPG engine system that works around the world.

LPG has many qualities that make it a practical option as an alternative fuel. Most importantly, LPG is significantly cheaper than gasoline or diesel with a cost of $2.705 per gallon compared to $3.379 for gasoline and $4.376 for diesel, which equates to a saving of over 20% and 38% per gallon respectively. The lower carbon to hydrogen ratio of LPG creates less CO_2 emissions during combustion, 12% less compared to diesel [6], and approximately 10% less than gasoline in equivalent displacement engines [7]. Similar to gasoline, LPG has a specific energy of 45 MJ/kg and its volume is reduced 260 times when compressed into a liquid [8]. LPG fuel tanks are significantly cheaper than CNG tanks [6], require a lower pressure of around 10 bar to liquefy, and LPG has higher energy density than CNG, 27 MJ/L compared to 9 MJ/L [9].

1.3 LPG Engines and Efficiency

Most LPG engines are simply gasoline engines that have been converted to run on LPG. Early versions of LPG engines used a converter that allowed the LPG to evaporate and mix with air before entering the intake valve to the combustion cylinder. The latest LPG engines use an injector similar to gasoline fuel injectors. There are no commercially available heavy duty LPG engines at this time, but there are medium duty LPG engines on the market. The Roush Cleantech Ford 6.8L V10 and the Power Solutions International 8.8L V8 are two examples of LPG engines derived from gasoline engines that are used in passenger buses. Cummins recently developed a purpose-built direct injected spark ignited (DISI) 6.7L LPG engine that reaches 41% brake thermal efficiency (BTE) at peak torque while also producing less CO_2 emissions than other

medium duty LPG engines [6]. The torque curves for the three previously mentioned engines are shown below in Figure 2.

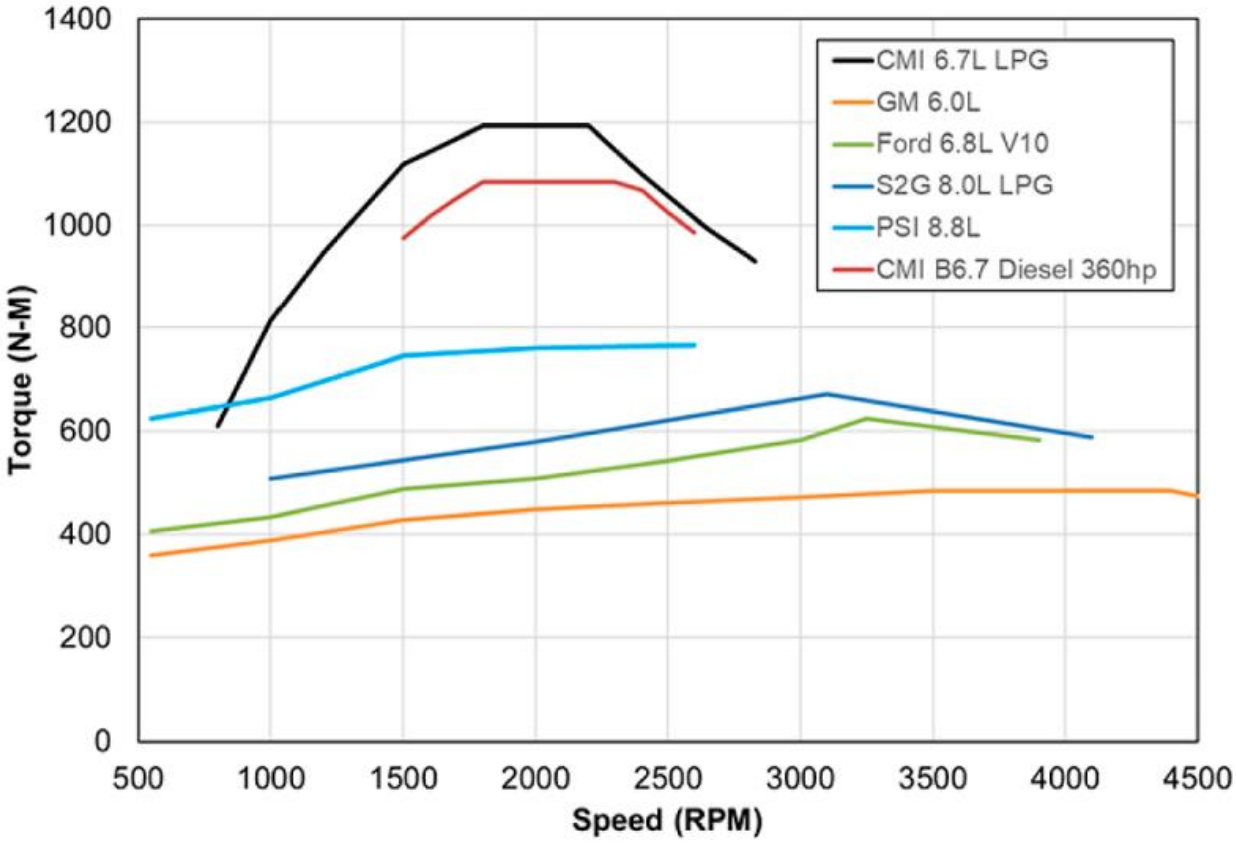

Figure 2: Torque curves for medium duty LPG engines with one diesel engine for reference [6].

1.4 Combustion Strategies

End-gas autoignition (EGAI), also known as knock, is one of the main limiting factors to improving engine efficiency. Increasing the compression ratio or turbocharged boost pressure would result in higher thermal efficiency, but it also leads to engine damage from uncontrolled combustion. Since the composition of LPG can vary within the limits of the HD-5 standard, the reactivity of the fuel and knock resistance can change. The research octane number (RON) for LPG can fluctuate based on composition since the experimental RON for propane and butane are 109.4 and 93.5, respectively [10].

Utilizing different compression ratios in a Ford 1.6L inline turbocharged DI engine, Krieck et al. found that LPG compositions with 70% propane or higher could run without knock onset at a compression ratio of 13:1, while also providing a 26% increase in brake specific efficiency at stoichiometric operation [7].

Along with mitigating the effects of knock, EGR also reduces NO_x emissions. Kim et al. found through varying the EGR levels during in-engine LPG testing that a cooled EGR system running at a 15% EGR rate reduced NO_x emissions by 34.4-46.5% depending on engine speed [11]. The implementation of the cooled EGR system caused fuel consumption to increase by about 2%, but that was offset by the implementation of stratified lean combustion to achieve significant improvement in brake specific fuel consumption (BSFC). Mustaffa et al. confirmed the use of direct injection to increase fuel efficiency of LPG by performing in-engine experiments with gasoline and LPG at various throttle positions and a constant 3000 rpm engine speed. The DI engine running on LPG produced more torque and consumed less fuel at all throttle positions than it did using gasoline [12]. In 2021, Splitter et al. [13] achieved 45% net thermal efficiency in a medium-duty single cylinder DI LPG engine through a combination of 16.8:1 compression and 30% cooled EGR. Most recently, Fosudo et al. [14] and Kar et al. [15,16] have performed extensive testing of LPG in a cooperative fuel research (CFR) engine. Their findings show that BTE is insensitive to LPG fuel composition, but the knock integral increases significantly with additional butane content. The addition of 25% EGR mitigated engine knock for all the fuel blends at an otherwise heavy knocking compression ratio. A computational fluid dynamic (CFD) study of the CFR engine supported the knock attenuating potential of EGR observed during the experiments.

1.5 Rapid Compression Machine Theory and Overview

A rapid compression machine (RCM) is a device that replicates the compression stroke of an internal combustion engine to study the ignition phenomena of a premixed fuel and oxidizer gas mixture. The compression stroke occurs very quickly and is assumed to be near-adiabatic. After compression, the piston remains fixed in place to maintain a constant volume in the reaction chamber. RCMs work on the assumption of the adiabatic core hypothesis, in which the compressed gas experiences heat loss to the reaction chamber walls, but only in a thin boundary layer between them. The piston compression creates a high temperature and pressure environment that can lead to volumetric autoignition of the mixture. If a single or two-stage ignition occurs, the ignition delay time (IDT) can be observed based on pressure changes inside the system.

Although they are only single shot machines and must use a premixed fuel/air mixture, RCMs provide the closest pressures and temperatures to a conventional internal combustion engine as shown below in Figure 3.

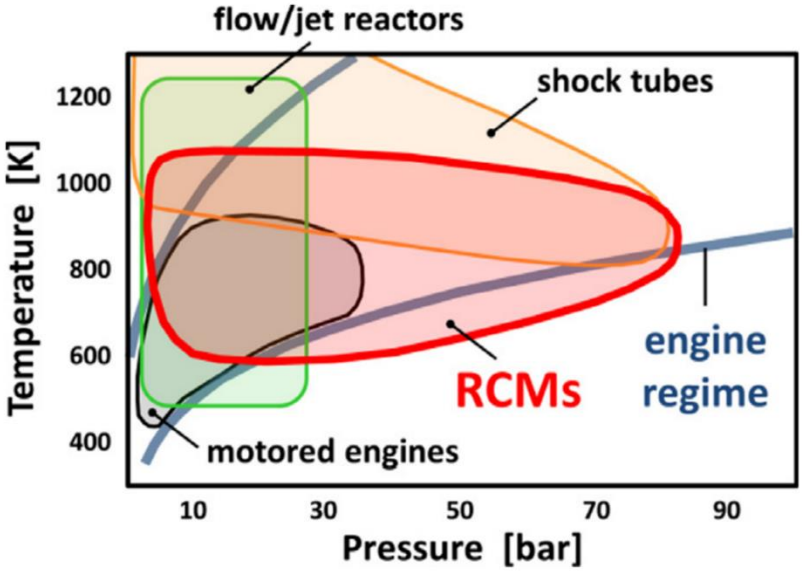

Figure 3: Typical temperature and pressure operating conditions for experimental combustion test facilities [17].

RCMs can reach the high pressure of a shock tube, while keeping temperatures low enough to study low temperature combustion and the negative temperature coefficient (NTC) regime. Most RCMs are pneumatically driven and hydraulically stopped, but there can be substantial differences in their design. A single piston RCM offers the ability to easily change the compression ratio by adjusting the end wall of the reaction chamber, and also offers more access to the reaction chamber for additional sensors or high-pressure gas sampling between compression and autoignition [18,19]. A dual piston RCM achieves faster compression times, with the inherent benefit of being a mechanically balanced system [20]. This reduces vibration and creates a quiescent zone in the gas medium between the piston faces if the pistons compress near-simultaneously. A free piston RCM involves pneumatically firing a sabot down a long cylinder before it lodges into the reaction chamber, sealing it off. The body of the RCM can be extended to achieve volumetric compression ratios as high as 37:1 and the reaction chamber end offers full optical access [21].

Facility effects is a term that is used to describe a variety of operating conditions that are unique to each individual RCM, and can have a substantial impact on measured IDTs. Some of these effects include mixture preparation methods, the duration of the compression stroke, post compression pressure loss from heat transfer, or turbulence due to piston design. Varying the ratios of inert gases in a mixture changes the heat capacity ratio and is used to change the temperature range that is tested in the RCM. This causes changes in IDT, as gases with differing thermal diffusivity will experience different amounts of heat loss from the adiabatic core. Wurmel et al. [22] studied the effects of diluent gases on IDT, showing that at equal TDC pressures and temperatures,

mixtures containing argon will have significantly longer IDTs. Wurmel also analyzed the effects of diluent gas composition on the pressure rise during the compression stroke. Di et al. [23] found that the makeup of the diluent gas had little impact on first-stage ignition of fuels, but had a significant impact on fuels with two-stage ignition behavior within the NTC regime. This occurred because of the differences in temperature rise in the various diluent gases after first-stage ignition based on their heat capacities. Goldsborough et al. [24] found that multi-stage ignition in RCMs with piston crevices could not be accurately predicted with the zero-dimensional isentropic expansion model because of heat loss to the cool crevice gases and required a multi-zone model instead. Ezzel et al. [25] conducted a virtual study of RCM configuration confirming Goldsborough's results as well as quantifying how piston crevice volume and compression speed impact IDT. Wadkar et al. [26] performed an extensive experimental study on how facility effects of the RCM as well as the mixture preparation method changed the IDT of ethanol. Ramalingam et al. [27] looked at the effects of extremely high RCM pressures on methane combustion, which included pre-ignition from hydraulic oil contamination and the need to recess pressure transducers to protect them from thermal shock. In a related study, Krause et al. [28] measured the impact of thermal shock on multiple piezoelectric pressure transducers in a spherical bomb, showing that even a thermally compensated pressure transducer's signal can be drastically improved with a thin layer of RTV silicone.

There has been a significant amount of research into the process of autoignition, beginning with Kaiser et a. in 2002 [29]. Using a homogeneous charge compression ignition (HCCI) engine, they found a sharp break in the ratio of CO to CO_2 at an air/fuel ratio of 75, indicating a transition from volumetric autoignition to a propagating flame. This

was followed by many studies to try to quantify the expected ignition behavior based on the physical and chemical mechanisms controlling autoignition. Im et al. [30] combined the prediction of mild or strong autoignition via the Sankaran criterion with the turbulent flow and scalar characteristics in terms of the Damköhler and Reynolds number to produce a regime diagram for homogeneous reactant mixtures. Grogan et al. [31] expanded the regime diagram and demonstrated its applicability to RCM experiments. Mansfield et al. [32] were able to use chemiluminescence to identify the strong ignition limits of iso-octane and show that the strong ignition limit shifted to higher temperatures with increased equivalence ratio. Goldsborough et al. [33] measured heat release rates during RCM experiments to show the point of mild autoignition initiation.

Recently, much work has been undertaken in showing how the presence of NO_x (NO and NO_2), as found in EGR, can promote or inhibit the reactivity of C_1 through C_3 hydrocarbons based on temperature and the amount of NO_x. NO_x has been shown to decrease ignition delay in a compression engine [34], RCM [35-38], shock tube [35, 39], flow reactor [40], and a jet stirred reactor [41]. These findings are especially important to the development of high compression ratio engines that utilize EGR substitution to prevent engine knock.

Propane has been used in various RCM studies, as it is the shortest hydrocarbon to exhibit NTC behavior in its ignition delay. RCM experiments involving propane have covered a wide variety of variables including equivalence ratio [20], high pressure [19], and dilution levels [42]. Ramalingam et al. [18] recently studied the IDT of four different European LPG samples, being the first to carry out RCM experiments with complex LPG mixtures. Imaging of the mild to strong ignition behavior of propane has been recorded

using a flame spectrometer [43] and chemiluminescence [44]. Their findings have major impacts on propane combustion modeling in the following ways. Simulated ignition delays can be changed significantly depending on the method used to calculate compressed gas temperatures, and that experimental measurements of IDT are systematically faster than model predictions when mild or mixed autoignition occurs. Figure 4 shows the location of the strong autoignition limit for propane based on compressed conditions.

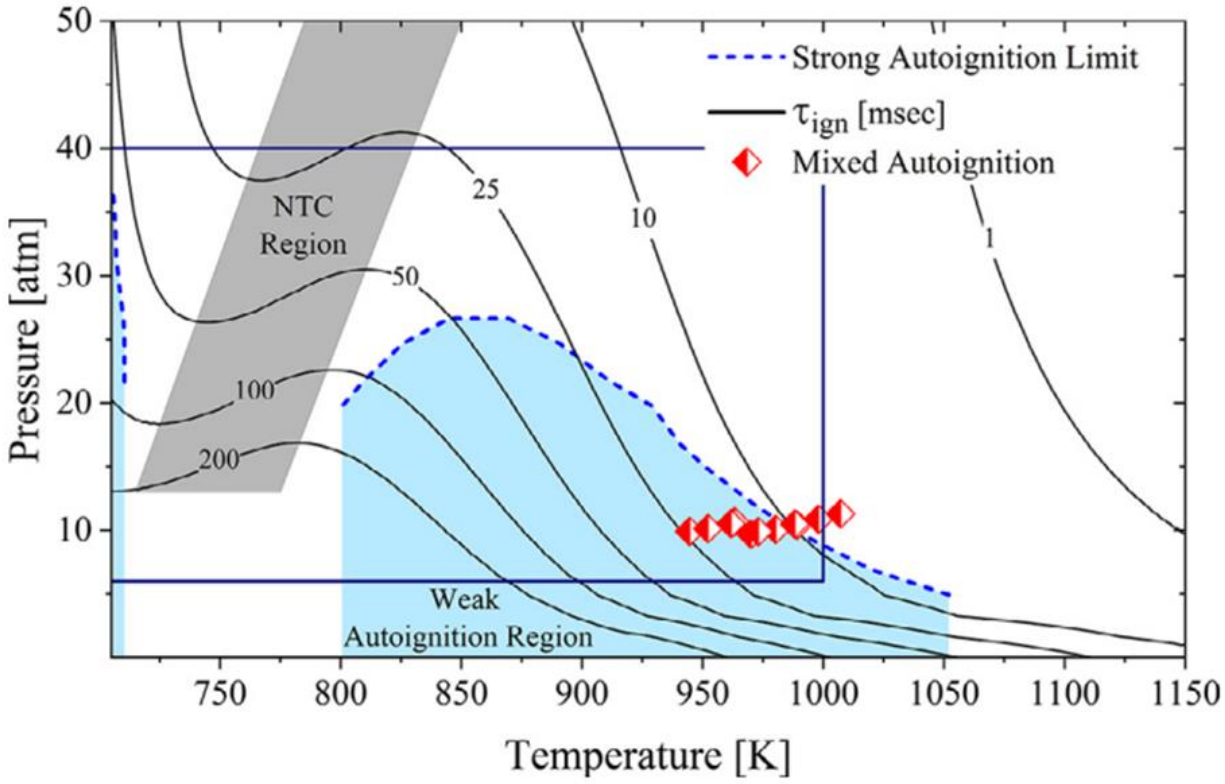

Figure 4: Propane autoignition regimes for an equivalence ratio of 0.50 [44].

1.6 Chemical Kinetic Mechanisms

A chemical kinetic mechanism is a list of species, reactions, and coefficients that are used to calculate a chemical reaction rate from the modified Arrhenius equation:

$$k(T) = AT^{b} exp\left(-\frac{E_a}{RT}\right) \quad (1)$$

where k is the reaction rate, T is the temperature in K, A is the pre-exponential factor in mol*cm*sec*K, b is the unitless temperature factor, E_a is the activation energy in cal/mole, and R is the universal gas constant. The reaction rate can then be used to solve for the rate of change in concentration of reactant species based on their initial concentrations:

$$\frac{d[A]}{dt} = -k[A][B] \tag{2}$$

where [A] and [B] are the concentrations of reactants A and B [45]. Chemical kinetic mechanisms also contain thermodynamic data, which includes coefficients for the polynomial fits of specific heat, enthalpy, and entropy. Thermodynamic data is necessary for solving the thermodynamic state after each iteration of chemical reaction processes. A program such as Chemkin-Pro numerically solves the differential equations governing the multi-species reaction rates and energy states of the system until chemical equilibrium has been reached. If the model includes any sort of fluid flow, such as a one-dimensional (1-D) laminar flame or a full three-dimensional (3-D) CFD simulation, then mass transport data must be included as part of the chemical kinetic mechanism as well to accurately predict diffusion between different point locations. The creation of detailed chemical kinetic mechanisms requires substantial experimental and theoretical studies, and the number of species and reactions in chemical kinetic mechanisms has grown by orders of magnitude as computing power continues to increase [46].

A 3-D CFD model of a combustion event may require millions of nodes to be solved simultaneously, therefore a simplified chemical kinetic mechanism is required in order to solve the system in a reasonable amount of time. The largest fuel species present in a mechanism typically determines the overall size of the mechanism. Often times, much of the mechanism is not actually required depending on the fuels being studied. Mechanism

reduction is a top-down approach to remove negligible species and reactions from a detailed chemical kinetic mechanism. Mechanism reduction uses data simulated from a detailed chemical kinetic mechanism to identify the least important species and reactions, and then sequentially remove them until a desired tolerance in predictive behavior is reached between the two mechanisms [47]. Pachler et. al [48] reduced AramcoMech 1.3 from 253 species to 70 species, achieving a 70.5% improvement in computation time with a 9.72% increase in error. However, it is possible to oversimplify a mechanism through reduction. The Sand Diego Mechanism, which is already a compact mechanism, was reduced by Bramlette and Depcik [49] to perform a 3-D simulation of a propane ramjet engine and the reduced mechanism lost significant accuracy in its ability to predict experimental shock tube ignition delay results, reinforcing that a reduced mechanism can only maintain accuracy under the chemical and thermodynamic conditions in which it was reduced.

1.7 Research Objectives

The goal of the present study is to develop a reduced chemical kinetic mechanism that can be used to accurately model three-dimensional, time-dependent, DISI, LPG engine simulations. The mechanism must predict ignition delay and flame speed across a range of fuel composition, temperature, pressure, equivalence ratios, and EGR substitution rates. Moreover, since previous work has shown reactive species such as nitric oxide (NO) present in EGR gas can affect autoignition propensity in the end-gas [50], the reduced LPG mechanism must also include NO_x/hydrocarbon chemistry. The reduced mechanism will be validated against experimental data available in the literature as well as new experiments performed in a rapid compression machine (RCM) under

engine-relevant conditions. The RCM experiments will include homogenous compression ignition experiments and laser ignited experiments, which enable measurement of flame speed and the heat release rate.

2. EXPERIMENTAL METHODS

2.1 Colorado State University RCM and Associated Instrumentation

Manufactured by Marine Technology, LTD of Galway, Ireland in 2014, CSU's rapid compression machine (RCM) features an opposed-piston design with a nominal compression ratio of 11.6:1 and compression duration of 15-25 ms. The machine's creviced pistons reduce turbulence during compression to create a quiescent zone and promote adiabatic core behavior. The major components of the RCM system are shown below in Figure 5.

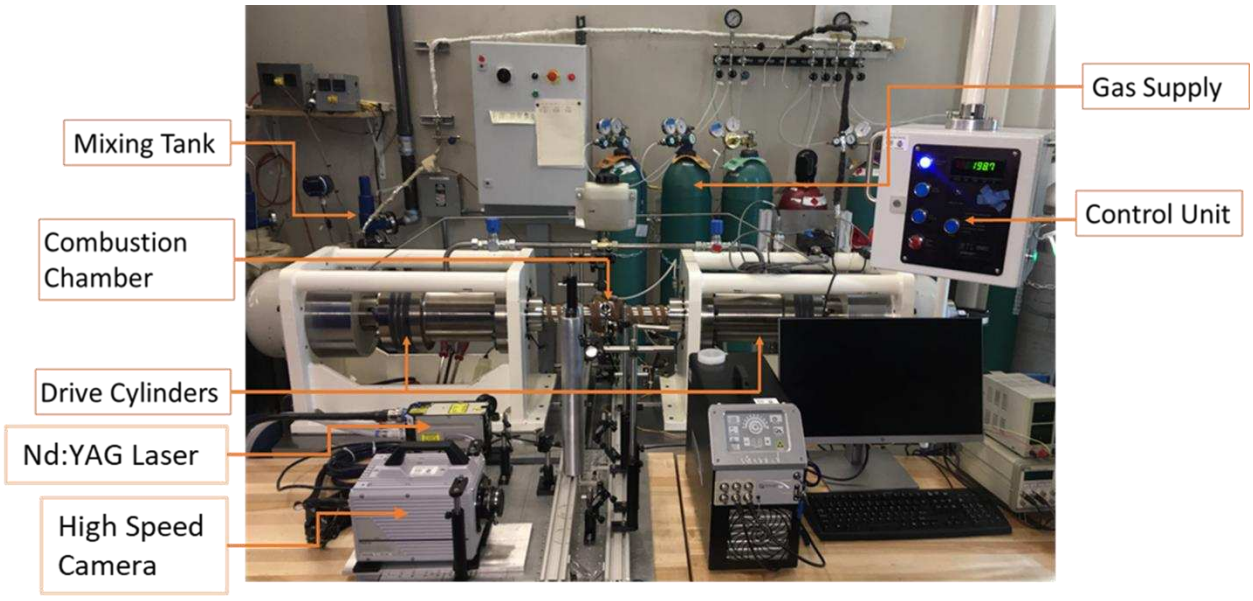

Figure 5: The CSU RCM and associated instrumentation.

In preparation to fire, the RCM's hydraulic locks are activated and the air bellows behind the drive cylinders are pumped to 200 psi. When fired, the locks are released and the cylinders are driven toward each other and held at top dead center (TDC), with a compressed volume of ~30.0 cm^3. Piston positions are measured using two Positek Limited p100 series linear transducers.

All tests during this study were performed using creviced pistons. Creviced pistons are essential to the adiabatic core hypothesis of an RCM in two ways. First, by diverting the colder gases from the thermal boundary layer with the wall to behind the piston faces they create a more uniform temperature profile across the diameter of the combustion chamber. Second, they prevent the formation of roll-up vortices that would disturb the quiescent zone created between the piston faces, maintaining a core volume largely free from fluid-dynamic disturbances as shown in Figure 6.

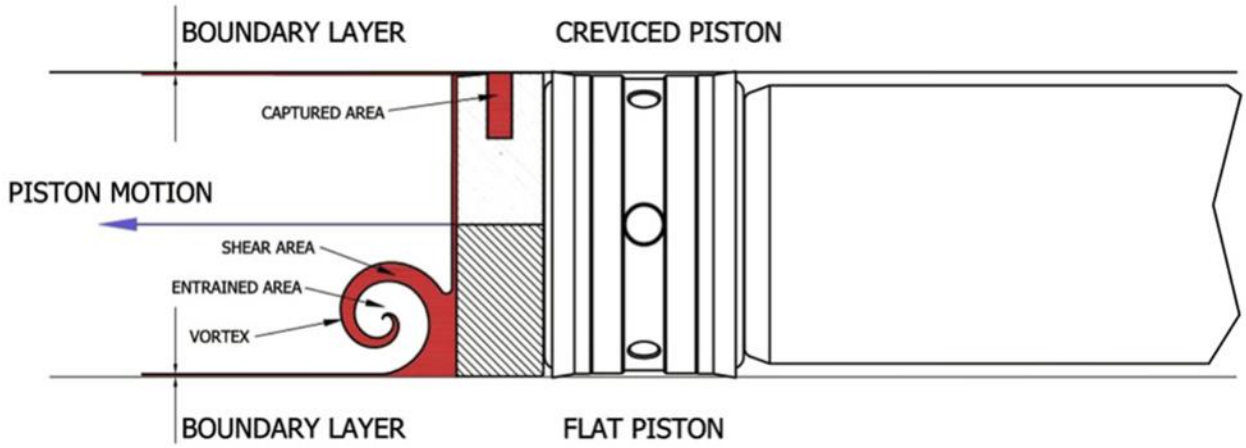

Figure 6: A creviced piston (upper half) traps gases from the boundary layer during piston motion that would create roll-up vortices if a flat piston (lower half) were used [51].

Creviced pistons have become ubiquitous in modern RCM experiments and much work has been done in showing the benefits of piston crevices [52,53], as well as the optimization of the crevice [54]. Some RCM facilities include an additional mechanism known as crevice containment for sealing off the cool gases in the crevice volume and fully preventing them from flowing back into the reaction chamber, while also preventing mass transfer from the high temperature core gases to the crevice [21,55,56].

The CSU RCM is equipped with a laser generated spark ignition system that allows for the initiation of a spherical flame at pressures and temperatures otherwise not attainable. The laser spark system was first implemented by Dumitrache et al. [57] in 2016

and is shown below in Figure 7. A Berkeley Nucleonics 555 pulse-delay generator is triggered by the rise of in-cylinder pressure to 10 bar and 14 ms later fires a 1064 nm, Q-switched, Quantel Q-smart 100 Nd:YAG laser with a pulse energy of 35 mJ, resulting in a laser spark approximately 10 ms after piston TDC. The laser passes through the first beam splitter and approximately 5% is sent toward a photodiode used to measure the spark timing relative to the in-cylinder pressure. A second beam splitter is directed toward an Ophir PE25BF-DIF-C energy sensor to indirectly measure the spark energy in the combustion chamber. The remainder of the laser beam is sent to the center of the combustion chamber through a 60 mm plano-convex focusing lens and a 12.7 mm sapphire window that protects the laser focusing assembly from the combustion event.

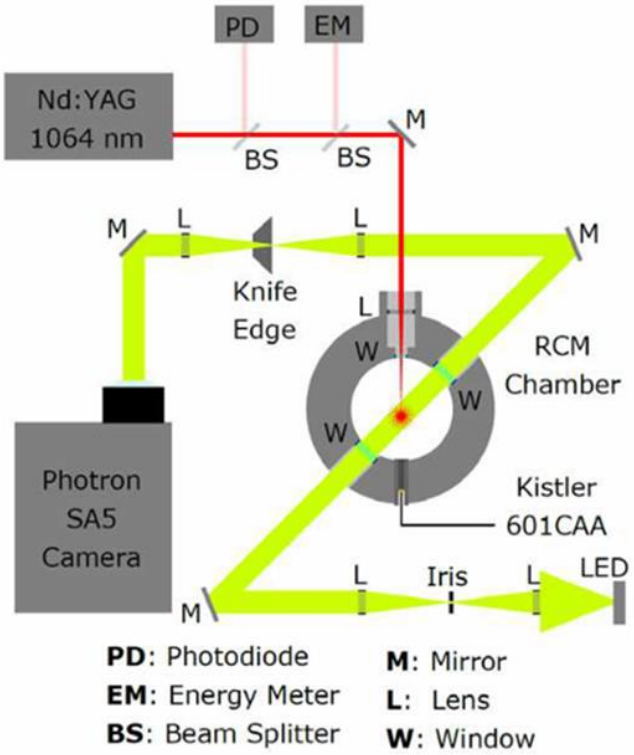

Figure 7: Schematic of the optical pathways for the laser ignition system (red) and schlieren collimated light (yellow) through the combustion chamber [58].

A schlieren optical system, also shown in Figure 7, is used to observe the laser spark and propagating flame. Light from a 404 ± 15 nm LED is collimated through a series

of lenses and mirrors before it passes through a 16.1 mm sapphire window and into the combustion chamber. The light passes through the combustion chamber and out the opposing sapphire window. It is then focused to a point and split with a knife edge. The light is re-collimated and reflected into a high-speed Photron SA5 camera operating at 50,000 frames per second and a resolution of 155 pixels/mm. The camera is controlled by the same pulse-delay generator as the laser but is set to activate immediately in order to start recording before the end of the compression stroke.

2.2 Mixture Formation and TDC Condition Control

All gas mixtures used in this study were prepared in a mixing tank with a volume of 19.23 L and a working pressure of 2 bar that can be used for gaseous or liquid fuels [59]. The mixing tank utilizes a PID controlled external heat wrap and a magnetic stir bar and allows the gaseous mixture to be sent consistently to the RCM combustion chamber. The mixing tank is evacuated by the vacuum pump prior to filling and the temperature is set to 303 K. Gasses are added to the mixture based on partial pressures, beginning with the species with the lowest mole fraction to ensure accuracy. An MKS 722B53TCD2FA Vacuum Pressure Transducer with an MKS PDR2000 Digital Power Supply and Digital Readout Capacitance Manometer Controller are used to observe the fill pressures. After filling, the mixture is allowed to stir for two hours, and the temperature is adjusted to match the desired temperature on the RCM combustion chamber. A diagram for the gas mixing system and how it connects to the RCM is shown in Figure 8.

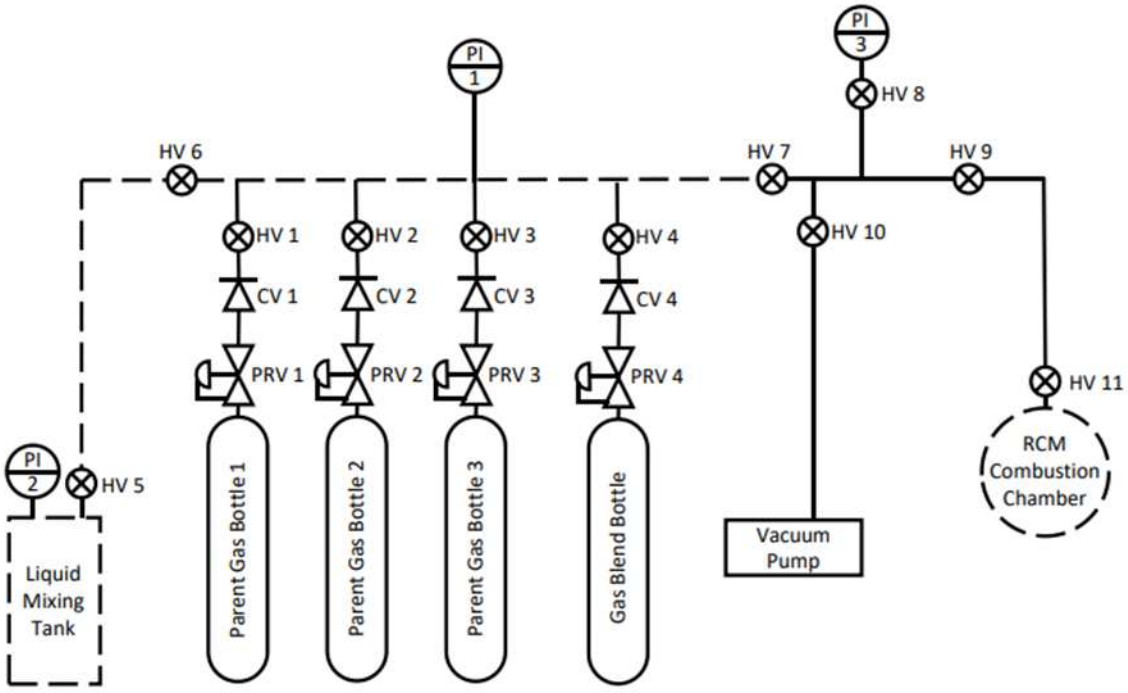

Figure 8: Piping and instrumentation diagram for the RCM gas mixing system. Dotted lines indicate temperature-controlled sections of piping. PI = pressure indicator, HV = hand valve, PRV = pressure regulated valve, CV = check valve [60].

The gases and purities used in this study were propane (99.99%), nitrogen (99.999%), argon (99.999%), carbon dioxide (99.995%), oxygen (99.994%), ethane (99.975%), propene (99.95%), n-butane (99.99%), and isobutane (99.99%). The R-EGR mixture was supplied by Airgas, while the NR-EGR was added to the mixing tank from the individual component bottles. The composition of both exhaust gas mixtures is shown below in Table 1.

Table 1: Gas composition of the R-EGR and NR-EGR mixtures.

	% 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%	-

In an internal combustion engine, the exhaust gas contains nitrogen as its main component instead of argon, but in the RCM, this would prevent the compressed gas from reaching sufficiently high temperatures required for low-reactivity experiments. The amount of NO in the R-EGR mixture was selected to be higher than the recorded engine out NO_x emission values of the 6.7 L Cummins LPG engine. EGR was added to the fuel/inert/oxidizer mixture on a mass substitution basis from 0 to 30% using Equation 3:

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

where m is the mass of a component species and subscripts indicate the type of component. One unforeseen effect of adding the R-EGR to the mixing tank with the fuel and air is the rapid conversion of NO to NO_2 in the presence of oxygen. The conversion of NO to NO_2 during mixture preparation was observed by Sahu et al. [35] during the course of this study. Based on their findings, it is false to assume that the fuel/air/R-EGR mixture contains the initial amount of NO by the time the gas mixture is delivered to the RCM. A Chemkin homogeneous constant volume reactor model based on the gas mixing tank was used to show that after the two-hour waiting period observed for gas mixing, almost all the NO was converted to NO_2. The time history of the NO oxidation is shown below in Figure 9. Based on these results, autoignition and flame propagation models were performed again using NO_2 in the gas mixture instead of NO.

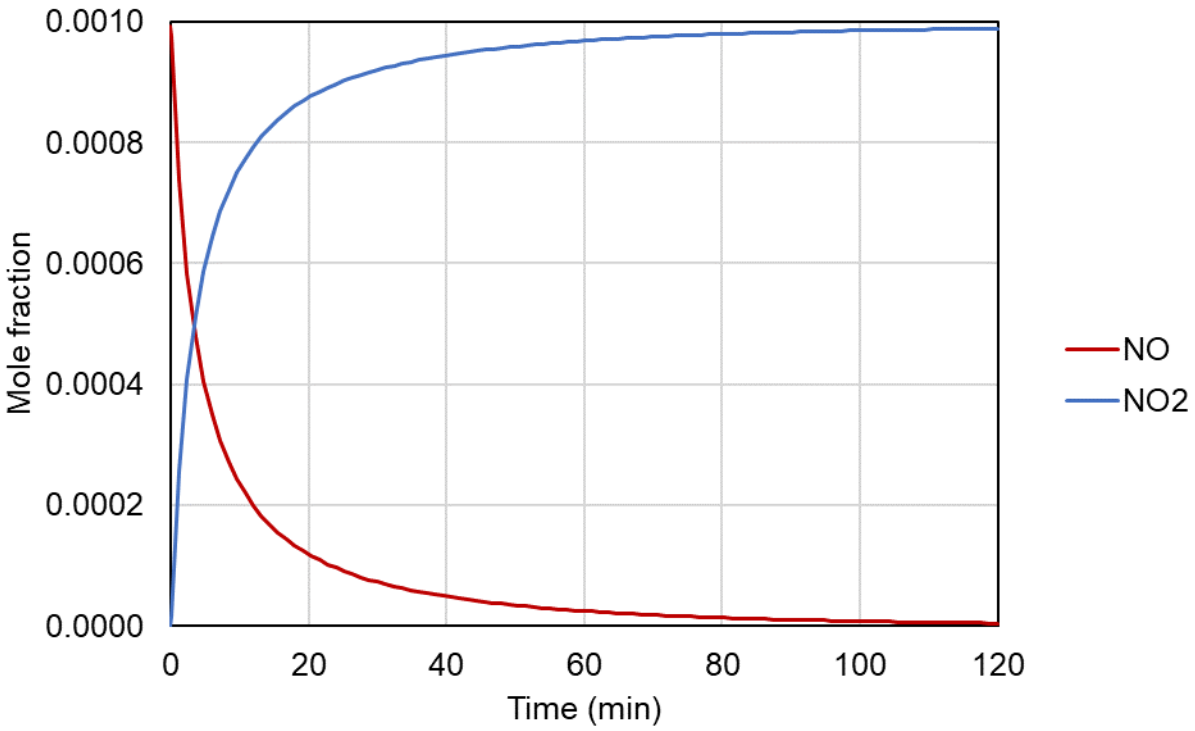

Figure 9: Conversion of NO to NO_2 over time in a model of the RCM mixing tank with 30% R-EGR and C_3H_8/air at 2 bar and 333 K.

The external temperature of the RCM combustion chamber and sleeves is maintained by an OMEGA SRT201 heat wrap with a Lightobject JLD612 PID controller. The temperature can be varied from 298 to 343 K depending on the desired temperature at piston TDC. Autoignition tests were performed by beginning at the low end of the temperature range for a mixture, and giving the RCM sufficient time for the external temperature to stabilize as temperature is increased. The TDC temperature range for each autoignition experimental case was approximately 700-900 K. Increasing the ratio of argon/nitrogen in the inert gas is also used to increase TDC temperature, while adding CO_2 to the inert gas will lower TDC temperatures. The initial pressure of the gas mixture inside the RCM is measured with a second MKS 722B53TCD2FA and MKS PDR2000. The initial pressure was allowed to vary between fuel/inert/oxidizer/EGR mixtures in order to maintain a nominal 24 bar TDC pressure. The RCM combustion chamber was

evacuated before filling with the appropriate gas mixture for the first time, and after piston retraction following each combustion event.

2.3 Ignition Delay Time Measurements

A thermally compensated, high speed Kistler 601CAA piezoelectric pressure transducer with a Kistler Type 5018 charge amplifier is used to record the dynamic pressure of the reaction chamber. The pressure data and piston positions are logged using a 12-bit Picoscope 4424 data acquisition system with a 2 MHz sample rate. A MATLAB script is used to process the homogeneous IDT experimental tests. First, the script averages the first 50 ms of high-speed pressure data and pegs that average to the initial chamber pressure measured by the absolute pressure transducer. This pegging process allows pressure trace to also contain the correct absolute pressures. The pressure trace is filtered using an 8^{th} order Butterworth filter followed by calculating the pressure derivative. The derivative of pressure is used to locate the moment of piston TDC, a local maximum, and the moment of autoignition, found with the maximum pressure rise. The time difference between these two points is the homogeneous IDT, demonstrated in Figure 10.

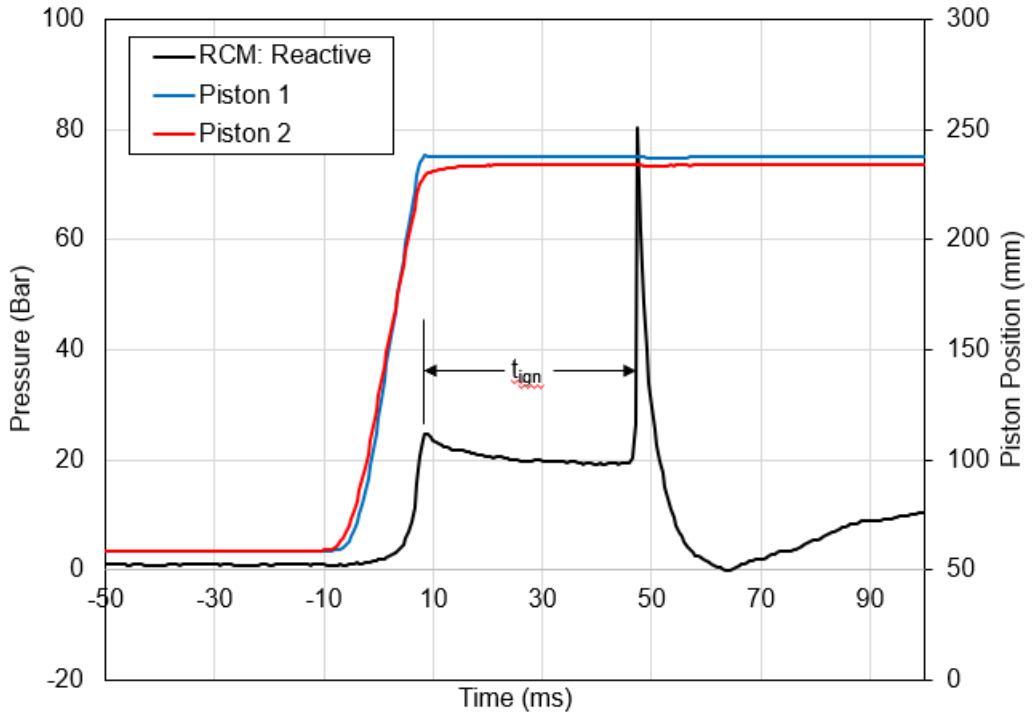

Figure 10: Recorded signals from an IDT experiment (Pc = 24 bar, Tc = 845 K, Φ = 1).

The temperature inside the RCM cannot be directly measured due to the speed at which it changes as well as the extreme conditions created by the combustion event, so it is necessary to calculate the TDC temperature based on an isentropic process:

$$\frac{T_c}{T_i} = \left(\frac{P_c}{P_i}\right)^{\frac{\gamma-1}{\gamma}} \tag{4}$$

where T_c is the compressed temperature at TDC, T_i is the initial mixture temperature, P_c is the compressed pressure, P_i is the initial pressure, and γ is the heat capacity ratio. Since the heat capacity ratio of a mixture changes with increasing temperature, the TDC temperature must be iterated toward. All TDC temperatures in this study were calculated using the adiabatic compression and expansion routine of Gaseq [61], which uses the initial mixture conditions and TDC pressure to solve the TDC temperature assuming frozen chemistry. A table of gas mixture compositions and TDC conditions for all autoignition experiments is available in Appendix A.

2.4 Estimation of Flame Propagation Rate

The series of schlieren images acquired during each test are run through a MATLAB script developed and utilized previously by Zdanowicz [62]. The script identifies the image which contains the spark ignition and then counts the pixels within the expanding flame front of each subsequent image as shown in figure 11.

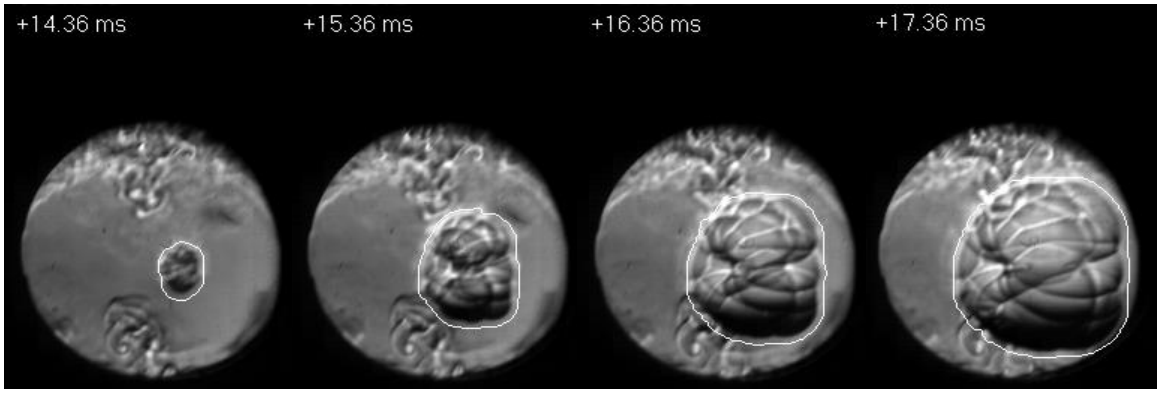

Figure 11: A representative sequence of images showing how the flame front is tracked from the moment after spark ignition until the flame front reaches the window perimeter.

Flame radius as a function of time is plotted by projecting the size of each flame image into a circle shown below in Figure 12.

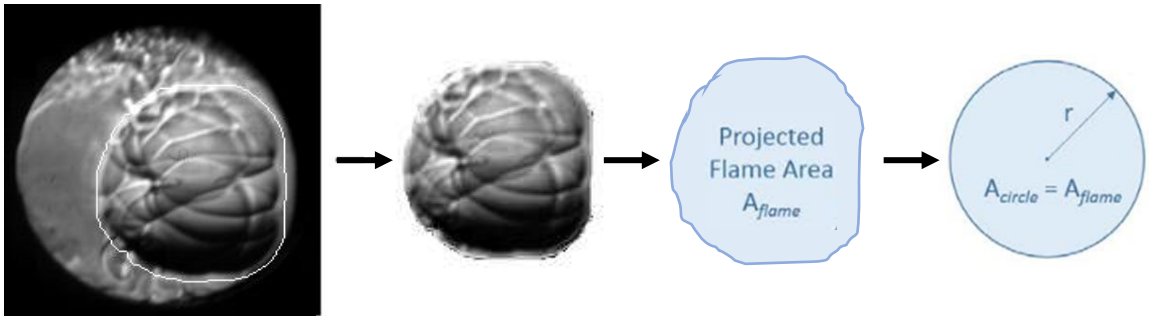

Figure 12: A conceptualization of the conversion of the flame front imagery to a circle with changing radius.

A second order polynomial is fit to the projected flame radius as a function of time. Non-linear extrapolation of the Kelley and Law method eliminates flame stretch effects and provides the zero-stretch burned gas flame speed according to Equation 5:

$$s_b = s_b^0 t + cr_f + 2L_b \ln(r_f) - 4\frac{L_b^2}{r_f} - \frac{8}{3}\frac{L_b^3}{r_f} \quad (5)$$

where s_b is the burned propagation rate found with the second-order polynomial in cm/s, s_b^0 is the zero-stretch burned propagation rate in cm/s, t is time in s, c is a measured constant, r_f is the projected spherical flame radius in cm, and L_b is the Markstein length in cm [63, 64]. Since Equation 5 is only valid for spherical laminar flames, experiments with piston offsets less than 2 ms were used to reduce the effects of turbulence. Equation 6 converts the extrapolated zero-stretch burned propagation rate to an unburned flame propagation rate by correcting for the change in density across the flame front [64]:

$$s_u = s_b \left(\frac{\rho_b}{\rho_u}\right) \quad (6)$$

where s_u and s_b are the unburned and burned flame propagation rates in cm/s and ρ_u and ρ_b are the unburned and burned gas density in kg/m^3. GASEQ calculated the unburned density using the initial RCM conditions and TDC pressure. 1-D flame speed simulations with NUIGMech1.1_HT in Chemkin approximated the burned gas density. A table of gas mixture compositions and TDC conditions for all flame propagation rate experiments is available in Appendix B.

2.5 Apparent Heat Release Rate

The apparent heat release rate (AHRR) is calculated from the high-speed pressure data. After the pistons reach TDC the reaction chamber is maintained at a constant volume, allowing the AHRR in W of the combustion event to be calculated by:

$$AHHR = \frac{dQ}{dt} = \frac{1}{\gamma - 1} V \frac{dP}{dt} \quad (7)$$

Where γ is the ratio of specific heats of the gas mixture provided by GASEQ at TDC conditions, V is the volume of the combustion chamber in m^3, P is the pressure in Pa, and

t is the time in s. $\frac{dQ}{dt}$ represents the net rate of external heat addition to the gas mixture that would result in the measured pressure rise $\frac{dP}{dt}$ but is actually the heat released by the combustion reaction, converting chemical energy into thermal energy. Changes to the species concentration as well as the specific heat ratio were not accounted for after TDC. The profile of the AHRR curve can be used to determine if and when EGAI occurs ahead of the flame front. An example of a laser ignited experiment and its associated AHRR curve are shown below in Figure 13.

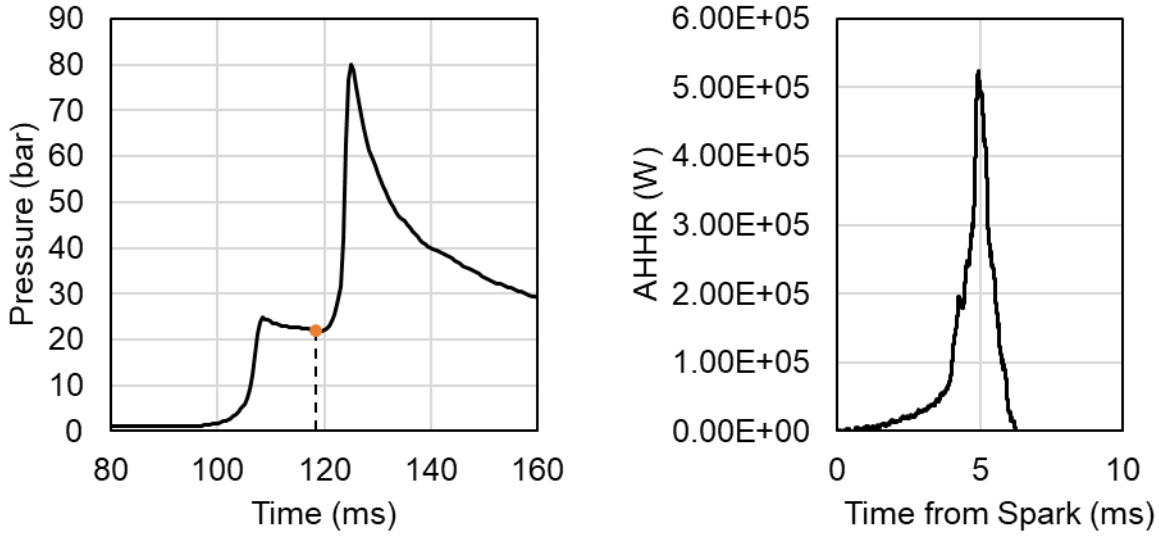

Figure 13: A pressure trace for a laser ignited test of $C_3H_8/N_2/O_2$ at 24 bar, 700 K, and Phi = 1.00 (left) with the spark timing denoted by an orange circle, and its calculated AHHR profile with no visible occurrence of EGAI (right).

3. CHEMICAL KINETIC MECHANISM DEVELOPMENT

3.1 Ignition Delay Time Models

All modeling in this study used ANSYS Chemkin-Pro 2021 R1. The Closed Homogeneous Batch Reactor was used for modeling ignition delay times. It is a zero-dimensional (0-D) model. 0-D models assume that chemical reactions proceed in a spatially uniform manner, all thermodynamic conditions are uniform, and only one thermodynamic state is needed to describe the reaction process [17]. The most basic approach to simulating autoignition is to use a constant volume, adiabatic reactor model that begins at the same temperature and pressure as the TDC conditions of an RCM experiment. This method was used for all experimental cases to determine the accuracy of the reduced mechanism to the chosen detailed mechanism. This is an oversimplification of most RCMs, however, and will produce simulated IDTs lower than those observed in experiments [51]. A constant volume reactor is missing two crucial pieces of information, the potential radical buildup already occurring during the compression stroke, and the heat loss from the compressed gases to the RCM combustion chamber walls. The most common way to replicate these conditions is using an effective volume profile. To calculate an effective volume profile, a non-reactive gas mixture of fuel, inert gases, and nitrogen replacing the oxygen is compressed in the RCM. An example of a reactive pressure trace and its corresponding non-reactive pressure trace are shown in Figure 14. In the case of propane mixtures, the non-reactive pressure trace should continuously decline after compression, while the reactive pressure trace

slightly rises due to the heat released into the gas mixture during radical buildup before autoignition.

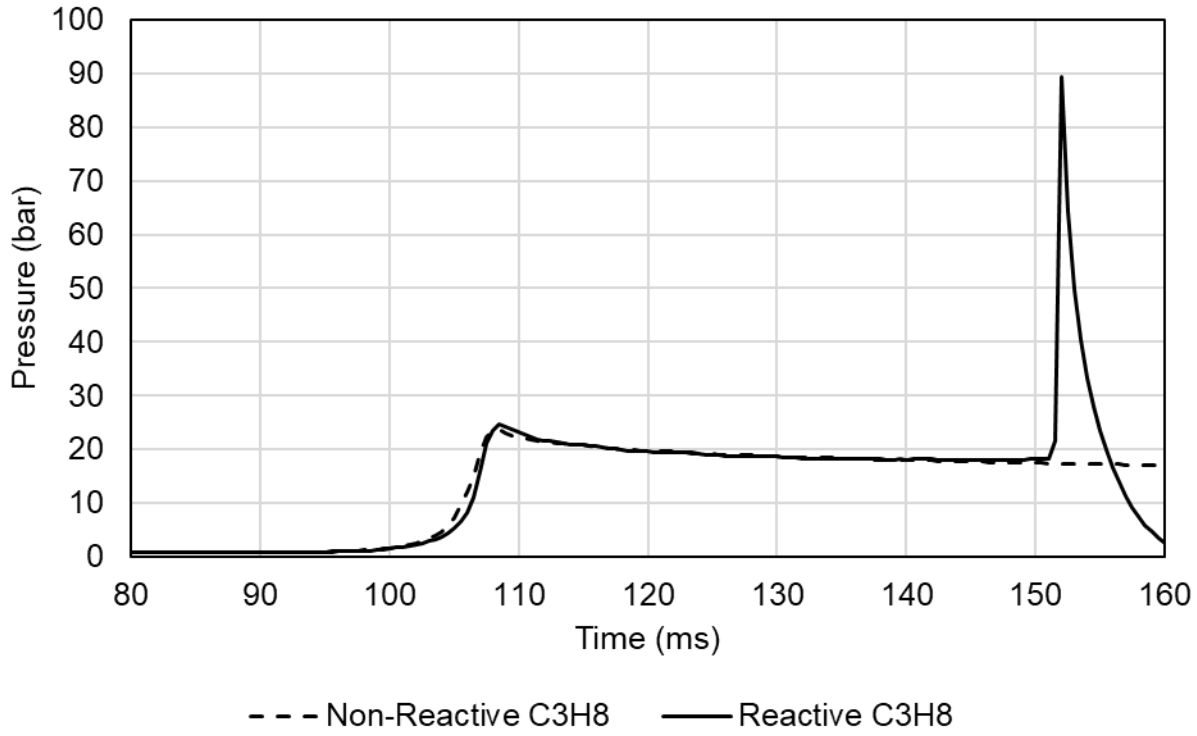

Figure 14: Recorded pressure trace from an autoignition test (solid line) of $C_3H_8/Ar/O_2$ and its associated non-reactive pressure trace of $C_3H_8/Ar/N_2$ (dashed line).

In this study the reactive pressure trace data until TDC was combined with the after TDC data of the non-reactive pressure trace to make a combined pressure trace as described by Dames et al. [65]. The combined pressure profile, along with the gas composition and initial conditions of the reactive pressure trace are used as inputs in a pressure constrained 0-D model with an initial volume of 1 m^3 and a gas reaction rate multiplier of zero. The model should reach the same TDC pressure and temperature observed in the reactive RCM test, but then decline similarly to the non-reactive test. Chemkin will export the reactor volume profile of the model. The volume profile will mimic the compression stroke of the RCM and then slowly expand to account for the pressure drop in the RCM due to heat loss. The volume profile can then be used as a constraint for the 0-D model,

which along with the proper initial pressure, temperature, and mixture conditions should recreate the conditions of the reactive pressure trace. The combined pressure trace and effective volume profile was used in the models for stoichiometric propane with and without 30% NR-EGR and 30% R-EGR to attempt to capture the facility effects of the CSU RCM.

3.2 Flame Propagation Rate Models

Laminar flame speed simulations were performed using the flame_speed__parameter_study.ckprj file located in the samples2010 folder of Chemkin. The mixture-averaged model was used for calculating the transport properties. Simulations were converged to a grid-independent solution with 300 as the maximum number of grid points. GRAD and CURV values were adjusted to 0.1 and both relative tolerance values were decreased to 1.0E-6. Inlet gas composition, temperature and pressure were adjusted to match published data for mechanism reduction, or RCM TDC conditions for modeling experimental data from this study.

3.3 Detailed Mechanism Selection

Eight detailed chemical kinetic mechanisms were evaluated to determine which were the most accurate at reproducing experimental data from literature and to select the mechanism that represents the best starting point for LPG mechanism reduction. The mechanisms that were evaluated are summarized below in Table 2.

Table 2: Detailed mechanisms selected for evaluation.

Detailed Mechanism	Origin	Species	Reactions
AramcoMech3.0	NUI Galway [66]	581	3,034
NUIGMech1.1	NUI Galway [67]	2,746	11,279
San Diego Mech	UC San Diego [68]	58	268
USC Mech Version II	University Southern California [69]	111	784
C1-C3 + NOx	Polytechnic University of Milan [70]	159	2,459
C1-C16 HT+LT+NOx	Polytechnic University of Milan [71]	537	18,250
Gaseous Fuels	ANSYS Chemkin-Pro [72]	1381	9,684
ARIES 82	Colorado State University [60]	82	519

Performance of the detailed chemical kinetic mechanisms was evaluated by comparing predicted ignition delay periods from constant volume, stoichiometric, 30 bar closed reactor simulations over a range of temperatures from 600-1000 K. The results of the simulations are shown below in Figure 15.

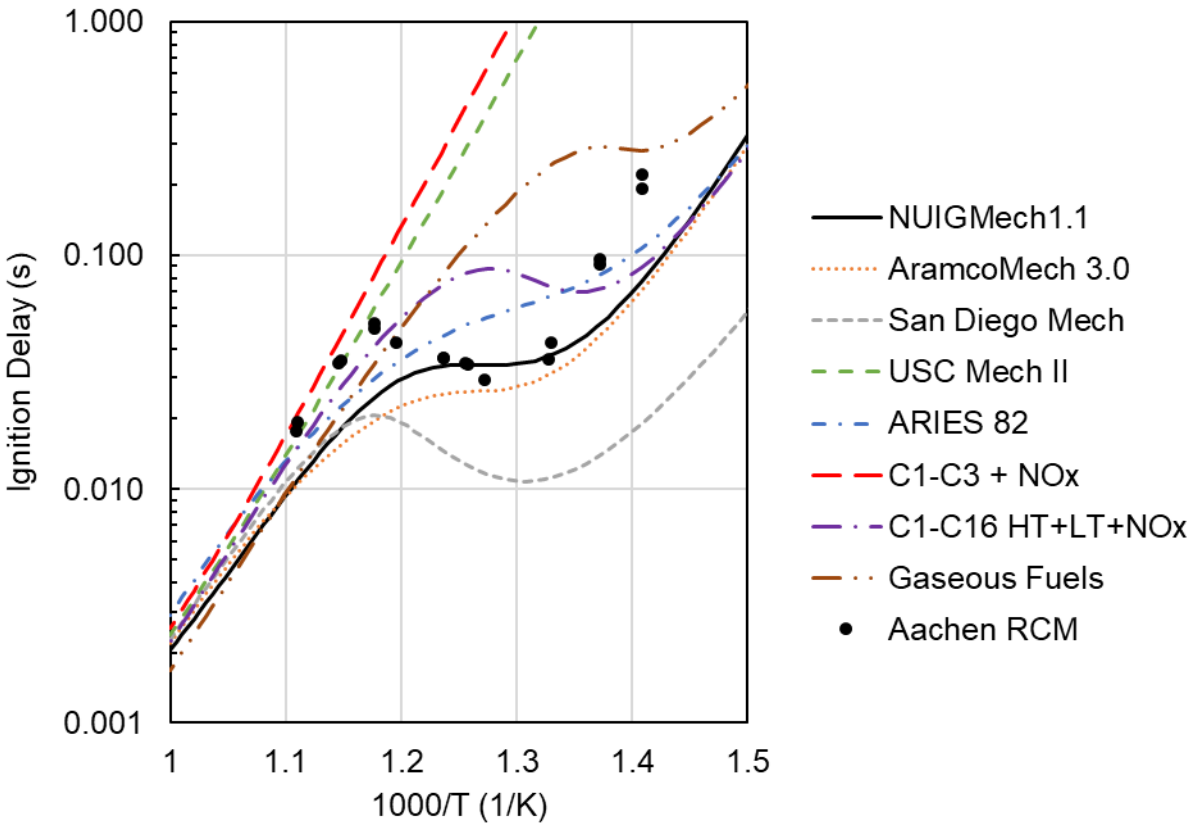

Figure 15: Fixed volume homogeneous autoignition of stoichiometric propane/air at 30 bar pressure as predicted by eight chemical kinetic mechanism (lines) in comparison with experimental results (black circles) from Ramalingam et al. [19].

All of the mechanisms showed reasonable agreement above 900 K. However, the USC Mech Version II mechanism and C1-C3 + NOx mechanism did not predict any low temperature reactivity and were eliminated as candidates for mechanism reduction. The San Diego Mechanism captured the NTC effect but appeared to be overly reactive at low temperatures. Both the C1-C16 HT+LT+NOx mechanism and the Gaseous Fuels mechanism predicted NTC behavior, but not in the same temperature range as the experimental data. ARIES 82 was developed for natural gas engines and lacks the propane chemistry necessary to fully predict NTC behavior. NUIGMech1.1 and AramcoMech 3.0 behave similarly with the former being slightly less reactive over the entire temperature range. Since NUIGMech1.1 contains recent updates to various sub-

mechanisms and contains detailed NOx chemistry, it was decided to proceed with NUIGMech1.1 for mechanism reduction.

3.4 Mechanism Reduction

Mechanism reduction was performed in Chemkin Reaction Workbench initially using the Directed Relation Graph with Error Propagation (DRGEP) method [73] with the autoignition results from stoichiometric propane combustion in air using NUIGMech1.1 as the target. The reduced mechanisms produced by this method became too inaccurate as the species count neared 100. In addition, both isobutane and n-butane were removed since they were not explicitly identified in the target model. Accordingly, more computationally intensive methods were used to improve the reduction results. A reduction operation sequence of DRGEP, Directed Relation Graph (DRG), DRG with Path Flux Analysis (DRGPFA), followed by the same three methods with added Sensitivity Analysis was used to achieve much greater accuracy in the reduced mechanisms [73]. This six-step reduction sequence was repeated until the reduced mechanism reached the specified error from the target mechanism. To ensure that the reduced mechanism contained all the needed reactions to predict ignition delay for the possible species present in LPG, autoignition of a fuel blend containing 60% propane, 10% ethane, 10% propene, 10% isobutane, and 10% n-butane was used as the target model. It was also necessary to constrain the mechanism reduction by the max NO mole fraction. Since NO created during the combustion event does not impact the IDT, Reaction Workbench will remove NOx chemistry from the reduced mechanism unless it is included as a target value. The details of the reduced mechanisms are listed in Table 3.

Table 3: Mechanism reduction schemes and reduction results for NUIGMech1.1.

Reduction Method	Fuel	Target	Tolerance	Species	Reactions
DRGEP	C_3H_8	IDT	5%	192	1,367
DRGEP	C_3H_8	IDT	10%	143	1,036
DRGEP	C_3H_8	IDT	15%	114	810
DRGEP, DRG, DRGPA, Sensitivity	Blend	IDT	1%	219	1761
DRGEP, DRG, DRGPA, Sensitivity	Blend	IDT	5%	128	965
DRGEP, DRG, DRGPA, Sensitivity	Blend	IDT	10%	102	717
DRGEP, DRG, DRGPA, Sensitivity	Blend	IDT / max NO mol fraction	1% / 10%	251	1,999
DRGEP, DRG, DRGPA, Sensitivity	Blend	IDT / max NO mol fraction	5% / 10%	153	1,227
DRGEP, DRG, DRGPA, Sensitivity	Blend	IDT / NO mol fraction	10% / 10%	100	670

Comparison of the reduced mechanisms to the NUIGMech1.1 target case showed that the 128 and 153 species reductions predicted IDT within 1 ms of the detailed mechanism at all but the lowest temperature point. The 219 and 251 species reductions were deemed too large to be computationally efficient in 3-D simulations. The 102 and 100 species reductions performed well at low and high temperatures but deviated to the maximum error allowed throughout the NTC regime. The 100 species mechanism also drastically underpredicted IDT for propane with 30% R-EGR, indicating that 100 species is simply too small for a mechanism required to accurately predict LPG reactivity across the full range of engine operating conditions. The 153 species reduction, hereafter referred to as ALPINE 153, was chosen as the optimal reduced mechanism. The full text of ALPINE 153 is listed in Appendix C.

ALPINE 153 was used to model the same experimental results from the RWTH Aachen University RCM in Figure 15, but this time using the more accurate variable volume modeling method with the effective volume profiles and initial conditions included in that study. Figure 16 shows the performance of ALPINE 153 and NUIGMech1.1 against the experimental IDTs. The IDTs predicted by the detailed and reduced mechanisms are never more than 1 ms apart and show good agreement with the experimental data.

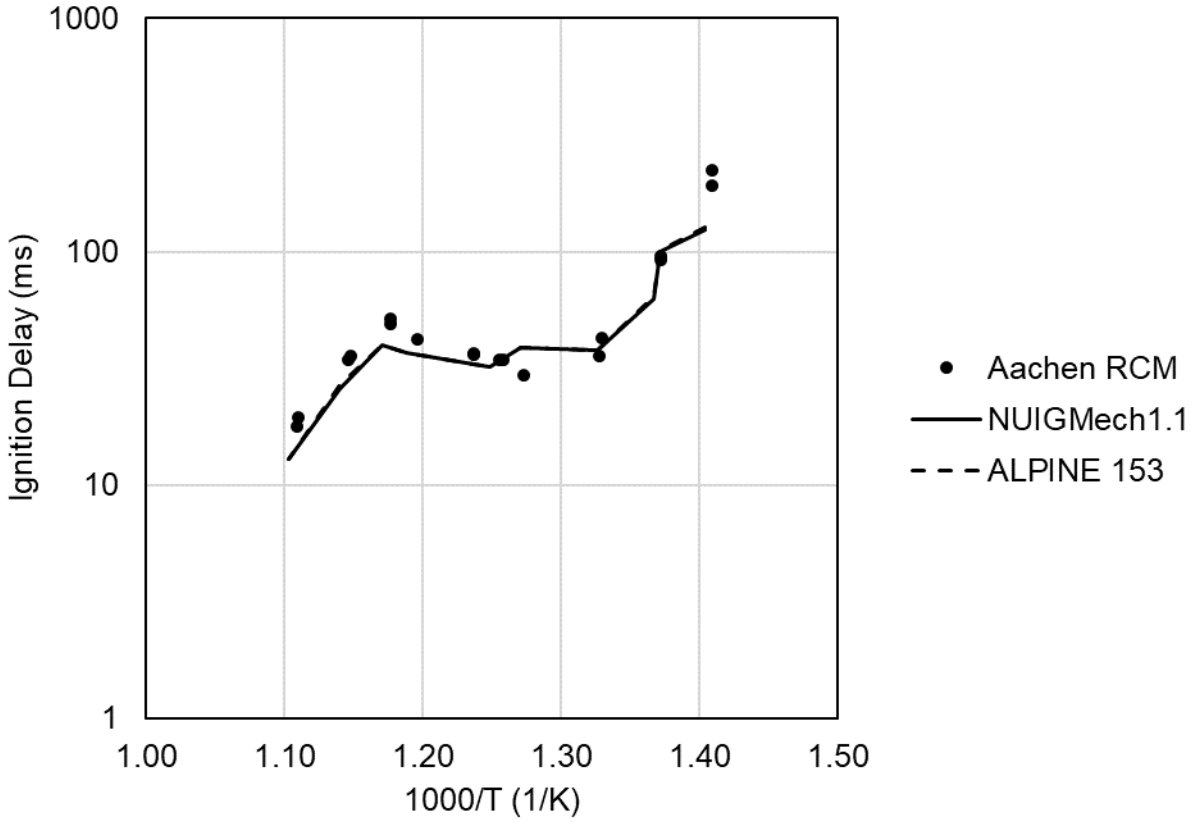

Figure 16: Variable volume homogeneous autoignition of stoichiometric propane/air at 30 bar pressure as predicted by NUIGMech1.1 and ALPINE 153 (lines) in comparison with experimental results (black circles) from Ramalingam et al. [19].

The RCM at RWTH Aachen University uses a single piston design, so it was also necessary to compare the reduced mechanism to a data set from a dual piston RCM, as they have different compression behavior and facility effects. The RCM at NUI Galway uses the same design as the RCM at CSU and has also been used to study propane

combustion at the same pressure and similar temperatures. Again, the modeled IDTs for both mechanisms match very well with the experimental data in Figure 17, only deviating from each other at the coldest temperature but still within the experimental IDT variation.

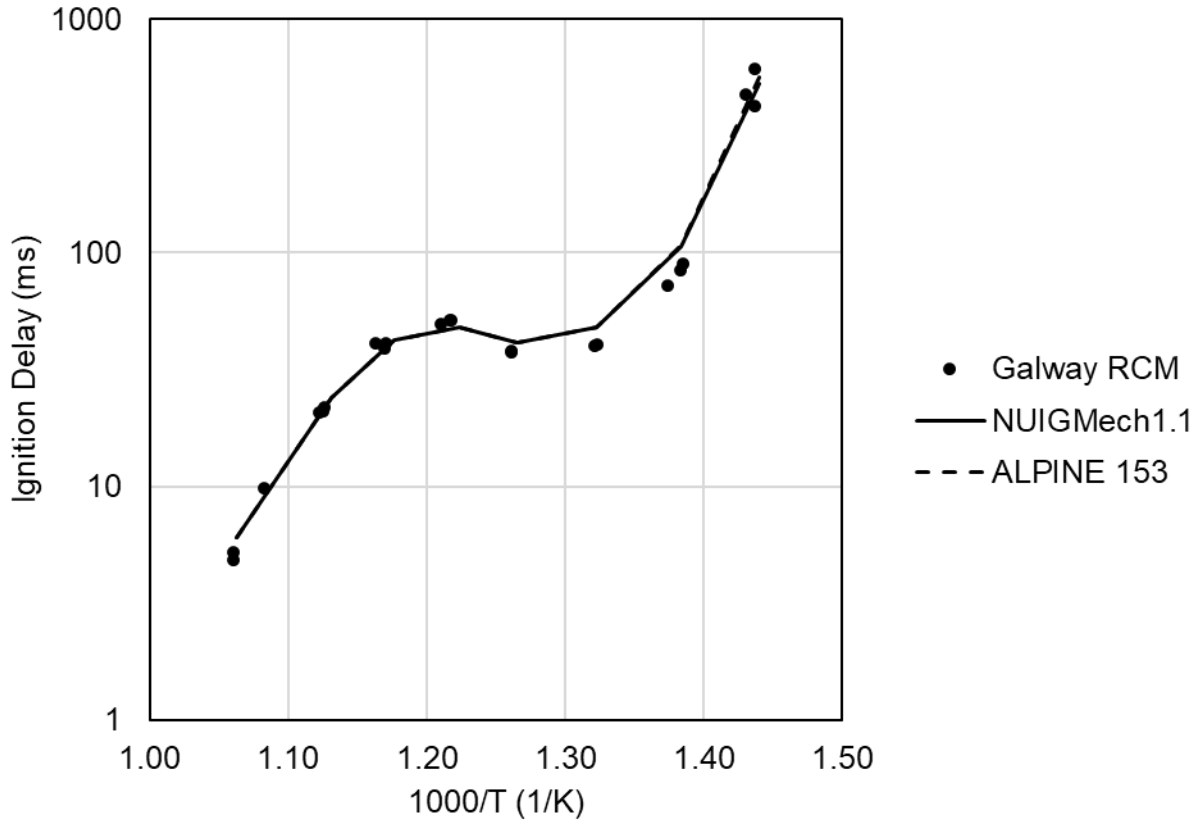

Figure 17: Variable volume homogeneous autoignition of stoichiometric propane/air at 30 bar pressure as predicted by NUIGMech1.1 and ALPINE 153 (lines) in comparison with experimental results (black circles) from Mohamed et al. [74].

Both NUIGMech1.1_HT and ALPINE 153 were compared to the same experimental data from literature used to validate NUIGMech1.1 for flame speed accuracy. NUIGMech1.1_HT is a high temperature version of NUIGMech1.1 that removes all the species and reactions that are not relevant to flame chemistry to be more computationally efficient. Both mechanisms perform very similarly to each other at low temperatures and pressures as seen in Figure 18, although it should be noted that as pressure increases, they also overpredict laminar flame speed in the lean condition.

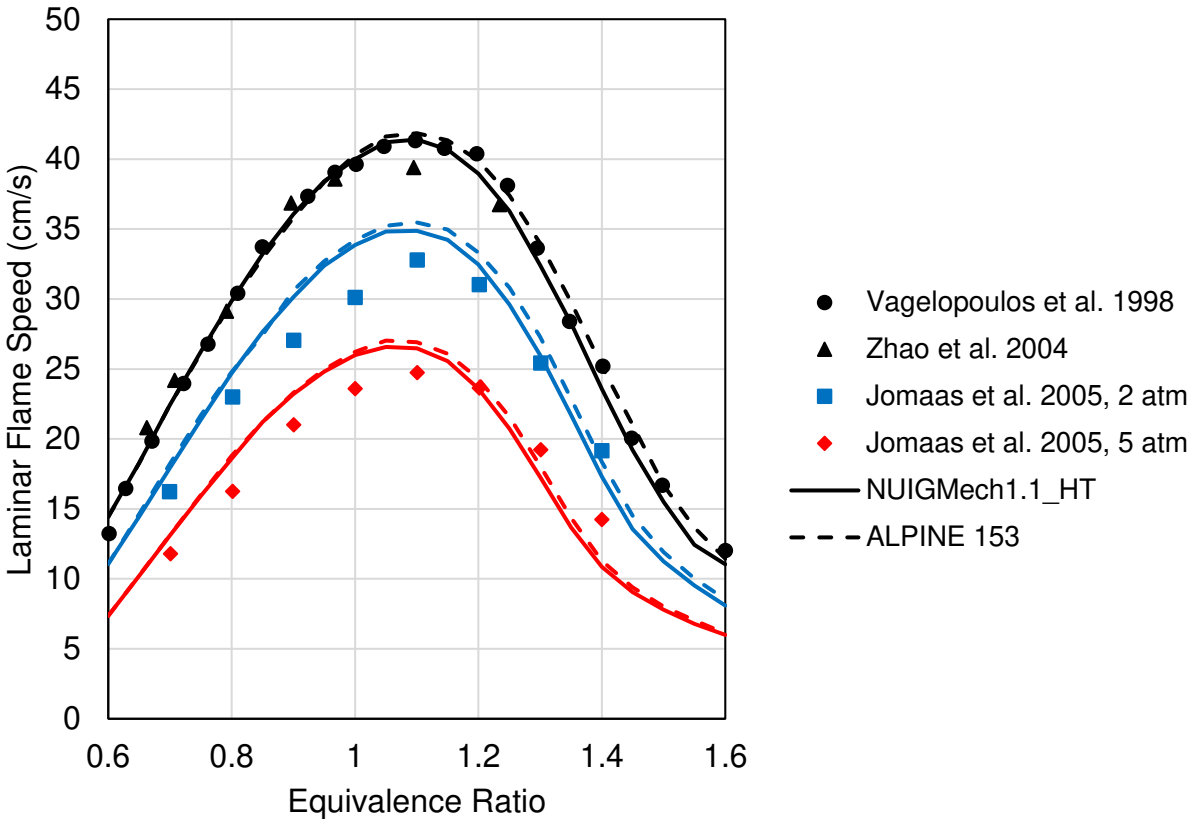

Figure 18: Simulated (lines) and experimentally measured (symbols) laminar flame speeds for pressures of 1, 2, and 5 atm at 298 K from literature [75-77].

4. EXPERIMENTAL RESULTS

4.1 Homogeneous Ignition Delay Time

Homogeneous ignition delay results for lean, stoichiometric, and rich propane/air mixtures with an equivalence ratio of 0.75, 1.0, and 1.5 respectively for nominal TDC pressure of 24 bar and approximate temperature range of 700 to 900 K are plotted below in Figure 19.

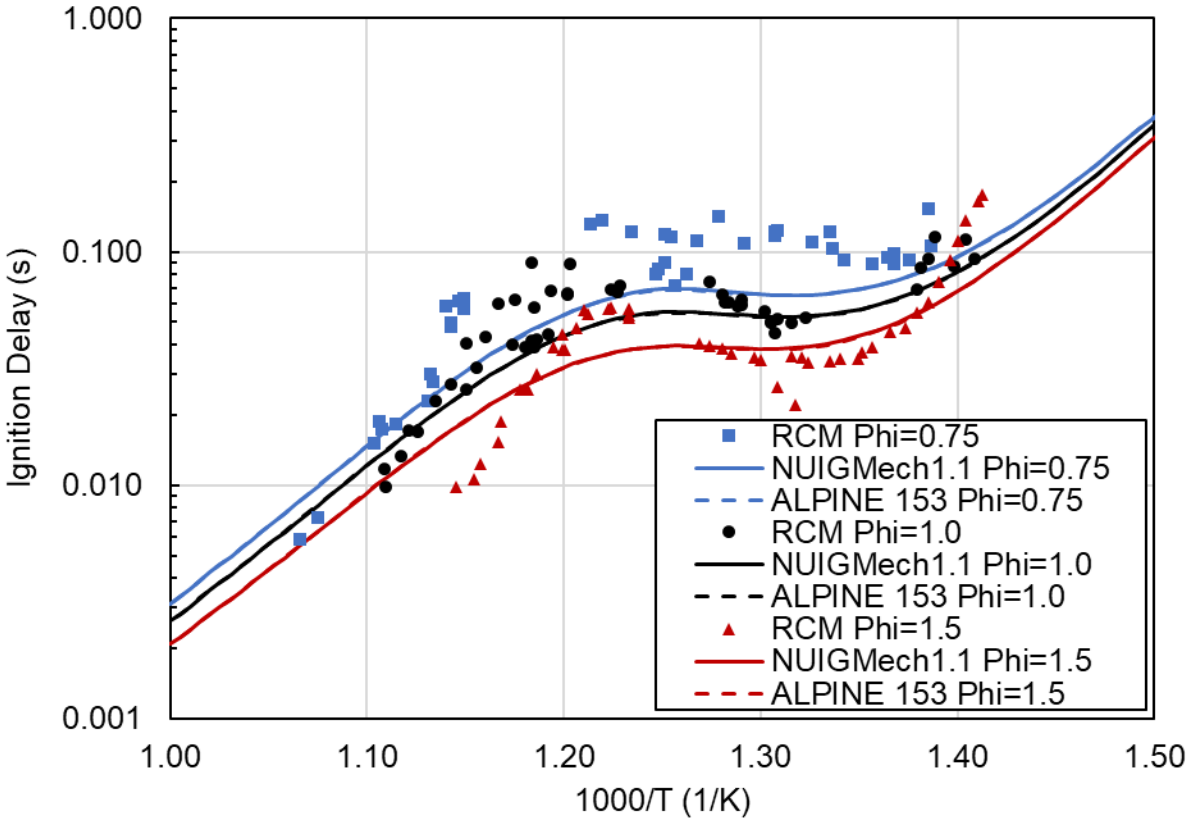

Figure 19: Experimental RCM ignition delay measurements (symbols) and simulated constant volume homogeneous autoignition delay of C_3H_8/inert/O_2 at 24 bar and varying equivalence using NUIGMech1.1 (solid lines) and ALPINE 153 (dashed lines).

Under these conditions, NTC behavior was observed for the rich, lean, and stoichiometric mixtures. The experimental results also showed that the rich fuel mixture exhibited the

shortest ignition delay periods, and the lean mixtures the longest for the full temperature range. ALPINE 153 AND NUIGMech1.1 both replicate these trends, as well as being almost indistinguishable from each other when plotted. The constant volume models are adequate at predicting low and high temperature autoignition but begin to diverge significantly at very low temperatures and the upper end of the NTC regime, leading to an average error of 18.99% for ALPINE 153 for stoichiometric propane. The longer experimental ignition delays allow more time for heat loss to the chamber walls and potential for cool piston crevice gas to flow back into the core, which is not accounted for in the adiabatic model. Although not the focus of this study, schlieren images of autoignition were occasionally recorded and they depict that for a majority of the temperature conditions tested, the propane mixtures were experiencing mild to mixed ignition. As discussed earlier, inhomogeneous autoignition cannot always be properly modeled in a 0-D, mixture averaged simulation.

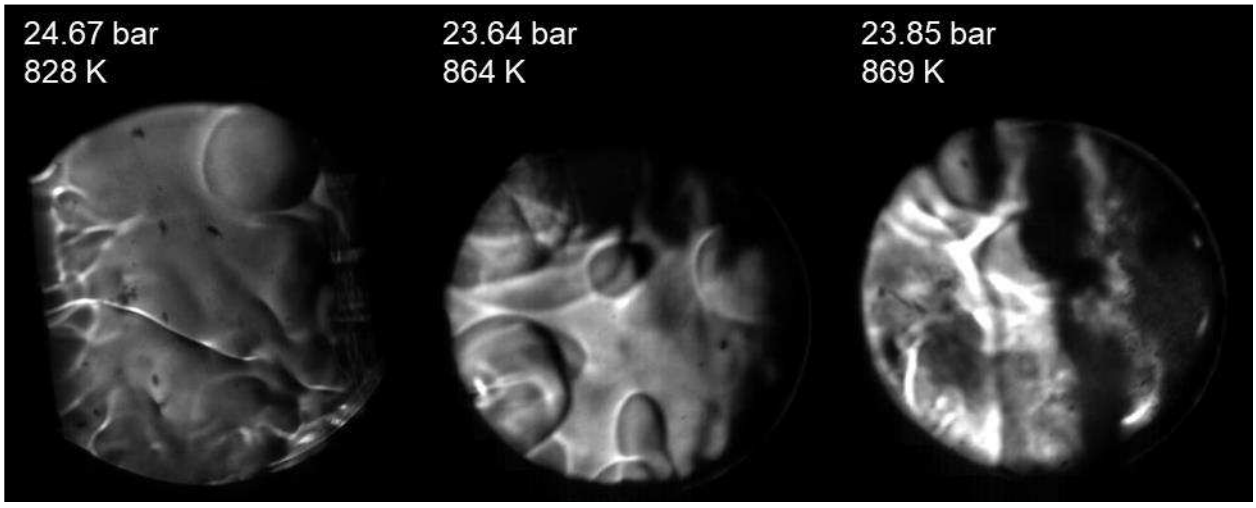

Figure 20: Schlieren images of mild (left), mixed (middle), and strong (right) autoignition for stoichiometric propane with their recorded TDC conditions.

The next set of ignition delay experiments shows the effect of the presence of NO_x in an EGR mixture. The R-EGR represents engine-out exhaust gas, which would be used

for high pressure EGR delivery to an engine cylinder. At 30% mass substitution, the R-EGR mixture contains approximately 1,000 ppm of NO_2 in the gas mixture, depending on the inert gas composition. The NR-EGR represents system-out exhaust gas which is used for low pressure EGR delivery. The expected engine-out NO_x level for the X-15 engine is below 5 ppm, an insignificant amount in regard to reaction kinetics. The results in Figure 21 show that NR-EGR increased ignition delay across the full temperature range as a result of mixture dilution and the lower heat capacity ratio from the CO_2 component gas. Again, the constant volume model does not predict the length of the IDT at the upper end of the NTC regime, but NUIGMech1.1 and ALPINE 153 predict the same values.

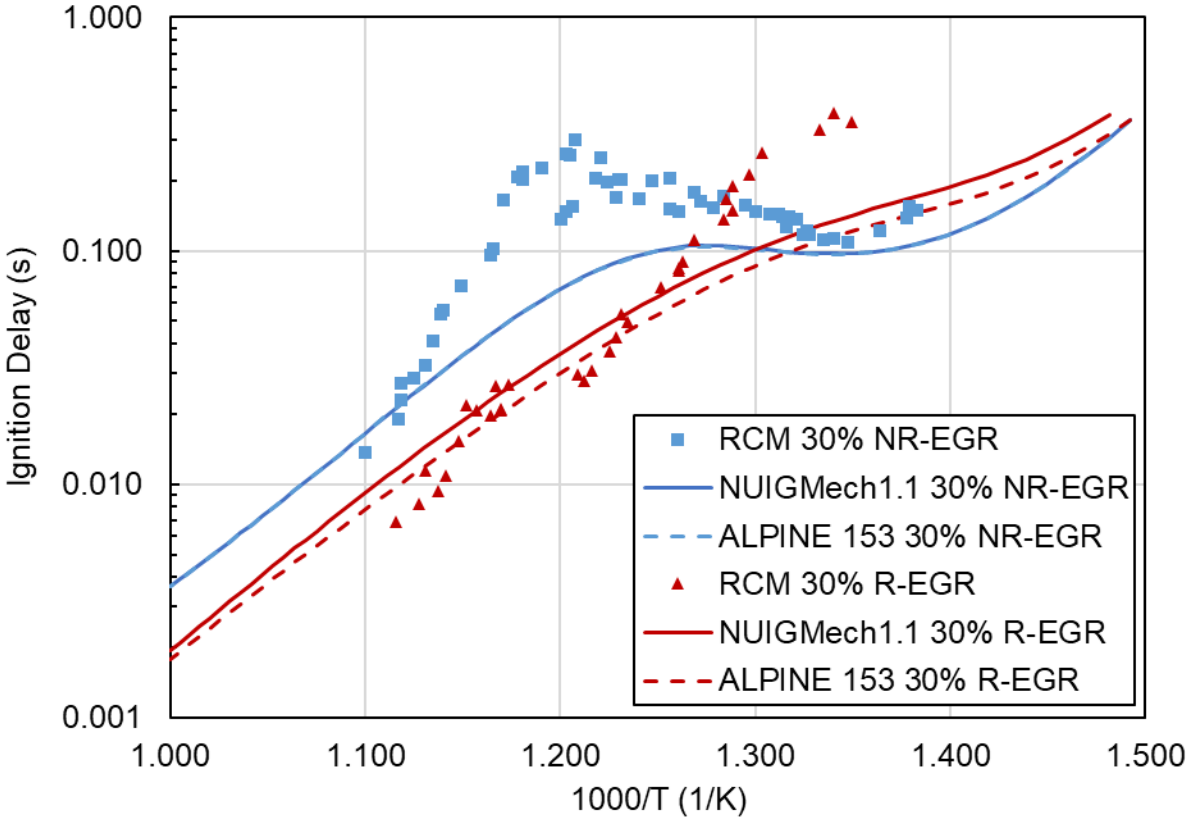

Figure 21: Experimental RCM ignition delay measurements (symbols) and simulated constant volume homogeneous autoignition delay of C_3H_8/inert/O_2/EGR at 24 bar and 30% EGR mass substitution using NUIGMech1.1 (solid lines) and ALPINE 153 (dashed lines).

The 30% R-EGR experiments show a much more pronounced effect than observed by Mohr et al. [50] for natural gas, as well as a completely unexpected behavior at low temperatures. At temperatures below 800 K, the NO_2 in the R-EGR suppresses autoignition even more than the NR-EGR mixture, while at temperatures above 800 K, the R-EGR promotes autoignition to times faster than the stoichiometric propane/air mixture from Figure 20. A closer look at intermediate species over time in the models shows that at low temperatures the NO_2 almost fully converts to HONO and causes a large buildup of H_2O_2 before autoignition, neither of which is present at higher temperatures. ALPINE 153 shows more reactivity than NUIGMech1.1 across the full temperature range for the 30% R-EGR case, indicating an oversimplification of the NO_x chemistry it contains, but still matching the behavior of the full mechanism.

The last set of IDT experiments were to determine the effect of variation in secondary fuel components of an LPG mixture. As discussed earlier, the amount of secondary fuels in HD-5 LPG is very small, but in the rest of the world LPG can be composed of over 50% C_4 hydrocarbons depending on location. To determine the impact of each secondary fuel type, stoichiometric mixtures of 80% propane with 20% of either ethane, propene, n-butane, or isobutane were used. The IDT for each mixture as well as the results of the constant volume model for NUIGMech1.1 and ALPINE 153 are shown in Figure 22. The mixtures show distinct differences in IDT with propane/ethane being the slowest, followed by propane/propene, propane/isobutane, and propane/n-butane in order of increasing reactivity. The propane/propene mixture showed a partial suppression of NTC behavior, which has also been displayed in other propane/propene mixtures in literature [67]. Both mechanisms predicted the same IDT values for the propane/ethane

mixtures, while only deviating by a few milliseconds from each other for the other mixtures. Due to the nature of mechanism reduction, it is expected that the error of ALPINE 153 in predicting IDT for LPG mixtures will go up if fuel composition does not consist of mostly propane.

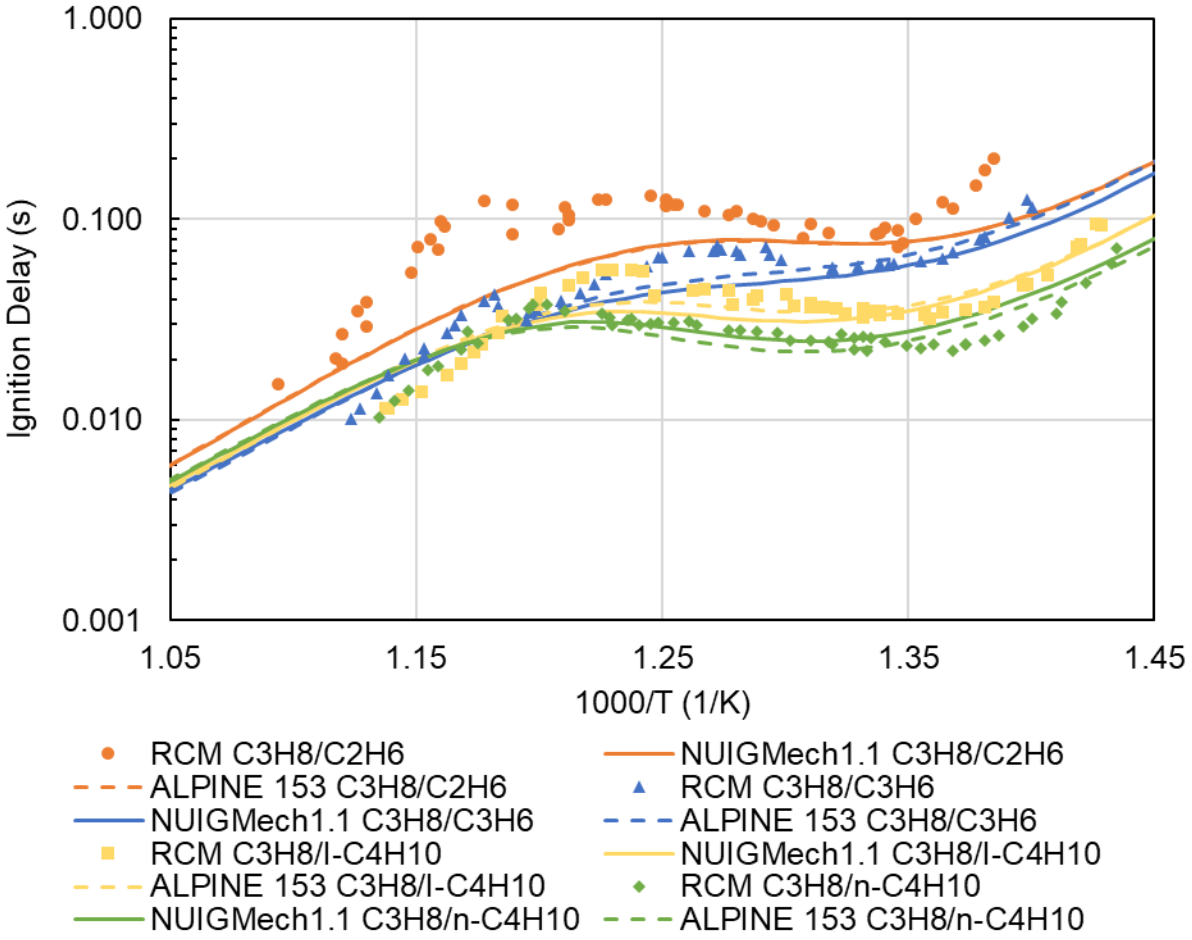

Figure 22: Experimental RCM ignition delay measurements (symbols) and simulated constant volume homogeneous autoignition delay of binary fuel/inert/O_2 at 24 bar and varying equivalence using NUIGMech1.1 (solid lines) and ALPINE 153 (dashed lines).

Effective volume models were only performed for stoichiometric propane/air or propane/air with either 30% NR-EGR or 30% R-EGR as this required performing every experimental case a second time to collect the appropriate non-reactive pressure traces for each mixture. Figure 23 shows the models predicted the correct shape of the ignition

delay curve for all experimental cases, including matching the slope of the NTC regime. However, the effective volume models show significant error from the experimental results, indicating a systematic error somewhere in either experimental data collection or in the design of the effective volume model.

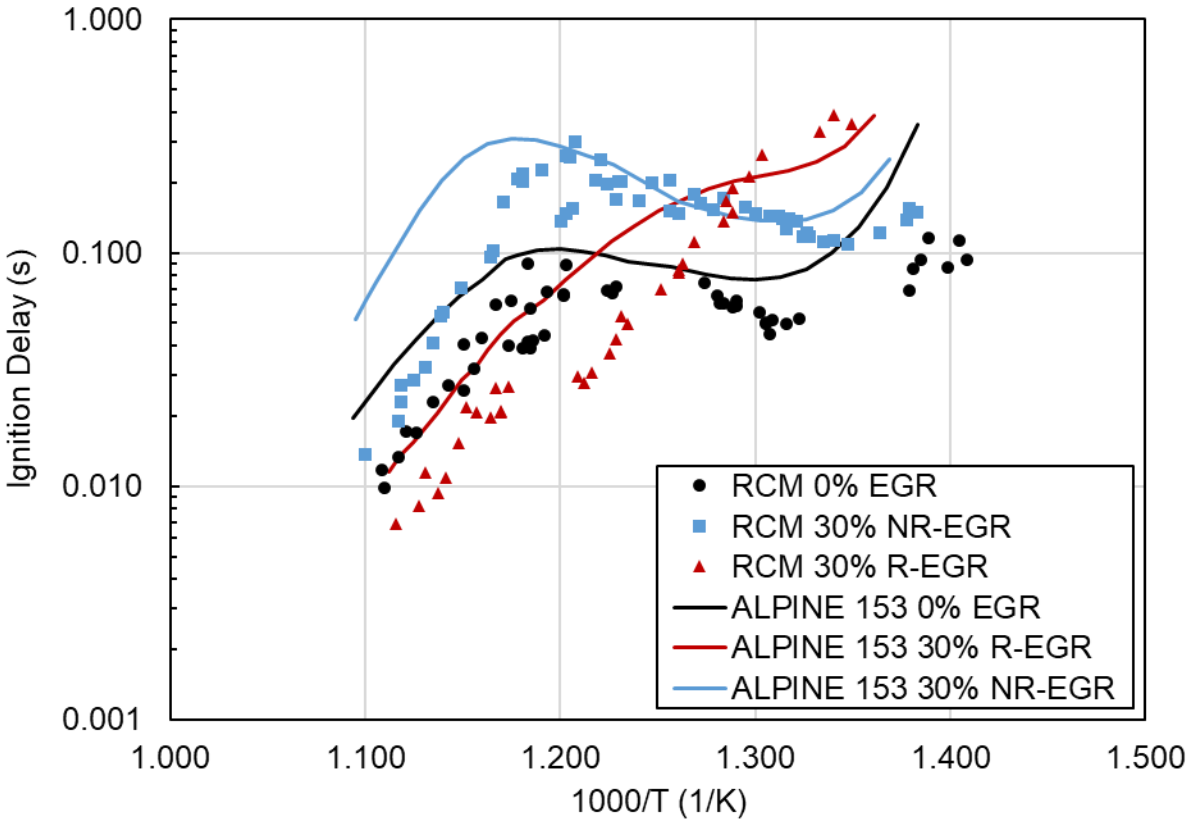

Figure 23: Experimental RCM ignition delay measurements (symbols) and simulated effective volume homogeneous autoignition delay of C_3H_8/inert/O_2/EGR at 24 bar and 0 or 30% EGR mass substitution using ALPINE 153 (solid lines).

Variation in IDT at a repeated condition can typically reach 15% [78], but the shift between the models and experiments is much higher in this case. Although not pictured in Figure 23, ALPINE 153 AND NUIGMech1.1 continued to provide almost identical IDT for the 0% and 30% NR-EGR cases, with the same consistent underprediction of IDT for 30% R-EGR cases that was observed in Figure 21. A comparison of the two mechanisms for the

three different gas mixtures at a TDC condition of 24 bar and 815 K can be seen in Figure 24.

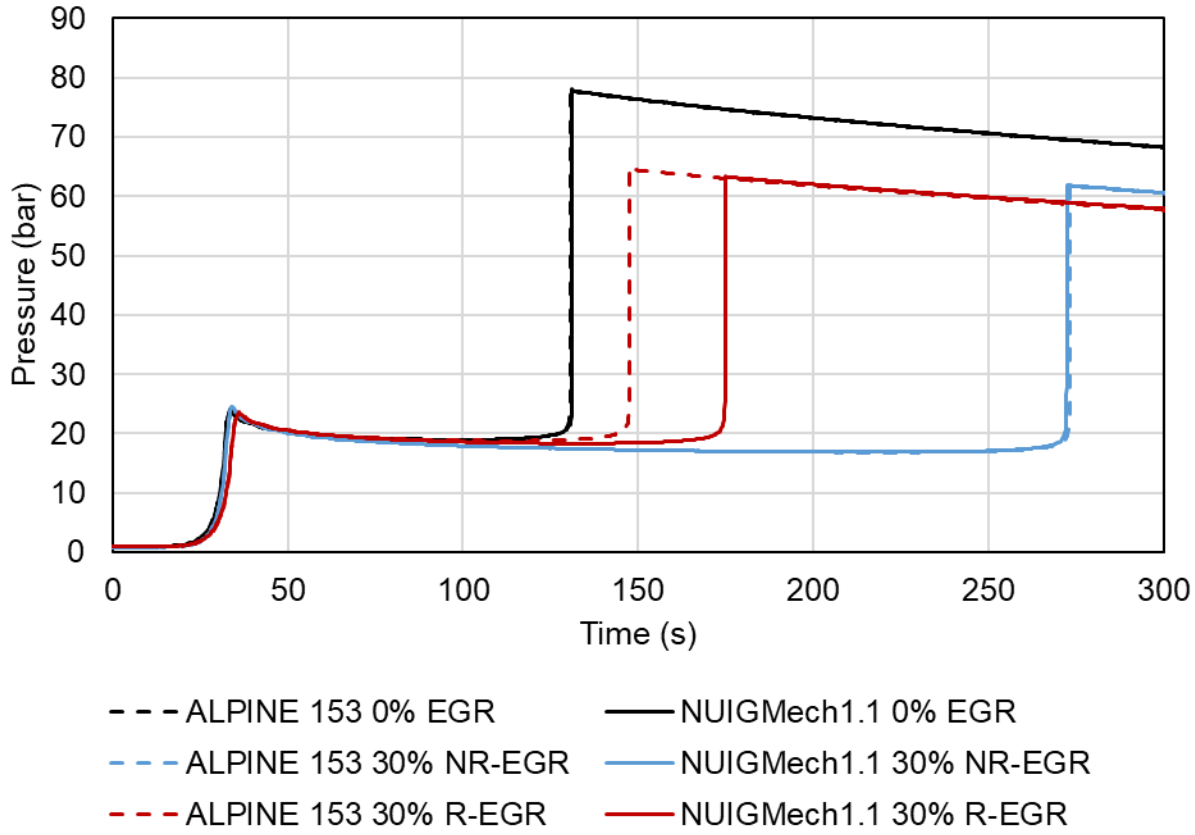

Figure 24: Simulated effective volume homogeneous autoignition delay of C_3H_8/inert/O_2/EGR at 24 bar and 815 K with 0 or 30% EGR mass substitution using NUIGMech1.1 (solid lines) and ALPINE 153 (dashed lines).

The shift between models and experiments necessitates a thorough examination of the calibration of RCM sensors and analysis of the signal processing methods used, as ALPINE 153 was able to match the data very closely from two different RCM's using their associated volume profiles in Figures 16 and 17. Weber et al. [79] have performed extensive work on the compounding uncertainties in RCM research, since TDC temperature is derived from several independent values. If measurement-based errors do exist in this work, the most likely sources are the initial chamber temperature, initial pressure, and the dynamic pressure. Processing errors could result from the pressure

pegging process, dynamic pressure trace filtering, or downsampling the pressure data to a more manageable size.

4.2 Flame Propagation Rate

Flame propagation rate was first tested as a function of equivalence ratio to determine if ALPINE 153 could predict lean, stoichiometric, and rich combustion scenarios as may be present in a stratified fuel injected engine. To ensure the effects of turbulence did not cause increasing flame speeds, all experiments with a piston offset greater than 2 ms were removed from the data sets. It has been shown previously that as piston offset increases, the measured flame propagation rate inside the RCM increases significantly [62]. To mitigate the effects of low temperature chemistry and ensure that the laser is igniting propane and not an intermediate species, a TDC temperature and pressure of 700 K and 24 bar was chosen for the equivalence sweep because propane will not autoignite in the CSU RCM at that condition. As observed in the spark timing matched schlieren images in Figure 25, the stoichiometric propane/air mixture was the fastest, with the lean flame moving slightly faster than the rich flame.

Figure 25: Schlieren images of flame propagation for propane with equivalence ratios of 0.75 (a), 1.0 (b), and 1.5 (c) at 24 bar, 700 K, and timestamps of 14.30, 14.84, 15.54, and 16.43 ms.

Measured flame propagation rates were compared to a 1-D Chemkin model using initial conditions that match the TDC conditions of the RCM. Both the full NUIGMech1.1_HT and the reduced ALPINE 153 mechanism accurately predict the flame propagation rate at stoichiometric and lean conditions, while overpredicting flame propagation in the lean region as shown below in figure 26. This same overprediction was observed for lean fuels in Figure 18 and the error appears to increase with increasing pressures. Error between the 1-D model and measured values of flame speed for stoichiometric propane was only 1.47%.

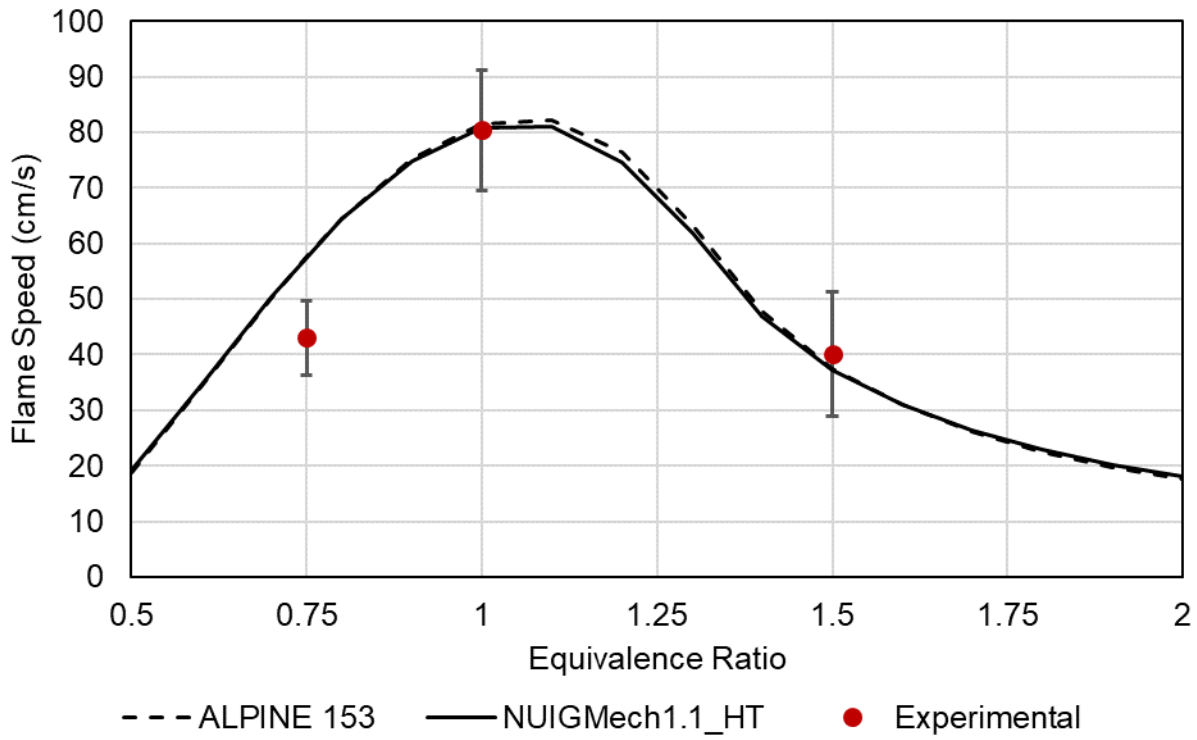

Figure 26: Experimental zero-stretch flame propagation rates at 24 bar and 700 K and simulated 1-D laminar flame speeds using NUIGMech1.1_HT and ALPINE 153 chemical kinetic mechanism for varying equivalence. Error bars represent standard deviation.

The next experimental parameter tested was the effect of increasing R-EGR amounts on flame propagation rates for stoichiometric propane/air mixtures. Again, a TDC condition of 24 bar and 700 K was used to prevent autoignition chemistry and the

amount of R-EGR was increased from 0-30% by mass. The increasing R-EGR amounts decreases the flame propagation rate in an almost linear behavior due to dilution of the fuel/air mixture shown below in Figure 27. The 30% R-EGR mixture in this data set contains 15% CO2 in the inert gas in order to maintain the 700 K TDC pressure and as such must be modeled as a discrete point because of the difference in thermal diffusivity from the other mixtures. Laminar flame speed models using NUIGMech1.1_HT and ALPINE 153 performed very accurately to the measured flame propagation rates except for the 20% R-EGR condition, although it is worth noting that the 20% R-EGR case also had much higher standard deviation than the others.

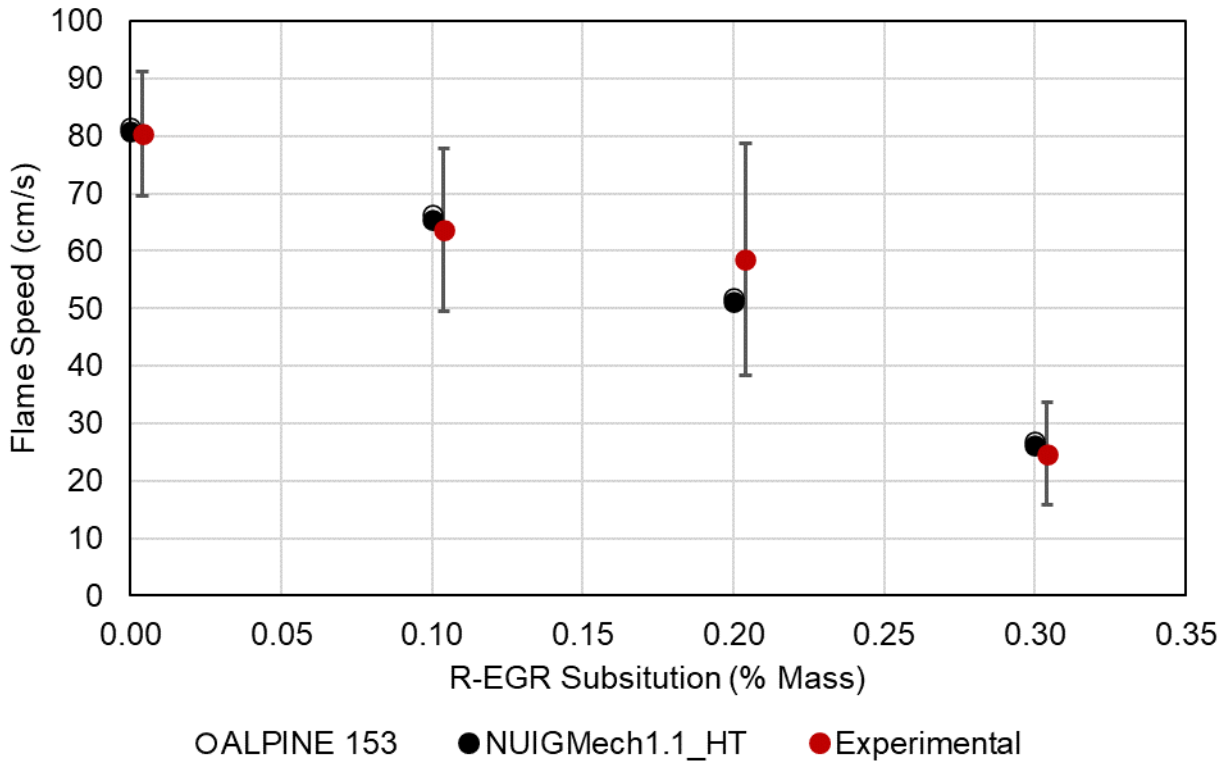

Figure 27: Experimental zero-stretch flame propagation rates at 24 bar and 700 K and simulated 1-D laminar flame speeds using NUIGMech1.1_HT and ALPINE 153 chemical kinetic mechanism for varying R-EGR amounts. Error bars represent standard deviation. Points staggered for clarity.

Since EGAI had not been observed in the 700 K flame propagation experiments, a higher temperature data set was necessary. The results of the 30% R-EGR autoignition

experiments and the significantly slower flame speeds provided by EGR dilution suggest that there is a conditional zone that would allow for visible EGAI in the RCM. The decreased flame speed because of EGR allows for a longer chemical induction period in the end gas which also has increased reactivity from high temperature NO_2. Based on a CFD model of the CSU RCM, 867 K was selected as the TDC temperature that was most likely to autoignite ahead of the flame front. The 867 K flame propagation rates were significantly faster than the 700 K flame results but still exhibited the almost linear decline as a function of R-EGR mass substitution shown in Figure 28. Both the NUIGMech1.1 and ALPINE 153 mechanisms predicted the flame propagation rate within the standard deviation of the experiments until 20% R-EGR substitution, after which they began to diverge significantly. ALPINE 153 overpredicts flame propagation rate at 30% R-EGR as compared to NUIGMech1.1 and demonstrates that there is a conditional range where the reduced mechanism is no longer valid for accurate simulations. At R-EGR percentages of 20 and higher, it appeared that EGAI was visibly occurring, but not until the flame had spread beyond the windows of the combustion chamber. Recreating the 30% R-EGR experiment in a different combustion chamber design with larger windows, 25.4 mm as compared to 16.1 mm, did provide visual confirmation that EGAI was occurring.

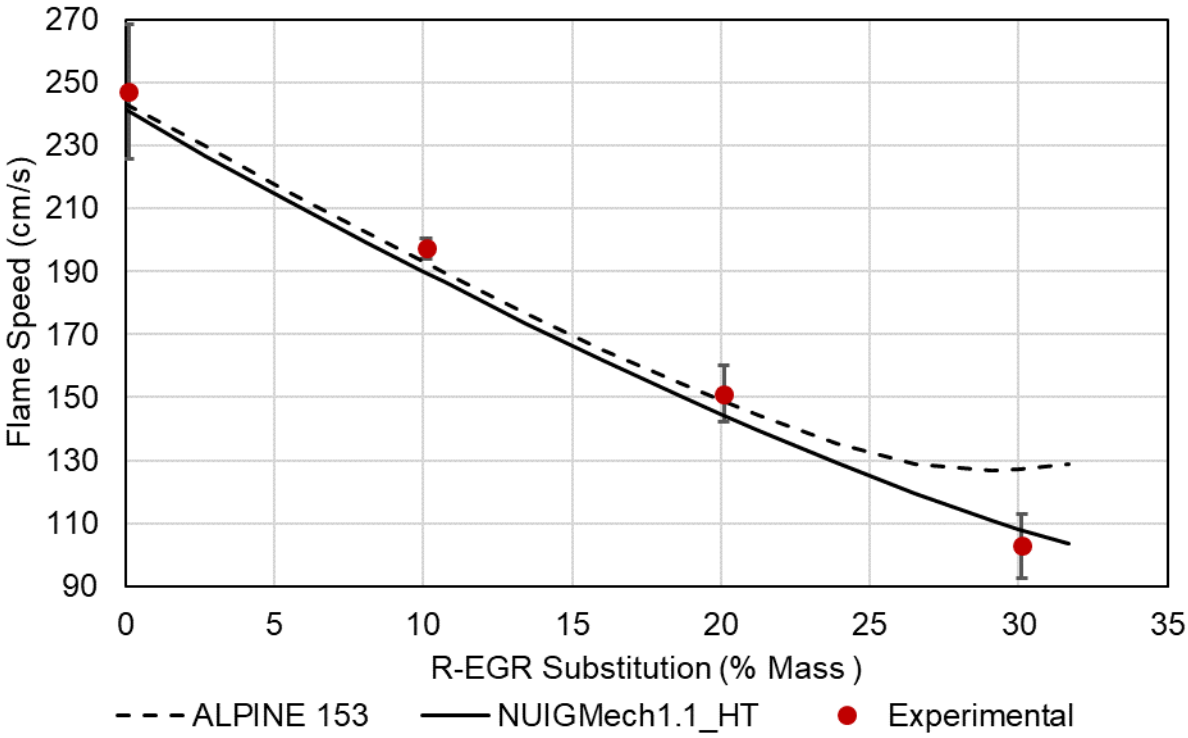

Figure 28: Experimental zero-stretch flame propagation rates at 24 bar and 867 K and simulated 1-D laminar flame speeds using NUIGMech1.1_HT and ALPINE 153 chemical kinetic mechanism for varying R-EGR amounts. Error bars represent standard deviation.

4.3 Apparent Heat Release Rate

The pressure traces for the flame propagation rate experiments in Section 4.2 were analyzed to derive the AHRR curves for each test condition. An example AHHR curve for the equivalence test of propane flame propagation rates at 24 bar and 700 K is shown below in Figure 29 Although the shape and magnitude of the 0.75 and 1.50 equivalence AHRR curves differ, the duration of the curves are very similar as would be expected from them having similar experimental flame speeds.

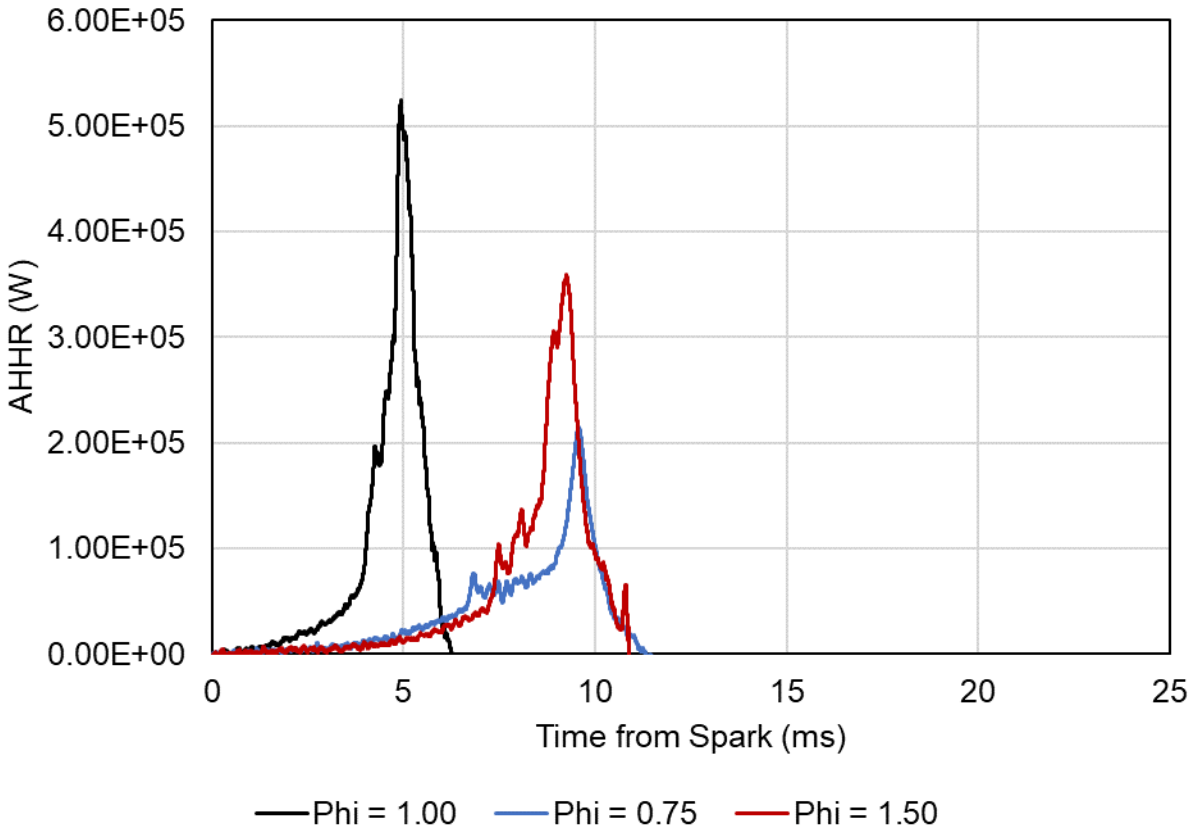

Figure 29: A representative AHRR curve for laser ignited stoichiometric, lean, and rich C_3H_8 at 24 bar and 700 K.

An AHRR curve from each of the flame propagation with increasing R-EGR data sets is included in Figure 30. The effect of the increasing R-EGR content is clearly displayed by the delayed heat release with each increment, as well as the diminishing curve size because of the dilution of the fuel/air mixture.

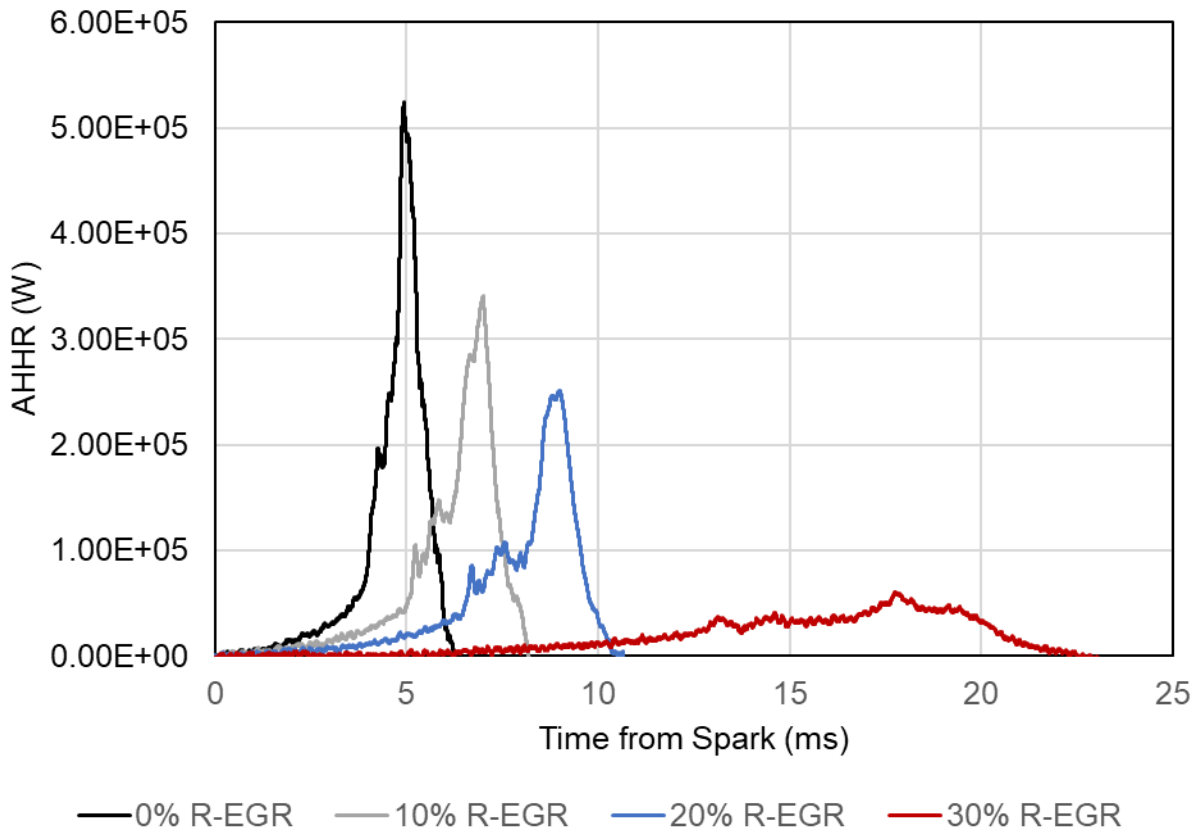

Figure 30: A representative AHRR curve for laser ignited stoichiometric C_3H_8 with 0, 10, 20, and 30% R-EGR by mass at 24 bar and 700 K.

The AHRR curves for the 867 K R-EGR examples in Figure 31 show a drastic change in behavior from those performed at 700 K. The maximum value of the heat release rates at 867 K is almost four times higher than the magnitudes at 700 K, occurring over a much shorter time scale. The AHRR profiles appear less noisy, but that is due to the signal being an order of magnitude higher, effectively smoothing the curves. The key takeaway is the change in the profile shape of the 30% R-EGR mixture between the 700 and 867 K cases, indicating the EGAI that was observed in the recorded schlieren videos.

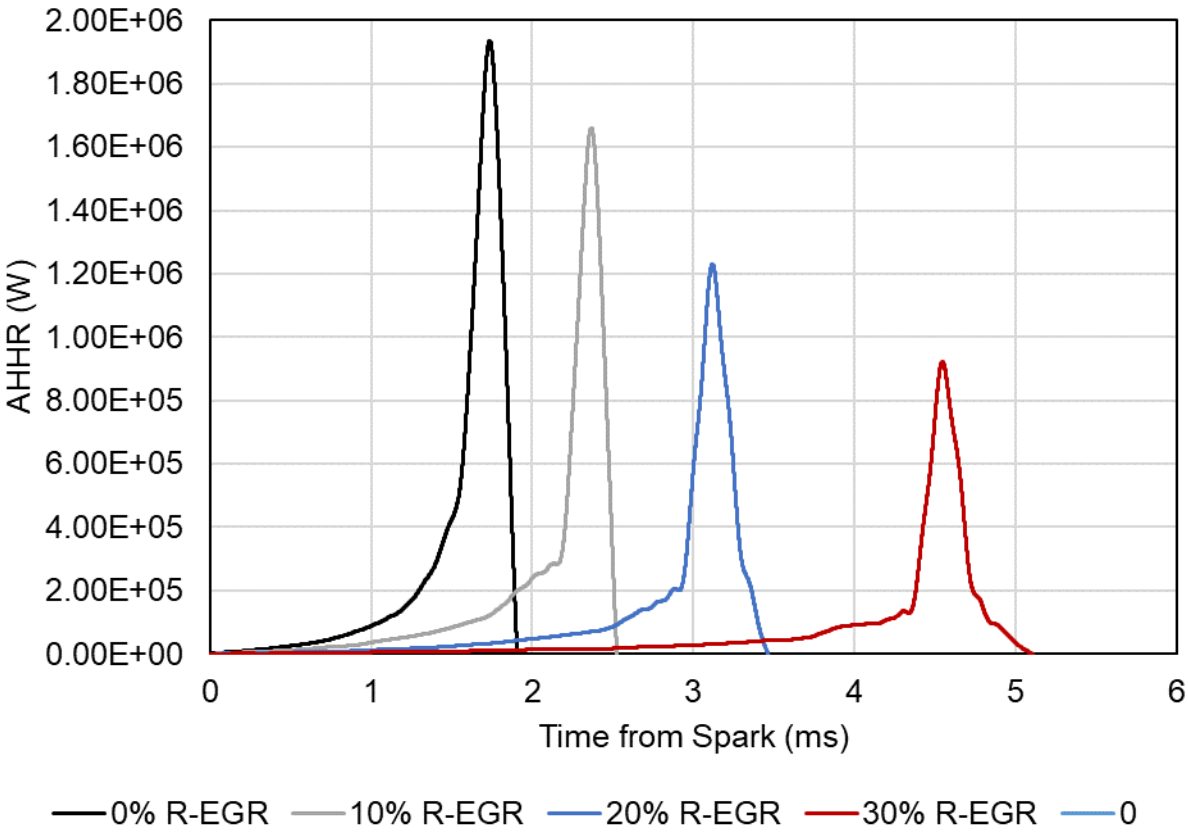

Figure 31: A representative AHRR curve for laser ignited stoichiometric C_3H_8 with 0, 10, 20, and 30% R-EGR by mass at 24 bar and 867 K.

5. CONCLUSION

5.1 Conclusion

The ignition delay times, flame propagation rate, and AHHR of various LPG mixtures as would be seen in spark ignited engine operation were measured in a rapid compression machine. The ignition delay times were performed for lean, stoichiometric, and rich propane/inert/oxygen mixtures at 24 bar and a temperature range of 700 to 900 K. Ignition delay times for stoichiometric propane/inert/oxygen with EGR with and without NO in the mixture were measured at similar conditions. The ignition delay behavior was significantly altered by the addition of the R-EGR mixture. Four binary fuels consisting of 80% propane with 20% ethane, propene, n-butane, or isobutane were also analyzed for ignition delay to determine the effect of secondary fuel on LPG reactivity, with longer hydrocarbons increasing reactivity.

Measured flame propagation rates were similar for 24 bar and 700 K propane at equivalence ratios of 0.75 and 1.5, with both flame fronts moving at almost half the speed of stoichiometric propane. R-EGR addition of 0 to 30% by mass was shown to decrease flame propagation rate in an almost linear behavior. At 867 K, R-EGR addition continued to decrease flame propagation rate. The slower flame speeds combined with the increased reactivity of the R-EGR mixture created the conditions for visible EGAI at 30% R-EGR mass substitution with sudden spike in the AHHR as compared to the same mixture at 700 K.

Eight detailed chemical kinetic mechanisms were modeled to determine their accuracy compared to published data. NUIGMech1.1 was selected as it most closely

predicted ignition delay times and included NO_x chemistry. Several iterations of mechanism reduction were performed until the optimal balance of size and accuracy was found. NUIGMech1.1 and the ALPINE 153 were used to model all of the experiments performed in the RCM.

The results of this study further the objectives of the ALPINE project by creating a robust, compact chemical kinetic mechanism that can accurately model ignition delay and flame speed for LPG combustion under a variety of engine like conditions. ALPINE 153 consists of 153 species and 1,227 reactions, which makes it suitable for 3-D combustion modeling. It contains the reactions necessary to simulate the combustion of C_1-C_4 hydrocarbons and includes NO_x chemistry. ALPINE 153 performs very well in simulations of laminar flame speeds at high temperatures and pressure, and predicts the changing reactivity based on LPG fuel content and EGR substitution.

Key Findings:

- R-EGR produced an unexpected effect in IDT due to NO_2 chemistry, suppressing autoignition at low temperatures while promoting it at high temperatures.
- ALPINE 153 was able to accurately predict laminar flame speeds at pressures and temperatures much higher than have previously been measured and match the IDT trends modeled by NUIGMech1.1.
- At very high temperatures, increasing amounts of R-EGR increased the heat release from end-gas autoignition upstream of the propagating flame.

5.2 Future Work

There are many avenues that exist for continuation of this research. The first is to generate a new reduced mechanism based on newer and improved detailed mechanisms. In the time since this study began, Martinez et al. [80] released NUIGMech1.2 which improved the predictions of the mechanism for multispecies short chain (C_1-C_3) hydrocarbon fuel blends in late 2021. This was followed with NUIGMech1.3

in 2022 from Mohamed et al. [74], which included changes to NO_x chemistry based on homogeneous ignition delay experiments involving propane, NO, NO_2, and N_2O. A new reduced mechanism following the same procedure as ALPINE 153 would incorporate the improved reaction rates in new iterations of NUIGMech.

There is potential for more research regarding the effect of NO_x on EGAI. A more thorough bracketing of the composition, pressure, and temperature conditions for laser ignited experiments would help to identify the conditional point where R-EGR contributes to knock instead of preventing it. This would be of great help to future engine simulations, as compression ratio and EGR levels increase in the pursuit of higher efficiency.

New reaction chamber designs and larger windows that allow much more chamber volume (including the piston faces) to be visible allow for the possibility of improving on the prediction of mild, mixed, and strong autoignition studies performed in other single piston RCMs. All three behaviors were observed over the course of this study in the schlieren imaging. This would be especially interesting for fuels in the NTC regime, to analyze if the autoignition event begins in the cooler thermal boundary layer instead of the adiabatic core.

Another interesting feature came up over the course of this experiment, which is that firing the laser at one side of the chamber produces a significantly larger EGAI event than firing at the center. It was observed several times when the laser fired low into the chamber that the upwardly propagating flame produced EGAI sooner than a similar spherically expanding flame from the center. By firing the laser toward the center of one piston face, the conditions of an internal combustion engine would be more closely replicated. Disabling one RCM piston and sealing that side of the combustion chamber

would also produce similar turbulence conditions to an engine. The results of this configuration could then be compared to 3-D CFD models of engine cylinders under similar conditions.

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APPENDIX A

RCM Test Conditions for Homogeneous Ignition Delay

Fuel (mole %)	Φ	EGR (mass %)	Inert Composition (mole %)	Avg. TDC Press. (bar)	TDC Temp. Range (K)
C_3H_8	1.00	0	75 N_2 : 25 Ar	23.65 ± 0.45	710 – 785
C_3H_8	1.00	0	65 N_2 : 35 Ar	23.88 ± 0.23	720 – 768
C_3H_8	1.00	0	36 N_2 : 64 Ar	24.21 ± 0.60	756 – 847
C_3H_8	1.00	0	100 Ar	23.75 ± 0.68	831 – 902
C_3H_8	0.75	0	60 N_2 : 40 Ar	23.72 ± 0.53	721 – 824
C_3H_8	0.75	0	100 Ar	23.80 ± 0.68	870 – 938
C_3H_8	1.50	0	45 N_2 : 55 Ar	23.97 ± 0.54	708 – 788
C_3H_8	1.50	0	100 Ar	23.63 ± 0.64	811 – 873
C_3H_8	1.00	30 NR-EGR	100 N2	23.86 ± 0.43	723 – 761
C_3H_8	1.00	30 NR-EGR	60 N_2 : 40 Ar	24.30 ± 0.43	754 – 833
C_3H_8	1.00	30 NR-EGR	16 N_2 : 84 Ar	23.96 ± 0.43	819 – 909
C_3H_8	1.00	30 R-EGR	73 N_2 : 27 Ar	23.82 ± 0.57	741 – 827
C_3H_8	1.00	30 R-EGR	100 Ar	24.31 ± 0.93	852 – 896
80 C_3H_8 20 C_2H_6	1.00	0	65 N_2 : 35 Ar	24.29 ± 0.77	722 – 747
80 C_3H_8 20 C_2H_6	1.00	0	45 N_2 : 55 Ar	24.11 ± 0.58	742 – 828
80 C_3H_8 20 C_2H_6	1.00	0	100 Ar	23.85 ± 0.92	841 – 914
80 C_3H_8 20 C_3H_6	1.00	0	100 N_2	24.48 ± 0.19	714 – 758
80 C_3H_8 20 C_3H_6	1.00	0	40 N_2 : 60 Ar	23.97 ± 0.32	770 – 837
80 C_3H_8 20 C_3H_6	1.00	0	20 N_2 : 80 Ar	23.85 ± 0.23	845 – 890
80 C_3H_8 20 i-C_4H_{10}	1.00	0	100 N_2	23.92 ± 0.18	700 – 763
80 C_3H_8 20 i-C_4H_{10}	1.00	0	50 N_2 : 50 Ar	23.94 ± 0.28	747 – 802
80 C_3H_8 20 i-C_4H_{10}	1.00	0	20 N_2 : 80 Ar	24.05 ± 0.17	805 – 879
80 C_3H_8 20 n-C_4H_{10}	1.00	0	100 N_2	23.56 ± 0.17	697 – 756
80 C_3H_8 20 n-C_4H_{10}	1.00	0	50 N_2 : 50 Ar	23.47 ± 0.24	749 – 813
80 C_3H_8 20 n-C_4H_{10}	1.00	0	20 N_2 : 80 Ar	24.04 ± 0.25	806 – 881

APPENDIX B

RCM Test Conditions for Flame Propagation Rate

Fuel	Φ	EGR (mass %)	Inert Composition (mole %)	Avg. TDC Press. (bar)	Avg. TDC Temp. (K)
C_3H_8	1.00	0	100 N2	24.33 ± 0.24	703.3 ± 2.0
C_3H_8	0.75	0	100 N2	24.05 ± 0.25	700.4 ± 0.9
C_3H_8	1.50	0	100 N2	24.01 ± 0.09	699.5 ± 1.1
C_3H_8	1.00	10 R-EGR	100 N2	23.91 ± 0.18	699.2 ± 1.3
C_3H_8	1.00	20 R-EGR	100 N2	24.31 ± 0.18	701.9 ± 1.1
C_3H_8	1.00	30 R-EGR	85 N_2 : 15 CO_2	23.79 ± 0.31	699.9 ± 1.8
C_3H_8	1.00	0	90 N_2 : 10 Ar	23.82 ± 0.43	866.7 ± 4.7
C_3H_8	1.00	10 R-EGR	90 N_2 : 10 Ar	24.03 ± 0.50	866.0 ± 1.2
C_3H_8	1.00	20 R-EGR	90 N_2 : 10 Ar	24.11 ± 0.17	867.6 ± 1.9
C_3H_8	1.00	30 R-EGR	90 N_2 : 10 Ar	24.22 ± 0.25	867.4 ± 3.5

APPENDIX C

ALPINE 153 Mechanism

```
ELEMENTS
C H N O AR
HE
END
SPECIES
AR N2 HE H2 H
O2 O H2O OH OHV
H2O2 HO2 CO CO2 CH3O2H
CH3O2 CH4 CH3 CH2 CH2(S)
CH CH3OH CH3O CH2OH HO2CHO
O2CHO OCHO CH2O HCO HCOH
C2H5O2H C2H5O2 C2H6 C2H5 C2H4
C2H3 C2H2 C2H C2H3O1-2 C2H5O
O2CH2CHO HO2CH2CO CH3CHO CH3CO CH2CHO
C2H3OH CH2CO HCCO CH3CO3H CH3CO3
CH3CO2 NC3H7O2H NC3H7O2 IC3H7O2H IC3H7O2
C3H6OOH1-3 C3H6OOH1-3O2 C3KET13 SC3H5OO TC3H5OO
OCHCH2CH2O C3H8 IC3H7 NC3H7 CH3CHCHO
C3H5O AC3H5OOH C3H6 C3H5-A C3H5-S
C3H5-T C3H4-A C3H3 TQJC3H6OH TQC3H6OI
QC3H5OHP IQJC3H6OH IQC3H6OT C3H6OH1-2 NC3H7O
C3H6OH2-1 IC3H7O CH3COCH2O2 CH3COCH2O C3KET21
CH3COCH3 CH3COCH2 C2H3CHO C2H3CO CH3CH(OO)CHO
QCH2CH(OOH)CHO QCH3CH(OOH)CO CYC2H3OCHO CH2CH2CHO SC4H9O
PC4H9O2 SC4H9O2 SC4H9O2H C4H8OOH1-3 C4H8OOH2-4
C4H8O1-3 C4H8OOH1-3O2 C4H8OOH2-4O2 NC4KET13 NC4KET24
C4H10 PC4H9 SC4H9 TC4H9O IC4H9O
IC3H5CHO IC4H9O2 TC4H9O2 IC4H8O2H-I IC4H8O2H-T
IC4H8OOH-IO2 IC4KETII IC4H7OOH TC4H9O2H IC4H10
IC4H9 TC4H9 IC4H7O IC4H8 IC4H7
C4H7O2-1 C4H8-1 C4H71-3 C4H8-2 NC3H7CHO
BC5H10 AC5H10 AC5H9-C C6H11OH1Q2-5 C6H11OH1Q2-3O2
C6H11OH1Q2-4O2 C6H11OH1Q2-5O2 C6H103OH1Q2 C6H104OH1Q2 C6H105OH1Q2
C6H10OH1KET2-3 NO HCN NH N
NNH HNO NO2 HONO N2O
HOCN NCO CH3NO2
END

THERMO ALL
  300.000  1000.000  5000.000
!
!(001_DILUENTS_001_UNDEFINED_UNDEFINED)
!\COMMENT:  G 5/97
AR                AR  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
!\COMMENT:  G 8/02
N2                N   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
!\COMMENT:  G 5/97
HE                HE  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
!(/001_DILUENTS_001_UNDEFINED_UNDEFINED)
!(002_H2_O2_001_H2_PYROSPEC)
!\COMMENT:  TPIS78
H2                H  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
!\COMMENT:  L 6/94
H                 H  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
!(/002_H2_O2_001_H2_PYROSPEC)
!(002_H2_O2_002_O2_PYROSPEC)
!\COMMENT:  RUS 89
O2                O  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
!\COMMENT:  L 1/90
O                 O  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
!(/002_H2_O2_002_O2_PYROSPEC)
!(002_H2_O2_003_H2O_PYROSPEC)
!\COMMENT:  L 5/89
H2O               H  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
!\COMMENT:  IU3/03
OH                H  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
!\COMMENT:  121286
OHV               H  1O  1        G    300.0    5000.0  1000.0     1
     2.88273E0   1.0139743E-3   -2.276877E-7   2.174683E-11  -5.126305E-16    2
      5.0265E4     5.595712E0     3.637266E0     1.85091E-4  -1.6761646E-6    3
   2.387202E-9  -8.431442E-13      5.00213E4    1.3588605E0                4
!(/002_H2_O2_003_H2O_PYROSPEC)
!(002_H2_O2_004_H2O2_PYROSPEC)
!\COMMENT:  T 8/03
H2O2              H  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
!\COMMENT:  T 1/09
HO2               H  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
!(/003_C1_001_CO_HTOXID)
!(003_C1_001_CO_PYROSPEC)
!\COMMENT:  RUS 79
CO                C  1O  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
!\COMMENT:  L 7/88
CO2               C  1O  2        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
!(/003_C1_001_CO_PYROSPEC)
!(003_C1_002_CH4_LTOXID)
!\COMMENT:  A 7/05
CH3O2H              C   1H   4O   2    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
!\COMMENT:
CH3O2               C   1H   3O   2    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
!(/003_C1_002_CH4_LTOXID)
!(003_C1_002_CH4_PYROSPEC)
!\COMMENT:  G 8/99
CH4                 C   1H   4        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
!\COMMENT:  IU0702
CH3                 C   1H   3        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
!\COMMENT:  IU3/03
CH2                 C   1H   2        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
!\COMMENT:  IU6/03
CH2(S)              C   1H   2        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
!\COMMENT:  IU3/03
CH                  C   1H   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
!(/003_C1_002_CH4_PYROSPEC)
!(003_C1_003_CH3OH_PYROSPEC)
!\COMMENT:  T06/02
CH3OH               C   1H   4O   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
!\COMMENT:  IU1/03
CH3O                C   1H   3O   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
!\COMMENT:  IU2/03
CH2OH               C   1H   3O   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
!(/003_C1_003_CH3OH_PYROSPEC)
!(003_C1_004_CH2O_LTOXID)
!\COMMENT:  6/26/95 THERM
HO2CHO              C   1H   2O   3    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
!\COMMENT:  6/26/95 THERM
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O2CHO               C   1H   1O   3    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
!\COMMENT:  ATCT/A
OCHO                C   1H   1O   2    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
!(/003_C1_004_CH2O_LTOXID)
!(003_C1_004_CH2O_PYROSPEC)
!\COMMENT:  T 5/11
CH2O                C   1H   2O   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
!\COMMENT:  T 5/03
HCO                 C   1H   1O   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
!\COMMENT:  MAR94
HCOH                C   1H   2O   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
!(/003_C1_004_CH2O_PYROSPEC)
!(004_C2_001_C2H6_LTOXID)
!\COMMENT:  9/ 1/12
C2H5O2H             C   2H   6O   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
!\COMMENT:  9/ 1/12
C2H5O2              C   2H   5O   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
!(/004_C2_001_C2H6_LTOXID)
!(004_C2_001_C2H6_PYROSPEC)
!\COMMENT:  G 8/88
C2H6                C   2H   6        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
!\COMMENT:  8/ 4/ 4 THERM
C2H5                C   2H   5        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
!(/004_C2_002_C2H4_HTOXID)
!(004_C2_002_C2H4_PYROSPEC)
!\COMMENT:  8/12/15
C2H4                C   2H   4        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
!\COMMENT:  8/12/15
C2H3                C   2H   3        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
!(/004_C2_003_C2H2_HTOXID)
!(004_C2_003_C2H2_PYROSPEC)
!\COMMENT:  G 1/91
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C2H2                C  2H  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
!\COMMENT:  T 5/10
C2H                 C  2H  1       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
!\COMMENT:  A 1/05
C2H3O1-2            C  2H  3O  1    G    200.0    6000.0  1000.0     1
  5.60158035E0  9.17613962E-3 -3.28028902E-6 5.27903888E-10-3.15362241E-14    2
  1.71446252E4  -5.47228512E0   3.58349017E0 -6.02275805E-3  6.32426867E-5    3
 -8.18540707E-8 3.30444505E-11   1.85681353E4   9.59725926E0                 4
!\COMMENT:  8/12/15
C2H5O               C  2H  5O  1    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
!(/004_C2_004_C2H5OH_PYROSPEC)
!(004_C2_005_CH3CHO_LTOXID)
!\COMMENT:  BOZ_03
O2CH2CHO            C  2H  3O  3    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
!\COMMENT:  BOZ_03
HO2CH2CO            C  2H  3O  3    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
!(/004_C2_005_CH3CHO_LTOXID)
!(004_C2_005_CH3CHO_PYROSPEC)
!\COMMENT:  L 8/88
CH3CHO              C  2H  4O  1    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
!\COMMENT:  IU2/03
CH3CO               C  2H  3O  1    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
!\COMMENT:
CH2CHO              C  2H  3O  1    G    298.0    3000.0  1000.0     1
   3.6302633E0  1.41239404E-2 -7.16478146E-6  1.76263004E-9-1.70391996E-13    2
  4.29875072E2   6.20577997E0  9.86311004E-1  2.24920216E-2 -1.64812936E-5    3
  5.86617239E-9-6.81551147E-13   1.07163704E3   1.95196726E1                 4
!(/004_C2_006_C2H3OH_LTOXID)
!(004_C2_006_C2H3OH_PYROSPEC)
!\COMMENT:  2/ 3/ 9 THERM
C2H3OH              C  2H  4O  1    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
!(/004_C2_006_C2H3OH_PYROSPEC)
!(004_C2_007_CH2CO_PYROSPEC)
!\COMMENT:
CH2CO               C  2H  2O  1    G    300.0    5000.0  1000.0     1
  5.35869367E0  6.95641586E-3 -2.64802637E-6 4.65067592E-10 -3.0864182E-14    2
 -7.90294013E3  -3.98525731E0   1.81422511E0   1.9900859E-2 -2.21416008E-5    3
  1.45028521E-8-3.98877068E-12  -7.05394926E3   1.36079359E1                 4
!\COMMENT:  T 4/09
HCCO                C  2H  1O  1    G    200.0    6000.0  1000.0     1
  5.91479333E0  3.7140873E-3  -1.3013701E-6 2.06473345E-10-1.21476759E-14    2
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  1.93596301E4 -5.50567269E0  1.87607969E0  2.21205418E-2 -3.58869325E-5    3
  3.05402541E-8-1.01281069E-11   2.0163384E4   1.3696829E1                  4
!(/004_C2_007_CH2CO_PYROSPEC)
!(004_C2_008_ACID_PYROSPEC)
!\COMMENT:  6/26/95 THERM
CH3CO3H             C  2H  4O  3    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
!\COMMENT:  4/ 3/ 0 THERM
CH3CO3              C  2H  3O  3    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
!\COMMENT:  2/14/95 THERM
CH3CO2              C  2H  3O  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
!(/005_C3_001_C3H8_HTOXID)
!(005_C3_001_C3H8_LTOXID)
!\COMMENT:  8/12/15
NC3H7O2H            C  3H  8O  2    G    300.0   5000.0  1392.0     1
  1.42246236E1  1.74340964E-2 -5.97063522E-6 9.27753851E-10-5.38585168E-14    2
 -2.88159737E4  -4.74357865E1   1.35815897E0  4.56683952E-2 -2.91646368E-5    3
  9.41701313E-9-1.22337394E-12  -2.41528416E4   2.23322825E1                  4
!\COMMENT: GOLDSMITH 2012
NC3H7O2             C  3H  7O  2    G    298.0   6000.0  1000.0     1
  1.13928391E1   1.8179582E-2 -6.36612872E-6  1.00817882E-9 -5.9500027E-14    2
 -9.53850281E3  -3.05901531E1  -2.18764216E0  6.63266676E-2 -8.85670635E-5    3
  7.52623609E-8-2.66793523E-11  -5.87082784E3   3.80774389E1                  4
!\COMMENT:  8/12/15
IC3H7O2H            C  3H  8O  2    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
!\COMMENT: GOLDSMITH 2012
IC3H7O2             C  3H  7O  2    G    298.0   6000.0  1000.0     1
  1.16518761E1  1.78468509E-2 -6.22317562E-6 9.82584904E-10-5.78627616E-14    2
 -1.18137559E4  -3.30378983E1  -1.26789412E0  6.59175817E-2 -9.14324526E-5    3
   7.8841997E-8 -2.7858959E-11  -8.43089252E3   3.17397573E1                  4
!\COMMENT: GOLDSMITH 2012
C3H6OOH1-3          C  3H  7O  2    G    298.0   6000.0  1000.0     1
   1.2753423E1  1.64990825E-2 -5.75149933E-6 9.07558827E-10-5.34133116E-14    2
 -1.89797992E3  -3.51115892E1  -1.53407267E0  7.04778409E-2 -9.92876404E-5    3
  8.31696376E-8-2.84706143E-11   1.69677071E3   3.60558537E1                  4
!\COMMENT: THERM  4/25/20
C3H6OOH1-3O2        C  3H  7O  4    G    300.0   5000.0  1390.0     1
   1.8814216E1  1.60762663E-2 -5.59675199E-6 8.79415836E-10-5.14552065E-14    2
 -2.31287645E4  -6.62090737E1   3.24156046E0  5.06140654E-2 -3.40549898E-5    3
  1.11982415E-8-1.43451545E-12  -1.75667823E4   1.80289601E1                  4
!\COMMENT: GOLDSMITH 2012
C3KET13             C  3H  6O  3    G    298.0   6000.0  1000.0     1
   1.4094982E1  1.56175081E-2 -5.50405747E-6 8.74852801E-10-5.17497813E-14    2
 -3.63943081E4  -4.16291747E1   5.41530167E0  4.35927794E-2 -5.43753738E-5    3
  4.93856476E-8-1.89868197E-11  -3.37525093E4   3.35182219E0                  4
!\COMMENT:  2/ 7/19 THERM
SC3H5OO             C  3H  5O  2    G    300.0   5000.0  1391.0     1
   1.3124657E1  1.17719171E-2 -4.06154905E-6  6.3436506E-10-3.69622374E-14    2
   3.1978525E3   -4.0625695E1   2.37869252E0  3.63937952E-2 -2.54689963E-5    3
  9.05375431E-9-1.30368839E-12   6.97002244E3   1.72448228E1                  4
!\COMMENT:  9/30/19
TC3H5OO             C  3H  5O  2    G    300.0   5000.0  1427.0     1
   1.1247595E1  1.18958685E-2 -3.79310732E-6 5.61099631E-10-3.14584401E-14    2
   1.36735441E3  -2.91220162E1   2.60844589E0  3.34570194E-2 -2.41496366E-5    3
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  9.1633332E-9-1.39948285E-12  4.16164345E3   1.6671437E1                4
!\COMMENT:  12 GMG
OCHCH2CH2O           C  3H  5O  2    G    100.0    5000.0 1195.86     1
  8.31103802E0  1.90269568E-2 -8.00643008E-6  1.48969891E-9 -1.0315926E-13   2
 -1.69017273E4  -1.28742885E1   2.3999549E0  3.02031615E-2 -1.12433758E-5   3
 -2.71630257E-9 2.03264811E-12 -1.48733375E4   1.92703545E1                4
!(/005_C3_001_C3H8_LTOXID)
!(005_C3_001_C3H8_PYROSPEC)
!\COMMENT:  8/12/15
C3H8                 C  3H  8        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
!\COMMENT:  8/12/15
IC3H7                C  3H  7        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
!\COMMENT:  8/12/15
NC3H7                C  3H  7        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
!(/005_C3_001_C3H8_PYROSPEC)
!(005_C3_002_C3H6_HTOXID)
!\COMMENT:
CH3CHCHO             C  3H  5O  1    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
!\COMMENT:  KPS12
C3H5O                C  3H  5O  1    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
!\COMMENT:  GOLDSMITH
AC3H5OOH             C  3H  6O  2    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
!(/005_C3_002_C3H6_LTOXID)
!(005_C3_002_C3H6_PYROSPEC)
!\COMMENT:  G 2/00
C3H6                 C  3H  6        G    200.0    6000.0  1000.0     1
  6.03870234E0  1.62963931E-2   -5.821308E-6 9.35936829E-10-5.58603143E-14   2
 -7.41715057E2  -8.43825992E0   3.83464468E0  3.29078952E-3  5.05228001E-5   3
 -6.66251176E-8 2.63707473E-11   7.88717123E2   7.53408013E0                4
!\COMMENT:  6/ 6/17 THERM
C3H5-A               C  3H  5        G    300.0    5000.0  1373.0     1
  8.83926244E0   1.0848952E-2 -3.76807987E-6 5.91217237E-10-3.45595703E-14   2
  1.60424092E4  -2.47555313E1  4.47889052E-1  2.79507544E-2 -1.69490036E-5   3
  5.54378883E-9-8.95719069E-13   1.92565554E4   2.13053621E1                4
!\COMMENT:
C3H5-S               C  3H  5        G    298.0    3000.0  1000.0     1
  2.88965689E0  2.06484496E-2 -1.02005529E-5  2.45220758E-9-2.32477736E-13   2
  3.04802242E4   1.02662579E1   1.5645165E0  2.36197016E-2 -1.07382165E-5   3
-8.68979222E-11 1.19817981E-12   3.08476047E4   1.72062874E1                4
!\COMMENT:
C3H5-T               C  3H  5        G    298.0    3000.0  1000.0     1
  2.36288328E0  2.15547888E-2 -1.07842989E-5  2.6198441E-9-2.50507107E-13   2
   2.8837747E4   1.33587759E1   2.47223165E0  1.75096865E-2  1.54166152E-6   3
 -1.03357169E-8 4.31484742E-12   2.89681156E4   1.36627279E1                4
!\COMMENT:  L 8/89
C3H4-A               C  3H  4        G    200.0    6000.0  1000.0     1
   6.3168722E0   1.1133728E-2  -3.9629378E-6  6.3564238E-10  -3.787554E-14   2
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  2.01300914E4 -1.09821592E1  1.32428134E0  2.30275933E-2 -1.33707079E-5    3
  3.73995006E-9-6.35687588E-13  2.16551584E4  1.54301401E1                  4
!\COMMENT:  T 7/11
C3H3               C  3H  3       G    200.0    6000.0  1000.0     1
  7.14221719E0  7.61902211E-3 -2.6746003E-6 4.24914904E-10-2.51475443E-14    2
  3.95710114E4 -1.25848129E1  1.34577946E0  3.27862233E-2 -4.75146967E-5    3
  3.77892551E-8-1.19201548E-11  4.07684638E4  1.52273792E1                  4
!(/005_C3_003_C3H4-AC3H4-P_PYROSPEC)
!(005_C3_004_NC3H7OH_LTOXID)
!\COMMENT:
TQJC3H6OH            C  3H  7O  3    G    300.0    5000.0  1411.0     1
  1.57530365E1  1.56289438E-2 -5.23690385E-6 8.01741456E-10-4.60590728E-14    2
 -3.24130576E4 -5.08911217E1  2.29728737E0  4.96725824E-2 -3.84714645E-5    3
  1.5603809E-8-2.56748169E-12  -2.8042951E4  2.03767936E1                  4
!\COMMENT:
TQC3H6OI             C  3H  7O  3    G    300.0    5000.0  1417.0     1
  1.71497525E1  1.47440875E-2 -4.99973196E-6 7.71920259E-10 -4.4617568E-14    2
 -2.30944769E4 -5.96032656E1  3.77984842E0  4.5124638E-2 -3.03819021E-5    3
  9.92338649E-9-1.22338206E-12 -1.84544341E4  1.23546787E1                  4
!\COMMENT:
QC3H5OHP             C  3H  7O  3    G    300.0    5000.0  1415.0     1
  1.65390643E1  1.45962463E-2 -4.89569717E-6  7.5019033E-10-4.31310565E-14    2
 -2.47102324E4 -5.34015731E1  1.76951547E0  5.23733147E-2  -4.1965818E-5    3
  1.72471815E-8-2.83710014E-12 -1.99859353E4  2.46273265E1                  4
!\COMMENT:
IQJC3H6OH            C  3H  7O  3    G    300.0    5000.0  1408.0     1
  1.55719527E1  1.57683363E-2 -5.28242575E-6 8.08628793E-10-4.64527621E-14    2
 -3.23985113E4 -4.97782092E1  1.74093905E0  5.10931764E-2 -4.02179535E-5    3
  1.66120004E-8-2.78425352E-12 -2.79317094E4  2.33734165E1                  4
IQC3H6OT             C  3H  7O  3    G    300.0    5000.0  1406.0     1
  1.67044548E1  1.52497437E-2 -5.19996341E-6 8.05676289E-10-4.66785083E-14    2
 -2.34693102E4 -5.83507487E1  2.97554636E0  4.80962295E-2 -3.51787999E-5    3
  1.3200846E-8-2.00208137E-12 -1.88187423E4  1.50392917E1                  4
!\COMMENT: SP_ZADOR
C3H6OH1-2            C  3H  7O  1    G    298.0    3000.0  1000.0     1
  2.00388719E1 -8.18078581E-3  1.5012071E-5 -6.40300256E-9 8.67342181E-13    2
 -1.49106099E4 -7.63464356E1  1.57941557E1 -6.10763187E-2  1.99166967E-4    3
 -1.99047331E-7 6.64970235E-11 -1.05679468E4 -3.83995345E1                  4
!\COMMENT:
NC3H7O               C  3H  7O  1    G    298.0    3000.0  1000.0     1
  3.71165592E0  2.98888018E-2 -1.50650214E-5  3.68054175E-9-3.53437601E-13    2
 -6.55169654E3  8.27016784E0  1.28341389E0  3.57266194E-2  -1.7696995E-5    3
  1.14202428E-9 1.40747781E-12 -5.88259252E3  2.09279823E1                  4
!\COMMENT: SP_FROM ZADOR
C3H6OH2-1            C  3H  7O  1    G    298.0    3000.0  1000.0     1
  6.11414519E0  2.4212332E-2 -1.12344701E-5  2.55293277E-9-2.30128197E-13    2
 -1.06549215E4 -2.82887333E0  2.73544355E0  3.56240446E-2 -2.51973981E-5    3
  9.75845743E-9-1.50573587E-12  -9.8740265E3  1.39971825E1                  4
!\COMMENT:
IC3H7O               C  3H  7O  1    G    298.0    3000.0  1000.0     1
  3.97830632E0  2.91186145E-2 -1.44865221E-5  3.50229508E-9-3.33520915E-13    2
 -7.90548136E3  5.3794563E0  9.86554785E-1  3.80805183E-2 -2.31947108E-5    3
  5.9982404E-9-9.14298018E-14  -7.1643567E3  2.05454298E1                  4
!(/005_C3_005_IC3H7OH_PYROSPEC)
!(005_C3_006_CH3COCH3_LTOXID)
!\COMMENT:  2/14/13 THERM
CH3COCH2O2           C  3H  5O  3    G    300.0    5000.0  1397.0     1
  1.65756401E1  1.06465489E-2 -3.61368681E-6 5.59053564E-10-3.23832271E-14    2
 -2.42541401E4 -5.45304899E1  1.19378141E0  4.98027161E-2 -4.17999508E-5    3
  1.74527607E-8-2.88198761E-12 -1.93244224E4  2.67877493E1                  4
!\COMMENT:  2/ 8/13 THERM
CH3COCH2O            C  3H  5O  2    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
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!\COMMENT:  2/14/13 THERM
C3KET21             C   3H   6O   3    G    300.0    5000.0  1394.0     1
  1.75768076E1  1.20311704E-2 -4.11633942E-6 6.40149366E-10-3.72127562E-14    2
 -4.15502347E4   -6.090971E1 -8.74352903E-1  6.12501498E-2 -5.51474542E-5    3
  2.48491014E-8-4.42613472E-12  -3.58060819E4   3.59306224E1                 4
!(/005_C3_006_CH3COCH3_LTOXID)
!(005_C3_006_CH3COCH3_PYROSPEC)
!\COMMENT:  8/12/15
CH3COCH3            C   3H   6O   1    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
!\COMMENT:  2/14/13 THERM
CH3COCH2            C   3H   5O   1    G    300.0    5000.0  1387.0     1
  1.09524298E1  1.11458668E-2 -3.86262877E-6 6.05088857E-10-3.53293362E-14    2
 -9.60833727E3  -3.15622776E1   1.13381826E0  3.25095045E-2 -2.10424651E-5    3
  6.64421151E-9-8.12618901E-13  -6.04868361E3   2.17158655E1                 4
!(/005_C3_006_CH3COCH3_PYROSPEC)
!(005_C3_007_C2H3CHO_PYROSPEC)
!\COMMENT:
C2H3CHO             C   3H   4O   1    G    298.0    3000.0  1000.0     1
  4.27745325E0  2.08995067E-2 -1.10621906E-5  2.80392911E-9-2.76871274E-13    2
 -1.01465486E4   2.26814496E0   1.30858881E0  2.90665687E-2 -1.85267312E-5    3
  5.10575873E-9 -3.1235785E-13  -9.34139504E3   1.75831373E1                 4
!\COMMENT:
C2H3CO              C   3H   3O   1    G    298.0    3000.0  1000.0     1
  4.57165627E0  1.67235781E-2 -8.58791816E-6  2.13315141E-9-2.07752945E-13    2
  9.48746848E3   3.10327903E0   1.67431562E0  2.53644779E-2 -1.74055511E-5    3
  5.43382478E-9-4.34352533E-13   1.02237218E4   1.78417413E1                 4
!\COMMENT:
CH3CH(OO)CHO          C   3H   5O   3    G    300.0    5000.0  1393.0     1
  1.43787605E1   1.3404919E-2  -4.9812814E-6 8.55523297E-10-5.36378095E-14    2
 -2.22169412E4  -4.39244104E1  5.13860198E-1  4.91794584E-2  -4.0971082E-5    3
  1.75184758E-8-3.02105145E-12  -1.77576548E4   2.93105958E1                 4
!\COMMENT:
QCH2CH(OOH)CHO        C   3H   5O   3    G    300.0    5000.0  1000.0     1
   6.8248196E0   2.2942498E-2  -7.8816911E-6    1.266793E-9 -7.8469708E-14    2
  -1.2513018E4    3.2035751E0   5.2640444E-1   5.9083462E-2  -6.5715773E-5    3
   3.7419547E-8 -8.2431935E-12   -1.2412302E4    2.9477829E1                 4
!\COMMENT:
QCH3CH(OOH)CO         C   3H   5O   3    G    300.0    5000.0  1406.0     1
  1.54753787E1  1.19855535E-2 -3.88647969E-6 5.82170268E-10-3.29481797E-14    2
 -2.12076656E4   -4.8562401E1 -2.34265079E-1   5.8011447E-2 -5.58943334E-5    3
  2.70757029E-8-5.10696754E-12  -1.67362113E4   3.24136213E1                 4
!\COMMENT:
CYC2H3OCHO            C   3H   4O   2    G    300.0    5000.0  1374.0     1
  8.70566732E0   1.8197935E-2 -7.29434992E-6   1.2469133E-9-7.70180076E-14    2
 -2.55049125E4  -2.12921665E1   7.12499787E0  4.70671619E-3  2.20592122E-5    3
 -1.80381528E-8 4.05467913E-12  -2.28419321E4  -6.04871852E0                 4
!\COMMENT:
CH2CH2CHO             C   3H   5O   1    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
!\COMMENT:
SC4H9O              C   4H   9O   1    G    300.0    5000.0  1411.0     1
  1.52130012E1  1.90029969E-2 -6.39004701E-6 9.80774402E-10-5.64493733E-14    2
 -1.59888805E4  -5.43195369E1   2.01772535E0  4.70083969E-2 -2.74726645E-5    3
  7.36290028E-9-6.30414237E-13  -1.11892176E4   1.74371746E1                 4
!(/006_C4_001_C4H10_HTOXID)
!(006_C4_001_C4H10_LTOXID)
!\COMMENT:  10/27/19
PC4H9O2             C   4H   9O   2    G    300.0    5000.0  1391.0     1
  1.66120049E1  2.04752336E-2 -7.01415262E-6   1.0901051E-9-6.32913959E-14    2
 -1.57901735E4  -5.79272276E1   1.80541406E0   5.2649306E-2 -3.30870383E-5    3
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 1.04593484E-8-1.32305701E-12 -1.03866773E4  2.24829685E1                4
!\COMMENT:  10/27/19
SC4H9O2             C  4H  9O  2    G    300.0    5000.0  1403.0     1
  1.68209433E1  1.98834074E-2 -6.71755569E-6  1.03411636E-9-5.96371075E-14    2
  -1.7581535E4  -5.95731156E1   2.27751066E0  5.44334651E-2 -3.82988187E-5    3
 1.42447767E-8-2.18864515E-12   -1.259091E4   1.83237264E1                4
!\COMMENT:  10/27/19
SC4H9O2H            C  4H  10O  2    G    300.0    5000.0  1402.0     1
  1.78075939E1  2.12546017E-2 -7.20960281E-6  1.11291271E-9-6.43060022E-14    2
 -3.48455718E4   -6.5801147E1   1.44010868E0  6.05300206E-2 -4.36262678E-5    3
 1.66226146E-8 -2.6155693E-12  -2.92631492E4   2.17354113E1                4
!\COMMENT:
C4H8OOH1-3          C  4H  9O  2    G    300.0    5000.0  1396.0     1
  1.61247782E1   2.0242098E-2 -6.88631475E-6  1.06534945E-9-6.16599545E-14    2
 -9.16802012E3  -5.26575415E1   2.46292502E0  4.70131194E-2 -2.42145198E-5    3
  4.6540781E-9 1.62198662E-14  -3.95787917E3   2.24569578E1                4
!\COMMENT:
C4H8OOH2-4          C  4H  9O  2    G    300.0    5000.0  1403.0     1
  1.72354039E1  1.91946365E-2 -6.49946502E-6  1.00210964E-9-5.78559962E-14    2
 -9.71158144E3   -5.9898615E1   1.82672511E0  5.69912331E-2 -4.24389492E-5    3
 1.67119278E-8-2.70635765E-12  -4.54629884E3   2.22051948E1                4
!\COMMENT:
C4H8O1-3            C  4H  8O  1    G    300.0    5000.0  1447.0     1
  1.32076917E1  1.77467973E-2 -5.69933762E-6 8.47771212E-10-4.77345874E-14    2
 -2.11717546E4   -4.7838642E1  -5.37284363E0  6.62224444E-2 -5.35318273E-5    3
 2.19451842E-8-3.54479816E-12  -1.54144887E4   4.98345472E1                4
!\COMMENT:
C4H8OOH1-3O2        C  4H  9O  4    G    300.0    5000.0  1400.0     1
   2.1573475E1  2.04528589E-2 -6.99497777E-6  1.08597818E-9-6.30071127E-14    2
 -2.88428166E4  -7.84560716E1   3.02241018E0  6.53862812E-2 -4.89645658E-5    3
 1.90437784E-8-3.02309317E-12  -2.25805572E4   2.05729328E1                4
!\COMMENT:
C4H8OOH2-4O2        C  4H  9O  4    G    300.0    5000.0  1400.0     1
   2.1573475E1  2.04528589E-2 -6.99497777E-6  1.08597818E-9-6.30071127E-14    2
 -2.88428166E4  -7.84560716E1   3.02241018E0  6.53862812E-2 -4.89645658E-5    3
 1.90437784E-8-3.02309317E-12  -2.25805572E4   2.05729328E1                4
!\COMMENT:
NC4KET13            C  4H  8O  3    G    300.0    5000.0  1411.0     1
  1.93085398E1  1.73455091E-2 -5.85046818E-6 9.00297947E-10-5.19274609E-14    2
 -4.51023813E4  -7.04869509E1   3.31775682E0  5.28482064E-2 -3.43211665E-5    3
 1.04562704E-8-1.12796519E-12  -3.94868388E4   1.58443308E1                4
!\COMMENT:
NC4KET24            C  4H  8O  3    G    300.0    5000.0  1394.0     1
  1.74146206E1  1.92744267E-2 -6.57971403E-6  1.02023879E-9-5.91418353E-14    2
 -4.60663138E4  -5.80320911E1   3.12062686E0  5.01343936E-2  -3.1019495E-5    3
 9.36512355E-9-1.07548923E-12   -4.0864427E4   1.96071994E1                4
!(/006_C4_001_C4H10_LTOXID)
!(006_C4_001_C4H10_PYROSPEC)
!\COMMENT:  8/12/15
C4H10               C  4H  10       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
!\COMMENT:  8/12/15
PC4H9               C  4H  9        G    300.0    5000.0  1393.0     1
  1.18547949E1  1.96962095E-2 -6.71054229E-6  1.03891144E-9-6.01513573E-14    2
  3.38182243E3  -3.72343446E1  4.09644702E-1  4.29511341E-2 -2.36582809E-5    3
 6.15744917E-9-5.64300671E-13   7.7431915E3   2.55312526E1                4
!\COMMENT:  8/12/15
SC4H9               C  4H  9        G    300.0    5000.0  1682.0     1
  9.25139144E0  2.24301385E-2 -7.82648592E-6  1.2355946E-9-7.26249864E-14    2
  3.11148804E3  -2.16080436E1  9.42662332E-1  3.7741453E-2 -1.58911963E-5    3
 1.75489317E-9  2.8972575E-13  6.20542636E3   2.42126605E1                4
!(/006_C4_001_C4H10_PYROSPEC)
!(006_C4_002_IC4H10_HTOXID)
```

!\COMMENT: 9/22/19
TC4H9O C 4H 9O 1 G 300.0 5000.0 1373.0 1
1.51889028E1 2.0147561E-2 -7.03124743E-6 1.10634275E-9-6.47863602E-14 2
-1.85728281E4 -5.68068356E1 4.11245323E0 3.82049645E-2 -1.49012588E-5 3
6.45321553E-10 5.86115592E-13 -1.38207918E4 5.66243109E0 4
!\COMMENT: 9/22/19
IC4H9O C 4H 9O 1 G 300.0 5000.0 1402.0 1
1.49421227E1 1.93741698E-2 -6.54752781E-6 1.0082861E-9-5.81656529E-14 2
-1.49775648E4 -5.33188211E1 1.09851986E0 5.02843927E-2 -3.22536137E-5 3
1.04323043E-8 -1.3354625E-12 -1.00529442E4 2.14919206E1 4
!\COMMENT:
IC3H5CHO C 4H 6O 1 G 300.0 5000.0 1396.0 1
1.33892118E1 1.3911542E-2 -4.75820958E-6 7.38736618E-10-4.28606559E-14 2
-1.97917448E4 -4.60146004E1 1.09372823E0 4.43315368E-2 -3.41918451E-5 3
1.39369607E-8 -2.3379146E-12 -1.56745978E4 1.94458467E1 4
!\COMMENT: 2/12/20
IC4H9O2 C 4H 9O 2 G 300.0 5000.0 1396.0 1
1.65502468E1 2.03894477E-2 -6.95256802E-6 1.07704804E-9 -6.2388229E-14 2
-1.63179416E4 -5.86704281E1 6.6428765E-1 5.92637819E-2 -4.4299953E-5 3
1.77847468E-8-2.97286552E-12 -1.09294589E4 2.61006936E1 4
!\COMMENT: 9/ 6/19
TC4H9O2 C 4H 9O 2 G 300.0 5000.0 1397.0 1
1.64403992E1 2.03443665E-2 -6.90545661E-6 1.06633114E-9-6.16257134E-14 2
-2.06885036E4 -6.05439541E1 1.79239003E0 5.67672897E-2 -4.27700336E-5 3
1.75928326E-8-3.02813253E-12 -1.57527539E4 1.74575453E1 4
!\COMMENT: 9/22/19
IC4H8O2H-I C 4H 9O 2 G 300.0 5000.0 1398.0 1
1.69514886E1 1.96565122E-2 -6.70712507E-6 1.03952009E-9-6.02352953E-14 2
-8.80398976E3 -5.81810331E1 2.36576125E-1 6.18274658E-2 -4.85588184E-5 3
2.03310238E-8-3.50400054E-12 -3.27357731E3 3.05430182E1 4
!\COMMENT: 9/22/19
IC4H8O2H-T C 4H 9O 2 G 300.0 5000.0 1385.0 1
1.58918892E1 2.06730298E-2 -7.0850682E-6 1.10147653E-9-6.39664273E-14 2
-1.09442141E4 -5.20875566E1 3.07062149E0 4.48451773E-2 -2.18981348E-5 3
3.8036668E-9 9.33329943E-14 -5.89846659E3 1.88457783E1 4
!\COMMENT: 22/19
IC4H8OOH-IO2 C 4H 9O 4 G 300.0 5000.0 1397.0 1
2.1603025E1 2.05744232E-2 -7.06861366E-6 1.10071529E-9 -6.3994598E-14 2
-2.79319407E4 -7.82672725E1 1.79333344E0 7.08585563E-2 -5.71423408E-5 3
2.41954633E-8-4.18040646E-12 -2.14284369E4 2.67425141E1 4
!\COMMENT: 9/22/19
IC4KETII C 4H 8O 3 G 300.0 5000.0 1396.0 1
1.80532391E1 1.8841121E-2 -6.45472857E-6 1.00330789E-9-5.82612587E-14 2
-4.39462527E4 -6.43254899E1 2.90712469E0 5.18272292E-2 -3.27937625E-5 3
1.00565978E-8 -1.1647857E-12 -3.84811883E4 1.7810076E1 4
!\COMMENT: 21/08/19 THERM
IC4H7OOH C 4H 8O 2 G 300.0 5000.0 1425.0 1
1.4477813E1 2.00176051E-2 -6.38000134E-6 9.43456882E-10-5.28823593E-14 2
-1.6720753E4 -4.61591612E1 -4.17611045E-1 5.77650805E-2 -4.27135576E-5 3
1.66549177E-8-2.61827018E-12 -1.19563554E4 3.26001977E1 4
!\COMMENT: 9/22/19
TC4H9O2H C 4H 10O 2 G 300.0 5000.0 1397.0 1
1.74091563E1 2.16498694E-2 -7.35726095E-6 1.13703858E-9-6.57512161E-14 2
-3.7916922E4 -6.66008499E1 1.0482232E0 6.25767968E-2 -4.78095308E-5 3
1.97968913E-8-3.41101635E-12 -3.24422541E4 2.04122472E1 4
!(/006_C4_002_IC4H10_LTOXID)
!(006_C4_002_IC4H10_PYROSPEC)
!\COMMENT: 8/12/15
IC4H10 C 4H 10 G 300.0 5000.0 1397.0 1
1.26422737E1 2.14133551E-2 -7.26711536E-6 1.12207226E-9-6.48434177E-14 2
-2.28293782E4 -4.66059659E1 -1.07413829E0 5.2461832E-2 -3.42407949E-5 3
1.18817533E-8-1.73238254E-12 -1.79218932E4 2.74851665E1 4
!\COMMENT: 10/ 4/19
IC4H9 C 4H 9 G 300.0 5000.0 1396.0 1
1.21140464E1 1.93954115E-2 -6.58728459E-6 1.01750858E-9-5.88134259E-14 2

```
   2.6441035E3  -4.00992454E1  5.58050275E-2  4.80008922E-2 -3.34035042E-5    3
  1.28484291E-8-2.11310293E-12   6.86745218E3   2.46372139E1                   4
!\COMMENT:  9/13/19
TC4H9               C   4H   9         G     300.0    5000.0  1381.0      1
  1.07073047E1  2.06651857E-2 -7.04353974E-6  1.09075877E-9-6.31649068E-14    2
  3.35244576E2  -3.21520645E1   1.98280167E0   3.3074392E-2 -8.97503566E-6    3
 -2.53990889E-9 1.26572569E-12   4.21272775E3   1.76148184E1                   4
!\COMMENT:  4/ 3/ 0 THERM
IC4H7O              C   4H   7O   1     G     300.0    5000.0  1386.0      1
  1.33457615E1  1.61218588E-2 -5.44376403E-6 8.38199374E-10 -4.8360828E-14    2
  6.11443644E2  -4.36818838E1   1.74700687E0   4.07783436E-2 -2.44750243E-5    3
  7.06502958E-9-7.51570589E-13   4.86979233E3   1.94535999E1                   4
!(/006_C4_003_IC4H8_LTOXID)
!(006_C4_003_IC4H8_PYROSPEC)
!\COMMENT:  8/12/15
IC4H8               C   4H   8         G     300.0    5000.0  1392.0      1
  1.11444028E1  1.81609265E-2 -6.17791116E-6 9.55481871E-10-5.52826092E-14    2
 -7.84024684E3  -3.68508829E1   5.72478139E-2   4.17768938E-2 -2.49095729E-5    3
  7.54294402E-9-9.23202212E-13  -3.72166259E3   2.35698905E1                   4
!\COMMENT:
IC4H7               C   4H   7         G     298.0    3000.0  1000.0      1
  3.82412534E0  2.95960754E-2 -1.46407966E-5   3.5266306E-9-3.35051666E-13    2
  1.41960801E4   4.75160803E0  -1.75459721E0   4.92910718E-2 -4.04373485E-5    3
  1.83479315E-8-3.47607453E-12   1.54490344E4   3.23361598E1                   4
!\COMMENT:  9/ 8/14
C4H7O2-1            C   4H   7O   1     G     300.0    5000.0  1684.0      1
   1.1268569E1   2.0172482E-2 -7.41925667E-6  1.21275519E-9-7.30115348E-14    2
  2.13876442E3  -3.15208064E1   5.16434924E0   2.53427725E-2 -1.39669041E-6    3
 -6.00713944E-9 1.76696879E-12   5.03210693E3   4.37441148E0                   4
!(/006_C4_004_C4H8-1_LTOXID)
!(006_C4_004_C4H8-1_PYROSPEC)
!\COMMENT:
C4H8-1              C   4H   8         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
!\COMMENT: CWZ ADDED FROM YL CALCULATION
C4H71-3             C   4H   7         G    298.15    2000.0  1000.0      1
  4.46811308E0  2.74302155E-2 -1.21179861E-5  2.27424125E-9-1.08909321E-13    2
    1.320203E4   2.39088817E0  2.79155108E-1   3.80223852E-2 -1.87607474E-5    3
 5.39086588E-10 1.86579489E-12   1.43480047E4   2.41411045E1                   4
!(/006_C4_005_C4H8-2_LTOXID)
!(006_C4_005_C4H8-2_PYROSPEC)
!\COMMENT:  8/12/15
C4H8-2              C   4H   8         G     300.0    5000.0  1383.0      1
  1.08652083E1  1.84123129E-2 -6.26886673E-6 9.70205962E-10-5.61638967E-14    2
 -7.09625867E3  -3.51547481E1   1.3079551E0   3.53136624E-2 -1.51866126E-5    3
  1.64112363E-9  3.4425762E-13  -3.19767852E3   1.81594717E1                   4
!(/006_C4_011_NC3H7CHO_LTOXID)
!(006_C4_011_NC3H7CHO_PYROSPEC)
!\COMMENT:  8/12/15
NC3H7CHO            C   4H   8O   1     G     300.0    5000.0  1679.0      1
  1.19789345E1  2.04894148E-2 -7.24831619E-6  1.15561709E-9-6.84119824E-14    2
  -3.0927213E4  -3.63929716E1   1.24208539E0   4.21277518E-2 -2.13832135E-5    3
  4.22614614E-9-1.03710908E-13  -2.71049353E4   2.21567167E1                   4
!(/007_C5_005_CC5H10BC5H10_LTOXID)
!(007_C5_005_CC5H10BC5H10_PYROSPEC)
!\AUTHOR:  KPS/JP  !\COMMENT:  [CC=C(C)C_[NA]_MESSPF]  [OPT//HR//HOF:  WB97XD/AUG-CC-PVTZ//WB97XD/6-311++G(D,P)//0KISODESMICS[CBS-
QB3/CBS-APNO/G3/G4]] GENERATED ON [2019_10_19_16_43_
BC5H10              C   5H  10         G     200.0    3000.0  1000.0      1
  2.43604039E0  4.26698394E-2 -2.06096382E-5  4.81426739E-9-4.41304814E-13    2
 -7.87742644E3   1.40425561E1   6.97870495E0 -2.46912236E-3  1.01782898E-4    3
 -1.25790376E-7 4.83670989E-11  -7.75864233E3  -2.06158545E0                   4
!(/007_C5_006_AC5H10_LTOXID)
!(007_C5_006_AC5H10_PYROSPEC)
```

!\AUTHOR: KPS/JP !\COMMENT: [C=C(C)CC_[WB97XD_6-31+GDP-GEOM_00018]_MESSPF] [OPT//HR//HOF: WB97XD/AUG-CC-PVTZ//WB97XD/6-311++G(D,P)//0KISODESMICS[CBS-QB3/CBS-APNO/G3/G4]] GENERAT
AC5H10 C 5H 10 G 200.0 3000.0 1000.0 1
3.5081941E0 4.19588686E-2 -2.07434721E-5 5.02272513E-9 -4.8268103E-13 2
-7.45892729E3 8.24526165E0 5.10075206E0 1.14618232E-2 7.48325605E-5 3
-1.03973288E-7 4.18417876E-11 -6.87753037E3 5.70417752E0 4
!\AUTHOR: KPS/JP !\COMMENT: [C=C(C)[CH]C_[NA]_MESSPF] [OPT//HR//HOF: WB97XD/AUG-CC-PVTZ//WB97XD/6-311++G(D,P)//0KISODESMICS[CBS-QB3/CBS-APNO/G3/G4]] GENERATED ON [2019_10_19_16_
AC5H9-C C 5H 9 G 200.0 3000.0 1000.0 1
4.15484073E0 3.80769147E-2 -1.8506506E-5 4.37669296E-9 -4.08431646E-13 2
9.33380689E3 5.11111559E0 4.35273311E0 1.34532681E-2 6.70816888E-5 3
-9.66735514E-8 3.9479372E-11 1.02033398E4 9.28513653E0 4
!\COMMENT: 5/19
C6H11OH1Q2-5 C 6H 13O 3 G 300.0 5000.0 1412.0 1
2.5454304E1 2.81820807E-2 -9.47614779E-6 1.45450255E-9 -8.37211984E-14 2
-3.84122947E4 -9.58658892E1 2.07747862E0 8.25818684E-2 -5.6841223E-5 3
1.97097674E-8 -2.69844211E-12 -3.03930829E4 2.95529406E1 4
!\COMMENT: 9
C6H11OH1Q2-3O2 C 6H 13O 5 G 300.0 5000.0 1405.0 1
3.04428303E1 2.91092976E-2 -9.90217854E-6 1.53184891E-9 -8.86572699E-14 2
-5.8147056E4 -1.19560974E2 2.12297527E0 9.97590267E-2 -7.78900492E-5 3
3.14238435E-8 -5.12837404E-12 -4.88370567E4 3.08119302E1 4
!\COMMENT: 19
C6H11OH1Q2-4O2 C 6H 13O 5 G 300.0 5000.0 1405.0 1
3.04428303E1 2.91092976E-2 -9.90217854E-6 1.53184891E-9 -8.86572699E-14 2
-5.8147056E4 -1.19560974E2 2.12297527E0 9.97590267E-2 -7.78900492E-5 3
3.14238435E-8 -5.12837404E-12 -4.88370567E4 3.08119302E1 4
!\COMMENT: 19
C6H11OH1Q2-5O2 C 6H 13O 5 G 300.0 5000.0 1405.0 1
3.04428303E1 2.91092976E-2 -9.90217854E-6 1.53184891E-9 -8.86572699E-14 2
-5.8147056E4 -1.19560974E2 2.12297527E0 9.97590267E-2 -7.78900492E-5 3
3.14238435E-8 -5.12837404E-12 -4.88370567E4 3.08119302E1 4
!\COMMENT: 15/19
C6H103OH1Q2 C 6H 12O 3 G 300.0 5000.0 1404.0 1
2.3818852E1 2.78678537E-2 -9.45603351E-6 1.46019748E-9 -8.43992106E-14 2
-4.5960714E4 -8.86173365E1 6.00523739E-1 8.32237696E-2 -5.99206769E-5 3
2.23635581E-8 -3.39822182E-12 -3.80566012E4 3.56015758E1 4
!\COMMENT: 15/19
C6H104OH1Q2 C 6H 12O 3 G 300.0 5000.0 1407.0 1
2.44796533E1 2.70582292E-2 -9.12175102E-6 1.40228253E-9 -8.07946078E-14 2
-4.71390048E4 -9.31529991E1 1.11310982E0 8.58599894E-2 -6.64232714E-5 3
2.69787976E-8 -4.46214907E-12 -3.94906526E4 3.07664621E1 4
!\COMMENT: 15/19
C6H105OH1Q2 C 6H 12O 3 G 300.0 5000.0 1407.0 1
2.51849996E1 2.65379826E-2 -8.95952672E-6 1.37874023E-9 -7.94953807E-14 2
-4.6247866E4 -9.67848978E1 8.91164787E-1 8.88766232E-2 -7.10737731E-5 3
2.97444803E-8 -5.04534646E-12 -3.84154662E4 3.16270523E1 4
!\COMMENT: 19
C6H10OH1KET2-3 C 6H 12O 4 G 300.0 5000.0 1380.0 1
3.00641028E1 2.52656245E-2 -8.70629746E-6 1.36009894E-9 -7.93026811E-14 2
-7.46249943E4 -1.20582898E2 2.04875611E0 9.05032044E-2 -6.66947833E-5 3
2.484605E-8 -3.74699068E-12 -6.49068074E4 2.99034977E1 4
!\COMMENT:
NO N 1O 1 G 298.15 3000.0 1000.0 1
2.79462839E0 2.12260586E-3 -1.11936971E-6 2.79521018E-10 -2.68625363E-14 2
1.00019069E4 8.88322674E0 4.15036687E0 -4.08890008E-3 9.38071726E-6 3
-7.50908901E-9 2.11742798E-12 9.77018679E3 2.53971032E0 4
!\COMMENT:
HCN C 1H 1N 1 G 298.15 3000.0 1000.0 1
2.92308097E0 4.44713874E-3 -2.18020741E-6 5.19245486E-10 -4.87687163E-14 2
1.47106866E4 6.27783116E0 2.22381158E0 8.91348548E-3 -1.13836313E-5 3
8.3241306E-9 -2.41730729E-12 1.4767077E4 9.23408445E0 4
!\COMMENT:
NH H 1N 1 G 298.15 3000.0 1000.0 1
2.95100955E0 9.09994439E-4 -8.35582439E-8 5.17312027E-11 1.13981436E-14 2

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  4.19707045E4  4.83056694E0  3.44697209E0  5.57847818E-4 -2.0028936E-6    3
 2.85952922E-9-1.12434284E-12  4.17899268E4  2.02990852E0                  4
!\COMMENT:  ATCT3E
N                N  1            G    200.0    6000.0  1000.0     1
  2.41604245E0  1.74663766E-4 -1.18864562E-7 3.01850054E-11-2.03260159E-15    2
  5.61051512E4  4.64905706E0  2.49976643E0  5.02149594E-7  1.93091211E-9    3
-4.94632629E-12 2.74089506E-15   5.6076071E4  4.19499326E0                  4
!\COMMENT:
NNH              H  1N  2        G   298.15    3000.0  1000.0     1
  2.90981142E0  4.44718211E-3 -1.82919152E-6 3.64004342E-10-3.13273352E-14    2
  2.92696472E4  9.11653812E0  4.09254871E0 -2.37173287E-3  1.15311297E-5    3
-1.06308423E-8  3.2393758E-12   2.9137498E4  3.93250587E0                  4
!\COMMENT:
HNO              H  1N  1O  1    G   298.15    3000.0  1000.0     1
  2.58819802E0  4.87708822E-3 -2.29243315E-6 5.82214028E-10-5.94811743E-14    2
  1.20213574E4  1.04315796E1  4.51988078E0 -5.42507623E-3  1.70239636E-5    3
-1.48708172E-8 4.44763498E-12  1.17637925E4  1.75618526E0                  4
!\COMMENT:
NO2              N  1O  2        G   298.15    3000.0  1000.0     1
  3.65239279E0  4.7163231E-3 -2.74591748E-6 7.45382834E-10-7.63891108E-14    2
  2.57216137E3   6.5268344E0  3.39100918E0  2.62448348E-3  5.09790306E-6    3
-7.62120493E-9 2.79960135E-12  2.78130679E3  8.57220275E0                  4
!\COMMENT:
HONO              H  1N  1O  2    G   298.15    3000.0  1000.0     1
  4.19966671E0  5.94217338E-3 -2.95404834E-6 7.19846187E-10-6.74909061E-14    2
 -1.08122769E4  5.08809833E0  3.49106617E0  6.81116875E-3  -1.3094312E-6    3
-2.34197204E-9 1.18931535E-12 -1.05722865E4  8.99803804E0                  4
!\COMMENT:
N2O              N  2O  1        G   298.15    3000.0  1000.0     1
  3.61316907E0  5.15970465E-3 -2.97227625E-6 8.00505298E-10-8.26331952E-14    2
  8.60075126E3  4.26880857E0  2.49126356E0  9.16224976E-3 -8.24847853E-6    3
 3.83289657E-9-7.19461784E-13  8.84938621E3  9.80262335E0                  4
!\COMMENT:
HOCN              C  1H  1N  1O  1G   298.15    3000.0  1000.0     1
  4.26758218E0  6.14779617E-3 -2.91885336E-6 6.92686313E-10-6.47954836E-14    2
 -3.34027063E3  2.82895438E0   2.7769203E0  1.2035926E-2 -1.16392715E-5    3
 6.43178073E-9-1.48093966E-12 -3.03841237E3  1.00391657E1                  4
!\COMMENT:
NCO              C  1N  1O  1    G   298.15    3000.0  1000.0     1
  3.77930605E0  5.23935486E-3 -3.11170901E-6 8.62141939E-10-9.12475403E-14    2
  1.34827126E4  4.10147682E0  2.80872271E0  7.96075832E-3 -5.45241934E-6    3
  1.2616856E-9 9.90990185E-14  1.37348757E4  9.07421285E0                  4
!\COMMENT:
CH3NO2             C  1H  3N  1O  2G   298.15    3000.0  1000.0     1
  3.29539268E0  1.82396763E-2 -9.53896025E-6  2.41170211E-9-2.37861517E-13    2
 -1.12915706E4  9.04148525E0  1.36489033E0  2.04311363E-2 -4.53032589E-6    3
-6.45793696E-9 3.36218562E-12 -1.06289427E4  1.97376805E1                  4
END

TRANSPORT ALL
AR 0 127.697 3.462 0.0 1.609 2.0
N2 1 97.839 3.61 0.0 1.756 4.0
HE 0 11.442 2.715 0.0 0.204 2.0
H2 1 304.69 2.19 0.0 0.775 280.0
H 0 541.672 1.53 0.0 0.666 0.0
O2 1 676.424 3.069 0.0 1.487 3.8
O 0 235.686 2.485 0.0 0.744 0.0
H2O 2 637.056 2.943 1.851 1.407 4.0
OH 1 514.598 2.582 1.635 1.077 0.0
OHV 1 80.0 2.75 0.0 0.0 0.0
H2O2 2 1361.148 3.179 1.702 2.239 3.8
HO2 2 963.003 3.129 2.146 1.959 3.8
CO 1 98.1 3.65 0.0 1.95 1.8
CO2 1 244.0 3.763 0.0 2.65 2.1
CH3O2H 2 481.8 3.626 0.0 0.0 1.0
```

CH3O2 2 481.8 3.626 0.0 0.0 1.0
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
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
HO2CHO 2 436.0 3.97 0.0 0.0 2.0
O2CHO 2 436.0 3.97 0.0 0.0 2.0
OCHO 2 498.0 3.59 0.0 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
C2H5O2H 2 470.6 4.41 0.0 0.0 1.5
C2H5O2 2 470.6 4.41 0.0 0.0 1.5
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
C2H2 1 265.3 3.721 0.0 0.0 2.5
C2H 1 265.3 3.721 0.0 0.0 2.5
C2H3O1-2 2 436.0 3.97 0.0 0.0 2.0
C2H5O 2 470.6 4.41 0.0 0.0 1.5
O2CH2CHO 2 275.049 5.428 0.0 0.0 1.0
HO2CH2CO 2 279.007 5.505 1.3 0.0 1.0
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
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
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
NC3H7O2H 2 481.5 4.997 1.7 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
C3H6OOH1-3 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
SC3H5OO 2 481.5 4.997 1.7 0.0 1.0
TC3H5OO 2 481.5 4.997 1.7 0.0 1.0
OCHCH2CH2O 2 459.9 5.0 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
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
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-S 2 316.0 4.22 0.0 0.0 1.0
C3H5-T 2 316.0 4.22 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
TQJC3H6OH 2 464.2 5.009 2.6 0.0 1.0
TQC3H6OI 2 464.2 5.009 2.6 0.0 1.0
QC3H5OHP 2 464.2 5.009 2.6 0.0 1.0
IQJC3H6OH 2 464.2 5.009 2.6 0.0 1.0
IQC3H6OT 2 464.2 5.009 2.6 0.0 1.0
C3H6OH1-2 2 487.9 4.82 0.0 0.0 1.0
NC3H7O 2 481.5 4.997 1.7 0.0 1.0

C3H6OH2-1 2 487.9 4.82 0.0 0.0 1.0
IC3H7O 2 459.5 5.036 1.7 0.0 1.0
CH3COCH2O2 2 502.115 5.429 0.0 0.0 0.0
CH3COCH2O 2 447.639 5.086 0.0 0.0 0.0
C3KET21 2 464.2 5.009 2.6 0.0 1.0
CH3COCH3 2 435.5 4.86 0.0 0.0 1.0
CH3COCH2 2 435.5 4.86 0.0 0.0 1.0
C2H3CHO 2 428.8 4.958 2.9 0.0 1.0
C2H3CO 2 443.2 4.12 0.0 0.0 1.0
CH3CH(OO)CHO 2 925.889 6.28 0.0 0.0 0.0
QCH2CH(OOH)CHO 2 925.889 6.28 0.0 0.0 0.0
QCH3CH(OOH)CO 2 925.889 6.28 0.0 0.0 0.0
CYC2H3OCHO 2 920.803 6.25 0.0 0.0 0.0
CH2CH2CHO 2 424.6 4.82 0.0 0.0 1.0
SC4H9O 2 496.0 5.2 0.0 0.0 1.0
PC4H9O2 2 496.0 5.2 0.0 0.0 1.0
SC4H9O2 2 496.0 5.2 0.0 0.0 1.0
SC4H9O2H 2 496.0 5.2 0.0 0.0 1.0
C4H8OOH1-3 2 496.0 5.2 0.0 0.0 1.0
C4H8OOH2-4 2 496.0 5.2 0.0 0.0 1.0
C4H8O1-3 2 496.0 5.2 0.0 0.0 1.0
C4H8OOH1-3O2 2 496.0 5.2 0.0 0.0 1.0
C4H8OOH2-4O2 2 496.0 5.2 0.0 0.0 1.0
NC4KET13 2 476.0 5.778 2.6 0.0 1.0
NC4KET24 2 476.0 5.778 2.6 0.0 1.0
C4H10 2 350.9 5.206 0.0 0.0 1.0
PC4H9 2 352.0 5.24 0.0 0.0 1.0
SC4H9 2 352.0 5.24 0.0 0.0 1.0
TC4H9O 2 496.0 5.2 0.0 0.0 1.0
IC4H9O 2 496.0 5.2 0.0 0.0 1.0
IC3H5CHO 2 436.4 5.352 0.0 0.0 1.0
IC4H9O2 2 502.252 5.43 0.0 0.0 0.0
TC4H9O2 2 502.252 5.43 0.0 0.0 0.0
IC4H8O2H-I 2 502.2 5.356 1.8 0.0 1.0
IC4H8O2H-T 2 502.2 5.356 1.8 0.0 1.0
IC4H8OOH-IO2 2 600.078 6.009 0.0 0.0 0.0
IC4KETII 2 549.655 5.716 0.0 0.0 0.0
IC4H7OOH 2 436.4 5.352 0.0 0.0 1.0
TC4H9O2H 2 505.54 5.45 0.0 0.0 0.0
IC4H10 2 335.7 5.208 0.1 0.0 1.0
IC4H9 2 352.0 5.24 0.0 0.0 1.0
TC4H9 2 352.0 5.24 0.0 0.0 1.0
IC4H7O 2 496.0 5.2 0.0 0.0 1.0
IC4H8 2 344.5 5.089 0.5 0.0 1.0
IC4H7 2 355.0 4.65 0.0 0.0 1.0
C4H7O2-1 2 436.4 5.352 0.0 0.0 1.0
C4H8-1 2 355.0 4.65 0.0 0.0 1.0
C4H71-3 2 357.1 4.72 0.0 0.0 1.0
C4H8-2 2 355.0 4.65 0.0 0.0 1.0
NC3H7CHO 2 464.2 5.009 2.6 0.0 1.0
BC5H10 2 391.4 5.55 0.0 0.0 1.0
AC5H10 2 386.6 5.532 0.5 0.0 1.0
AC5H9-C 2 396.8 5.458 0.0 0.0 1.0
C6H11OH1Q2-5 2 495.31 6.276 0.0 13.3 1.0
C6H11OH1Q2-3O2 2 495.31 6.276 0.0 13.3 1.0
C6H11OH1Q2-4O2 2 495.31 6.276 0.0 13.3 1.0
C6H11OH1Q2-5O2 2 495.31 6.276 0.0 13.3 1.0
C6H103OH1Q2 2 495.31 6.276 0.0 13.3 1.0
C6H104OH1Q2 2 495.31 6.276 0.0 13.3 1.0
C6H105OH1Q2 2 495.31 6.276 0.0 13.3 1.0
C6H10OH1KET2-3 2 493.406 6.262 0.0 13.13 1.0
NO 1 139.32 3.339 0.2 1.76 4.0
HCN 1 569.0 3.63 0.0 0.0 1.0
NH 1 80.0 2.65 0.0 0.0 4.0
N 0 71.4 3.298 0.0 0.0 0.0

```
NNH 2 71.4 3.798 0.0 0.0 1.0
HNO 2 170.0 3.43 1.62 0.0 1.0
NO2 2 333.59 3.852 0.4 0.0 1.0
HONO 2 350.0 3.95 1.639 0.0 1.0
N2O 1 232.4 3.828 0.0 0.0 1.0
HOCN 2 232.4 3.828 0.0 0.0 1.0
NCO 1 232.4 3.828 0.0 0.0 1.0
CH3NO2 2 232.4 3.828 0.0 0.0 1.0
END

REACTIONS MOLES CAL/MOLE
!++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++++++++++++++++++++++++++++++++++++++
!\KINETICS_MODULE: H2_O2
!++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++++++++++++++++++++++++++++++++++++++
!------------------------------------------------------------------------------------------------------------------------------
!\SUBMECH: H2
!------------------------------------------------------------------------------------------------------------------------------
!____________________________________________________________________________________________________________
!\REACTIONCLASS: RH(=)PRODUCTS
!____________________________________________________________________________________________________________
!\Author: AK !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
H2+M=2H+M    4.577E19 -1.4 1.044E5
   HE/0.83/
   CO/1.9/
   CH4/2.0/
   H2/2.5/
   C2H6/3.0/
   CO2/3.8/
   H2O/12.0/
!____________________________________________________________________________________________________________
!\REACTIONCLASS: RH+R_ABSTRACTION
!____________________________________________________________________________________________________________
!\Author: SP !\Ref: BAULCH, D. L.; BOWMAN, C. T.; COBOS, J PHYS CHEM REF DATA 2005, 34, 757-1397. !\Comment: WARNING
O+H2=OH+H    3.8E12 0.0 7.948E3
   DUP
!\Author: SP !\Ref: BAULCH, D. L.; BOWMAN, C. T.; COBOS, J PHYS CHEM REF DATA 2005, 34, 757-1397. !\Comment: WARNING
O+H2=OH+H    8.8E14 0.0 1.9175E4
   DUP
!\Author: UB !\Ref: J.V.MICHAEL SUTHERLAND, J.PHYS.CHEM. 92(1988) 3853 !\Comment: WARNING
H2+OH=H+H2O    2.2E8 1.51 3.43E3
!____________________________________________________________________________________________________________
!\REACTIONCLASS: TERMOLECULARREACTIONH+O2+R(=)RH+O2!!AUTHOR
!____________________________________________________________________________________________________________
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
2H+O2=H2+O2    8.8E22 -1.835 8.0E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
2H+O2=2OH    4.0E22 -1.835 8.0E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
H+O2+O=OH+O2    7.35E22 -1.835 8.0E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
H+O2+OH=H2O+O2    2.56E22 -1.835 8.0E2
!------------------------------------------------------------------------------------------------------------------------------
!\ENDSUBMECH: H2
!------------------------------------------------------------------------------------------------------------------------------
!------------------------------------------------------------------------------------------------------------------------------
!\SUBMECH: O2
!------------------------------------------------------------------------------------------------------------------------------
!____________________________________________________________________________________________________________
!\REACTIONCLASS: RH(=)PRODUCTS
!____________________________________________________________________________________________________________
!\Author: AK !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
2O+M=O2+M    6.165E15 -0.5 0.0E0
   HE/0.83/
```

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   AR/0.83/
   CO/1.9/
   CH4/2.0/
   H2/2.5/
   C2H6/3.0/
   CO2/3.8/
   H2O/12.0/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONH
!_____________________________________________________________________________________________________
!\Author: AK !\Ref: HONG ET AL. PROC. OF THE COMB. INST. 33(2011) 309?16 !\Comment: 2 PARAMETER FIT
O2+H=O+OH    1.04E14 0.0 1.5286E4
!-----------------------------------------------------------------------------------------------------
!\ENDSUBMECH: O2
!-----------------------------------------------------------------------------------------------------
!-----------------------------------------------------------------------------------------------------
!\SUBMECH: H2O
!-----------------------------------------------------------------------------------------------------
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RH(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: ABS_TEST SP !\Ref: SELLEVAG, S. R.;J. PHYS. CHEM. A 2008, 112, 50855095 ! !\Comment: WARNING
H+OH(+M)=H2O(+M)    2.5E13 0.234 -1.14E2
   AR/0.4/
   HE/0.57/
   O2/1.0/
   N2/1.0/
   H2/1.5/
   H2O/13.0/
   LOW/4.53E21 -1.81E0 4.92E2/
   TROE/7.3E-1 1.0E-30 1.0E30 1.0E30/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RH+R_ABSTRACTION
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: G. ALTINAY, J. PHYS. CHEM. A, 118(2014), PP. 38-54 !\Comment: WARNING
2OH=H2O+O    2.88E6 1.79 -1.75E3
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ALPHA_SCISSION
!_____________________________________________________________________________________________________
!\Author: AK !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
O+H+M=OH+M    4.714E18 -1.0 0.0E0
   AR/0.75/
   HE/0.75/
   CO/1.5/
   CH4/2.0/
   CO2/2.0/
   H2/2.5/
   C2H6/3.0/
   H2O/12.0/
!=====================================================================================================
!\SUBSPECIES: OHV
!=====================================================================================================
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ALPHA_SCISSION
!_____________________________________________________________________________________________________
!\Author: ABS !\Ref: HALL AND PETERSEN IJCK 2006 !\Comment: WARNING
H+O+M=OHV+M    4.43E14 0.0 1.0E4
   AR/0.4/
   O2/0.8/
   CO2/2.0/
   H2/2.0/
   CH4/2.0/
   H2O/12.0/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: THIRD_BODY_DEACTIVATION
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!_____________________________________________________________________________________________________
!\Author: ABS !\Ref: HALL AND PETERSEN IJCK 2006 !\Comment: WARNING
OHV+H2O=OH+H2O    5.92E12 0.5 -8.6E2
!\Author: ABS !\Ref: HALL AND PETERSEN IJCK 2006 !\Comment: WARNING
OHV+H2=OH+H2    2.95E12 0.5 -4.44E2
!\Author: ABS !\Ref: WARNING !\Comment: WARNING
OHV+N2=OH+N2    2.1E12 0.5 -4.82E2
!\Author: ABS !\Ref: HALL AND PETERSEN IJCK 2006 !\Comment: WARNING
OHV+OH=2OH    1.5E12 0.5 0.0E0
!\Author: ABS !\Ref: HALL AND PETERSEN IJCK 2006 !\Comment: WARNING
OHV+H=OH+H    1.5E12 0.5 0.0E0
!\Author: ABS !\Ref: HALL AND PETERSEN IJCK 2006 !\Comment: WARNING
OHV+AR=OH+AR    2.17E10 0.5 2.06E3
!\Author: ABS !\Ref: HALL AND PETERSEN IJCK 2006 !\Comment: WARNING
OHV=OH    1.4E6 0.0 0.0E0
!\Author: ABS !\Ref: HALL AND PETERSEN IJCK 2006 !\Comment: WARNING
OHV+O2=OH+O2    2.1E12 0.5 -4.82E2
!\Author: ABS !\Ref: HALL AND PETERSEN IJCK 2006 !\Comment: WARNING
OHV+CO2=OH+CO2    2.75E12 0.5 -9.68E2
!\Author: ABS !\Ref: HALL AND PETERSEN IJCK 2006 !\Comment: WARNING
OHV+CO=OH+CO    3.23E12 0.5 -7.87E2
!\Author: ABS !\Ref: HALL AND PETERSEN IJCK 2006 !\Comment: WARNING
OHV+CH4=OH+CH4    3.36E12 0.5 -6.35E2
!\Author: ABS !\Ref: HALL AND PETERSEN IJCK 2006 !\Comment: WARNING
OHV+O=OH+O    1.5E12 0.5 0.0E0
!=====================================================================================================
!\ENDSUBSPECIES: OHV
!=====================================================================================================
!-----------------------------------------------------------------------------------------------------
!\ENDSUBMECH: H2O
!-----------------------------------------------------------------------------------------------------
!-----------------------------------------------------------------------------------------------------
!\SUBMECH: H2O2
!-----------------------------------------------------------------------------------------------------
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RH(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: UB !\Ref: TROE, COMBUST. FLAME, 158 !\Comment: RATE CONSTANT IS FOR N2,
H2O2(+M)=2OH(+M)    2.0E12 0.9 4.8749E4
   HE/0.44/
   O2/0.79/
   CO2/1.06/
   N2/1.5/
   CO/2.8/
   H2/3.7/
   H2O/5.1/
   H2O2/5.2/
   LOW/2.3530181E24 -2.2929358E0 4.8743405E4/
   TROE/4.3E-1 1.0E-30 1.0E30/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RH+R_ABSTRACTION
!_____________________________________________________________________________________________________
!\Author: AK !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
H2O2+H=H2O+OH    2.41E13 0.0 3.97E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
H2O2+H=HO2+H2    5.02E6 2.07 4.3E3
!\Author: AK !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
H2O2+O=OH+HO2    9.55E6 2.0 3.97E3
!\Author: AK !\Ref: HONG ET AL. J. PHYS. CHEM. A 114(2010) 5718-5727 !\Comment: WARNING
H2O2+OH=H2O+HO2    1.74E12 0.0 3.18E2
   DUP
!\Author: AK !\Ref: HONG ET AL. J. PHYS. CHEM. A 114(2010) 5718-5727 !\Comment: WARNING
H2O2+OH=H2O+HO2    7.59E13 0.0 7.269E3
   DUP
!_____________________________________________________________________________________________________
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!\REACTIONCLASS: R+R(=)PRODUCTS
!________________________________________________________________________________________________________
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
HO2+H=H2+O2    2.8E6 2.09 -1.451E3
!\Author: AK !\Ref: MUELLER ET AL., INT. J. CHEM. KINET. 31(10)(1999) 705724. !\Comment: WARNING
HO2+H=2OH    7.079E13 0.0 2.95E2
!\Author: AK !\Ref: BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21 !\Comment: WARNING
HO2+O=OH+O2    3.25E13 0.0 0.0E0
!\Author: UB !\Ref: M.P. BURKE, S.J. KLIPPENSTEIN, L.B. HARDING, PROC. COMBUST. INST. 34(2013) 547-555 !\Comment: WARNING
OH+HO2=H2O+O2    1.93E20 -2.49 5.8424E2
   DUP
!\Author: UB !\Ref: M.P. BURKE, S.J. KLIPPENSTEIN, L.B. HARDING, PROC. COMBUST. INST. 34(2013) 547-555 !\Comment: WARNING
OH+HO2=H2O+O2    1.21E9 1.24 -1.30758E3
   DUP
!\Author: UB !\Ref: M.P. BURKE, S.J. KLIPPENSTEIN, L.B. HARDING, PROC. COMBUST. INST. 34(2013) 547-555 !\Comment: WARNING
2HO2=H2O2+O2    1.214E10 0.422 -1.48052E3
   DUP
!\Author: UB !\Ref: M.P. BURKE, S.J. KLIPPENSTEIN, L.B. HARDING, PROC. COMBUST. INST. 34(2013) 547-555 !\Comment: WARNING
2HO2=H2O2+O2    1.688E16 -0.681 1.293166E4
   DUP
!________________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ALPHA_SCISSION
!________________________________________________________________________________________________________
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
H+O2(+M)=HO2(+M)    4.66E12 0.44 0.0E0
   HE/0.52/
   AR/0.65/
   O2/0.9/
   H2/1.35/
   CH4/2.0/
   CO2/3.25/
   H2O/16.6/
   C2H6/3.0/
   CO/3.0/
   LOW/1.225E19 -1.2E0 0.0E0/
   TROE/5.0E-1 1.0E0 1.0E10/
!--------------------------------------------------------------------------------------------------------------------------------
!\ENDSUBMECH: H2O2
!--------------------------------------------------------------------------------------------------------------------------------
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+++++++++++++++++++++++++++++++++++++++
!\END_KINETICS_MODULE: H2_O2
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+++++++++++++++++++++++++++++++++++++++
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+++++++++++++++++++++++++++++++++++++++
!\KINETICS_MODULE: C1
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+++++++++++++++++++++++++++++++++++++++
!--------------------------------------------------------------------------------------------------------------------------------
!\SUBMECH: CO
!--------------------------------------------------------------------------------------------------------------------------------
!________________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONO
!________________________________________________________________________________________________________
!\Author: ?? !\Ref: MEULLER 99 * 0.76 !\Comment: WARNING
CO+O(+M)=CO2(+M)    1.362E10 0.0 2.384E3
   HE/0.7/
   AR/0.7/
   CO/1.75/
   H2/2.0/
   CO2/3.6/
   H2O/12.0/
   LOW/1.173E24 -2.79E0 4.191E3/
!________________________________________________________________________________________________________
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!\REACTIONCLASS: RADICAL_ADDITIONOH
!_____________________________________________________________________________________________________
!\Author: UB !\Ref: J.P. SENOSIAIN, S.J. KLIPPENSTEIN, J.A. MILLER, PROC. COMBUST. INST. 30(2005) 945-953. !\Comment: WARNING
CO+OH=CO2+H    2.3E7 1.35 9.74E2
   PLOG/1.315E-2 2.1E5 1.9E0 -1.064E3/
   PLOG/1.315E-1 2.5E5 1.88E0 -1.043E3/
   PLOG/1.315E0 8.7E5 1.73E0 -6.85E2/
   PLOG/1.3158E1 6.8E6 1.48E0 4.8E1/
   PLOG/1.3158E2 2.3E7 1.35E0 9.74E2/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONHO2
!_____________________________________________________________________________________________________
!CO+HO2(=)CO2+OH                                +8.55000000E+003 +2.52000000E+000 +1.55600000E+004 !\Author: UB !\Ref: S.J.KLIPPENSTEIN, PROC.
COMBUST. INST. 36(2017) 77-111 !\Comment: WARNING
CO+HO2=CO2+OH    8.35E3 2.55 1.656E4
!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+O2(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: ?? !\Ref: 86TSA / HAM * 0.44 !\Comment: WARNING
CO+O2=CO2+O    1.119E12 0.0 4.77E4
!=====================================================================================================
!\SUBSPECIES: CO2
!=====================================================================================================
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONH
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: CURRAN ESTIMATE !\Comment: WARNING
H+CO2=OCHO    7.5E13 0.0 2.9E4
!=====================================================================================================
!\ENDSUBSPECIES: HOCO
!=====================================================================================================
!-----------------------------------------------------------------------------------------------------
!\ENDSUBMECH: CO
!-----------------------------------------------------------------------------------------------------
!-----------------------------------------------------------------------------------------------------
!\SUBMECH: CH4
!-----------------------------------------------------------------------------------------------------
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RH(=)PRODUCTS
!_____________________________________________________________________________________________________
!J.TROE, V.G. USHAKOV, J. CHEM. PHYS. 136(2012) 214309 !\Comment: WARNING
CH3+H(+M)=CH4(+M)    6.47E13 0.185 -5.4E1
   H2/4.0/
   H2O/12.0/
   CO/2.3/
   CO2/4.0/
   AR/1.0/
   CH4/5.0/
   C2H6/4.0/
   N2/1.5/
   HE/0.7/
   CH3OH/6.0/
   O2/1.5/
   LOW/8.54E32 -4.69E0 2.2E3/
   TROE/5.16194E-1 3.6378482E3 1.0E0 1.0E30/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RH+R_ABSTRACTION
!_____________________________________________________________________________________________________
!\Author: UB !\Ref: J.W.SUTHERLAND, M.-C.SU, J.V.MICHAEL, INT.J.CHEM.KINET. 33(2001) 669-684 !\Comment: WARNING
CH4+H=CH3+H2    4.08E3 3.16 8.756E3
!\Author: UB !REF !\Ref: WARNING !\Comment: WARNING
CH4+O=CH3+OH    4.9E6 2.2 7.591E3
!\Author: UB !\Ref: ULTAN LEAST SQUARES FIT TO AVAILABLE EXPERIMENT 27-6-2018 !\Comment: WARNING
CH4+OH=CH3+H2O    5.65476E6 1.93695 2.6562698E3
!\Author: WARNING !\Ref: J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A(2008) 112(30) !\Comment: 1.695E+001 IN ARAMCOMECH1.3(WITH AX1.5)
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CH4+HO2=CH3+H2O2    1.12E1 3.74 2.1009E4
!\Author: SP !\Ref: H-H CARSTENSEN, A.M. DEAN, O. DEUTSCHMANN, PROC. COMBUST. INST. 31(2007) 149-157 ! !\Comment: WARNING
CH4+O2CHO=CH3+HO2CHO    3.22E3 3.13 1.52E4
!\Author: WARNING !\Ref: NEW FIT FROM HJC !\Comment: WARNING
CH4+CH3O2=CH3+CH3O2H    9.6E-1 3.77 1.781E4
!\Author: WARNING !\Ref: ZHU AND LIN ET AL. !\Comment: WARNING
CH3+HO2=CH4+O2    1.819E3 2.83 -3.73E3
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONCH2
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: GRI 3.0 !\Comment: WARNING
CH4+CH2=2CH3    2.46E6 2.0 8.27E3
!=====================================================================================================
!\SUBSPECIES: CH2(S)
!=====================================================================================================
!_____________________________________________________________________________________________________
!\REACTIONCLASS: THIRD_BODY_DEACTIVATION
!_____________________________________________________________________________________________________
!\Author: UB !\Ref: F.HAYES, W.D.LAWRENCE, W.S.STAKER, K.D.KING, J. PHYS. CHEM. 100(1996) 11314-11318 !\Comment: WARNING
CH2(S)+N2=CH2+N2    1.26E13 0.0 4.3E2
!\Author: UB !\Ref: F.HAYES, W.D.LAWRENCE, W.S.STAKER, K.D.KING, J. PHYS. CHEM. 100(1996) 11314-11318 !\Comment: WARNING
CH2(S)+AR=CH2+AR    6.62E12 0.0 4.54E2
!\Author: UB !\Ref: F.HAYES, W.D.LAWRENCE, W.S.STAKER, K.D.KING, J. PHYS. CHEM. 100(1996) 11314-11318 !\Comment: WARNING
CH2(S)+H2O=CH2+H2O    5.48E13 0.0 -4.3E2
!\Author: UB !\Ref: F.HAYES, W.D.LAWRENCE, W.S.STAKER, K.D.KING, J. PHYS. CHEM. 100(1996) 11314-11318 !\Comment: WARNING
CH2(S)+CO=CH2+CO    1.26E13 0.0 4.3E2
!\Author: UB !\Ref: F.HAYES, W.D.LAWRENCE, W.S.STAKER, K.D.KING, J. PHYS. CHEM. 100(1996) 11314-11318 !\Comment: WARNING
CH2(S)+CO2=CH2+CO2    5.48E13 0.0 -4.3E2
!_____________________________________________________________________________________________________
!\REACTIONCLASS: MISC
!_____________________________________________________________________________________________________
!\Author: UB !\Ref: P.-F. LEE, H. MATSUI, W.-Y. CHEN, C.-S. WANG, J. PHYS. CHEM. A, 116(2012) 9245-9254 !\Comment: WARNING
CH2(S)+O2=>H+OH+CO    1.2014E12 0.0 0.0E0
!\Author: UB !\Ref: P.-F. LEE, H. MATSUI, W.-Y. CHEN, C.-S. WANG, J. PHYS. CHEM. A, 116(2012) 9245-9254 !\Comment: WARNING
CH2(S)+O2=CO+H2O    5.1488E11 0.0 0.0E0
!\Author: WARNING !\Ref: GRI 3.0 !\Comment: WARNING
CH2(S)+O=CO+H2    1.5E13 0.0 0.0E0
!\Author: WARNING !\Ref: GRI 3.0 !\Comment: WARNING
CH2(S)+O=HCO+H    1.5E13 0.0 0.0E0
!\Author: WARNING !\Ref: GRI 3.0 !\Comment: WARNING
CH2(S)+H2=CH3+H    7.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: GRI 3.0 !\Comment: WARNING
CH2(S)+H=CH+H2    3.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: GRI 3.0 !\Comment: WARNING
CH2(S)+OH=CH2O+H    3.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: GRI 3.0 !\Comment: WARNING
CH2(S)+CO2=CH2O+CO    1.4E13 0.0 0.0E0
!\Author: UB !\Ref: W. HACH ET AL. BER. BUNSENGES. PHYS. CHEM. 93, 165(1989) !\Comment: WARNING
C2H2+CH2(S)=C2H2+CH2    4.0E13 0.0 0.0E0
!=====================================================================================================
!\ENDSUBSPECIES: CH2(S)
!=====================================================================================================
!=====================================================================================================
!\SUBSPECIES: CH2
!=====================================================================================================
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ALPHA_SCISSION
!_____________________________________________________________________________________________________
!\Author: UB !\Ref: GRI3.0 !\Comment: WARNING
H+CH2(+M)=CH3(+M)    6.0E14 0.0 0.0E0
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   H2/2.0/
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   C2H6/3.0/
   H2O/6.0/
   LOW/1.04E26 -2.76E0 1.6E3/
   TROE/5.62E-1 9.1E1 5.836E3 8.552E3/
!\Author: UB !\Ref: GRI3.0 !\Comment: WARNING
CH+H2(+M)=CH3(+M)    1.97E12 0.43 -3.7E2
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   H2/2.0/
   C2H6/3.0/
   H2O/6.0/
   LOW/4.82E25 -2.8E0 5.9E2/
   TROE/5.78E-1 1.22E2 2.535E3 9.365E3/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: MISC
!_____________________________________________________________________________________________________
!\Author: UB !\Ref: PRIVATE COMMUNICATION WITH S.J. KLIPPENSTEIN !\Comment: WARNING
CH2+O2=CH2O+O    1.3E5 2.4202 1.604E3
!\Author: UB !\Ref: PRIVATE COMMUNICATION WITH S.J. KLIPPENSTEIN !\Comment: WARNING
CH2+O2=>CO2+2H    1.05E9 0.9929 -2.69E2
!\Author: UB !\Ref: PRIVATE COMMUNICATION WITH S.J. KLIPPENSTEIN !\Comment: WARNING
CH2+O2=>CO+H+OH    6.5E5 0.9929 -2.69E2
!\Author: WARNING !\Ref: GRI 3.0 !\Comment: WARNING
CH2+O=>CO+2H    5.0E13 0.0 0.0E0
!\Author: UB !\Ref: ARAMCOMECH1.3, COMBINING GRI3.0 AND S.W.MAYER, ET AL. 11TH INT. SYMP. COMBUST. !\Comment: WARNING
CH2+H=CH+H2    1.0E18 -1.56 0.0E0
   DUP
!\Author: UB !\Ref: ARAMCOMECH1.3, COMBINING GRI3.0 AND S.W.MAYER, ET AL. 11TH INT. SYMP. COMBUST. !\Comment: WARNING
CH2+H=CH+H2    2.7E11 0.67 2.57E4
   DUP
!\Author: UB !\Ref: K-W LU, H MATSUI, C-L HUANG, P RAGHUNATH, N-S WANG, MC LIN, J. PHYS. CHEM. A 2010, 114, 54935502 !\Comment: WARNING
CH2+H2=CH3+H    4.4E5 2.39 7.35E3
!\Author: WARNING !\Ref: GRI 3.0 !\Comment: WARNING
CH2+OH=CH+H2O    1.13E7 2.0 3.0E3
!_____________________________________________________________________________________________________
!\REACTIONCLASS: MISC
!_____________________________________________________________________________________________________
!\Author: ABS !\Ref: HALL AND PETERSEN IJCK 2006 !\Comment: WARNING
CH+O2=CO+OHV    3.24E14 -0.4 4.15E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH+O2=HCO+O    3.24E14 -0.4 4.15E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH+O2=>H+CO+O    4.86E14 -0.4 4.15E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH+O2=H+CO2    4.86E14 -0.4 4.15E3
!\Author: WARNING !\Ref: MESSING ET AL.,J. CHEM. PHYS. 74, 3874(1981) !\Comment: WARNING
CH+O=CO+H    5.7E13 0.0 0.0E0
!\Author: WARNING !\Ref: GLARBORG, MILLER, AND KEE, WESTERN STATES SECTION, SAN ANTONIO(1985) !\Comment: WARNING
CH+OH=HCO+H    3.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: BERGEAT ET AL., CHEM. PHYS. LETT. 480, 21(2009) !\Comment: WARNING
CH+H2O=H+CH2O    1.774E16 -1.22 2.38E1
!\Author: WARNING !\Ref: BERMAN, FLEMING, HARVEY AND LIN, 19TH SYMP. COMB. P. 73, 1982 !\Comment: X0.5
CH+CO2=HCO+CO    1.7E12 0.0 6.85E2
!=====================================================================================================
!\ENDSUBSPECIES: C
!=====================================================================================================
!=====================================================================================================
!\SUBSPECIES: CH3
!=====================================================================================================
!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+O2(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: ?? !\Ref: R.X. FERNANDES ET AL.,J PHYS. CHEM. A,(2006) 110 !\Comment: WARNING
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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/
!\Author: ?? !\Ref: N. K. SRINIVASAN ET AL.,J. PHYS. CHEM. A 109, 7902-7914(2005) !\Comment: WARNING
CH3+O2=CH3O+O    7.546E12 0.0 2.832E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3+O2=CH2O+OH    2.641E0 3.283 8.105E3
!_____________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONO
!_____________________________________________________________________________________________
!\Author: UB !\Ref: HARDING AND KLIPPENSTEIN 2B04, 30TH SYMP 2004. !\Comment: REVERTING TO ORIGINAL PRODUCTS DUE TO CONVERGENCE
PROBLEMS
CH3+O=CH2O+H    5.54E13 0.05 -1.36E2
!_____________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONOH
!_____________________________________________________________________________________________
!\Author: ?? !\Ref: FROM JASPER / KLIPP,J.PHYS.CHEM A 111,19,3932-3950 !\Comment: WARNING
CH3+OH=CH2+H2O    4.293E4 2.568 3.9978E3
!\Author: ?? !\Ref: FROM JASPER / KLIPP,J.PHYS.CHEM A 111,19,3932-3950 !\Comment: ONLY INCLUDING TRANS HCOH FOR SIMPLICITY, DO NOT HAVE
TO COMBINE THE K'S. IT
CH3+OH=CH2(S)+H2O    8.433E19 -1.962 8.244E3
   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/
!\Author: ?? !\Ref: FROM JASPER / KLIPP,J.PHYS.CHEM A 111,19,3932-3950 !\Comment: WARNING
CH3+OH=CH2O+H2    9.494E18 -2.199 9.769E3
   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/
!\Author: UB !\Ref: FROM JASPER / KLIPP,J.PHYS.CHEM A 111,19,3932-3950 !\Comment: 1.3*A\
CH3+OH=CH2OH+H    2.3335E14 -0.186 8.6E3
   PLOG/1.0E-2 1.05365E10 9.65E-1 3.21E3/
   PLOG/1.0E-1 1.17455E10 9.5E-1 3.25E3/
   PLOG/1.0E0 3.0459E10 8.33E-1 3.57E3/
   PLOG/1.0E1 9.9125E12 1.34E-1 5.64E3/
   PLOG/1.0E2 2.3335E14 -1.86E-1 8.6E3/
!\Author: ?? !\Ref: FROM JASPER / KLIPP,J.PHYS.CHEM A 111,19,3932-3950 !\Comment: WARNING
CH3+OH=H+CH3O    5.242E10 0.551 1.307E4
   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/
!\Author: ?? !\Ref: FROM JASPER / KLIPP,J.PHYS.CHEM A 111,19,3932-3950 !\Comment: WARNING
CH3+OH=HCOH+H2    7.25E20 -2.402 9.639E3
   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/
!_____________________________________________________________________________________________
!\REACTIONCLASS: R+HO2(=)PRODUCTS
!_____________________________________________________________________________________________
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3+HO2=CH3O+OH    1.0E12 0.269 -6.875E2
!=============================================================================================
!\ENDSUBSPECIES: CH3
!=============================================================================================
!=============================================================================================
!\SUBSPECIES: CH3O2
!=============================================================================================
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!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+R(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991, 87(19), 3213--3220. !\Comment: WARNING
CH3O2+O=CH3O+O2    3.6E13 0.0 0.0E0
!\Author: WARNING !\Ref: LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991, 87(19), 3213--3220. !\Comment: WARNING
CH3O2+H=CH3O+OH    9.6E13 0.0 0.0E0
!\Author: WARNING !\Ref: LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991, 87(19), 3213--3220. !\Comment: WARNING
CH3O2+OH=CH3OH+O2    6.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: LIGHTFOOT,P.D. ET AL., ATMOS. ENVIRON. PART A !\Comment: WARNING
CH3O2+HO2=CH3O2H+O2    2.47E11 0.0 -1.57E3
!\Author: WARNING !\Ref: !REF !\Comment: ADDED 29 / 07 / 2015
CH3O2+H2O2=CH3O2H+HO2    2.41E12 0.0 9.936E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3O2+CH3=2CH3O    5.849E11 0.353 -1.46E3
!\Author: WARNING !\Ref: LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991, 87(19), 3213--3220. !\Comment: WARNING
2CH3O2=>CH2O+CH3OH+O2    3.11E14 -1.61 -1.051E3
!\Author: WARNING !\Ref: LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991, 87(19), 3213--3220. !\Comment: WARNING
2CH3O2=>O2+2CH3O    1.4E16 -1.61 1.86E3
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RH+R_ABSTRACTION
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: TSANG _ HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986 !\Comment: WARNING
H2+CH3O2=H+CH3O2H    1.5E14 0.0 2.603E4
!_____________________________________________________________________________________________________
!\REACTIONCLASS: KHP_HOMOLYTIC_FISSION
!_____________________________________________________________________________________________________
!\Author: SP !\Ref: A.W.JASPER, S.J.KLIPPENSTEIN, L.B.HARDING, PROC.COMBUST.INST. 32(2009) 279-286 !\Comment: WARNING
CH3O2H(+M)=CH3O+OH(+M)    4.04972E19 -1.153 4.425049E4
   LOW/3.80285E42 -7.502E0 4.6756097E4/
   TROE/8.375E-1 3.6562E4 4.988E2 9.99E3/
!\Author: UB !\Ref: A.W.JASPER, S.J.KLIPPENSTEIN, L.B.HARDING, PROC.COMBUST.INST. 32(2009) 279-286 !\Comment: WARNING
CH3O+OH=CH2O+H2O    3.6192E2 2.4976 1.889448E3
!=====================================================================================================
!\ENDSUBSPECIES: CH3O2
!=====================================================================================================
!-----------------------------------------------------------------------------------------------------
!\ENDSUBMECH: CH4
!-----------------------------------------------------------------------------------------------------
!-----------------------------------------------------------------------------------------------------
!\SUBMECH: CH3OH
!\MECHCOMMENTS: HCOH IS FORMED FROM CH3+OH, IT IS NOT NECESSARY FOR FORMALDEHYDE OXIDATION, AND MINOR FOR CH4 /CH3OH
!-----------------------------------------------------------------------------------------------------
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RH(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: SP !\Ref: FROM JASPER / KLIPP,J.PHYS.CHEM A 111,19,3932-3950 !\Comment: NEGLECTING HCOH CHANNELS AS THEY ARE NOT IMPORTANT
CH3OH(+M)=CH3+OH(+M)    2.084E18 -0.615 9.25406E4
   LOW/1.5E43 -6.995E0 9.79922E4/
   TROE/7.656E-1 5.951E1 1.91E3 9.374E3/
!\Author: SP !\Ref: FROM JASPER / KLIPP,J.PHYS.CHEM A 111,19,3932-3950 !\Comment: NEGLECTING HCOH CHANNELS AS THEY ARE NOT IMPORTANT
CH3OH(+M)=CH2(S)+H2O(+M)    3.121E18 -1.017 9.1712E4
   LOW/1.43E47 -8.227E0 9.94171E4/
   TROE/9.922E-1 4.731E4 9.43E2 4.711E4/
!\Author: SP !\Ref: FROM JASPER / KLIPP,J.PHYS.CHEM A 111,19,3932-3950 !\Comment: NEGLECTING HCOH CHANNELS AS THEY ARE NOT IMPORTANT
CH3OH(+M)=CH2OH+H(+M)    7.896E-3 5.038 8.44674E4
   LOW/3.39E42 -7.244E0 1.052303E5/
   TROE/6.843E-1 4.1493E4 3.7049E4 3.98E3/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RH+R_ABSTRACTION
!_____________________________________________________________________________________________________
!\Author: UB !\Ref: J.T.JODKOWSKI, ET AL, J. PHYS. CHEM.A, 103(1999) 3750-3765 \ !COMMENT !\Comment: WARNING
CH3OH+H=CH2OH+H2    1.35E3 3.2 3.488E3
!\Author: UB !\Ref: J.I.MOSES ET AL. J. ASTROPHYS. 737(2011) 15 !\Comment: WARNING
CH3OH+H=CH3O+H2    4.1E4 2.658 9.221E3
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!\Author: UB !\Ref: H.F.LEFEVRE ET AL. INT. J. CHEM. KINET. 4(1972) 103 !\Comment: WARNING
CH3OH+O=CH3O+OH    1.7E12 0.0 2.285E3
!\Author: UB !\Ref: TSANG, JPC REF. DATA, 16 !\Comment: WARNING
CH3OH+O=CH2OH+OH    3.88E5 2.5 3.08E3
!\Author: UB !\Ref: XU ET AL. PROC 31 2007 159-166 !\Comment: WARNING
CH3OH+OH=CH3O+H2O    1.5E2 3.03 -7.63E2
!\Author: UB !\Ref: XU ET AL. PROC 31 2007 159-166 !\Comment: WARNING
CH3OH+OH=CH2OH+H2O    3.08E4 2.65 -8.067E2
!\Author: UB !\Ref: MOUSAVIPOUR, S. H.; HOMAYOON, Z. J PHYS CHEM A 2011, 115, 3291-3300 !\Comment: WARNING
CH3O+HO2=CH3OH+O2    1.4E11 0.0 0.0E0
!\Author: UB !\Ref: S. J. KLIPPENSTEIN, L. B. HARDING, M. J. DAVIS, A. S. TOMLIN, R. T. SKODJE, PCI, 33(2011) 351-357 !\Comment: ULTAN ADDED 21 /
08 / 15
CH3OH+O2=CH2OH+HO2    3.58E5 2.27 4.27645E4
!\Author: UB !\Ref: M. ALTARAWNEH, A. H. AL-MUHTASEB, B. Z. DLUGOGORSKI, E. M. KENNEDY, J. C. MACKIE, J. COMP. CHEM. 32(2011) 1725-1733
!\Comment: ULTAN ADDED
CH3OH+HO2=CH3O+H2O2    1.22E12 0.0 2.00707E4
!\Author: UB !\Ref: M. ALTARAWNEH, A. H. AL-MUHTASEB, B. Z. DLUGOGORSKI, E. M. KENNEDY, J. C. MACKIE, J. COMP. CHEM. 32(2011) 1725-1733
!\Comment: EA INCREASE
CH3OH+HO2=CH2OH+H2O2    3.26E13 0.0 1.87822E4
!\Author: UB !\Ref: I. M. ALECU, D. G. TRUHLAR, J. PHYS. CHEM. A, 115(2011) 14599-14611 !\Comment: ULTAN ADDED 21 / 08 / 15
CH3OH+CH3=CH2OH+CH4    2.13E-1 3.953 7.0551E3
!\Author: UB !\Ref: I. M. ALECU, D. G. TRUHLAR, J. PHYS. CHEM. A, 115(2011) 14599-14611 !\Comment: ULTAN ADDED 21 / 08 / 15
CH3OH+CH3=CH3O+CH4    3.22E3 2.425 8.5795E3
!\Author: UB !\Ref: TSANG, JPC REF. DATA, 16 !\Comment: WARNING
CH3OH+HCO=CH2OH+CH2O    9.63E3 2.9 1.311E4
!\Author: UB !\Ref: TSANG, JPC REF. DATA, 16 !\Comment: WARNING
CH3OH+CH3O=CH2OH+CH3OH    3.0E11 0.0 4.074E3
!\Author: UB !\Ref: TSANG, JPC REF. DATA, 16 !\Comment: WARNING
CH3OH+CH3O2=CH2OH+CH3O2H    1.81E12 0.0 1.371E4
!=============================================================================================================
!\SUBSPECIES: CH2OH
!=============================================================================================================
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: R+R(=)RH+RH
!_____________________________________________________________________________________________________________
CH2OH+O2=CH2O+HO2    7.2E13 0.0 3.736E3
   DUP
CH2OH+O2=CH2O+HO2    2.9E16 -1.5 0.0E0
   DUP
!\Author: SP !\Ref: XU K XU ZF LIN MC MOL PHYS 105 !\Comment: WARNING
CH2OH+H=CH2O+H2    4.0E6 1.86 1.47E2
!\Author: WARNING !\Ref: NORTON, T.S ET AL., IJCK.(1991). !\Comment: WARNING
CH2OH+HO2=CH2O+H2O2    1.2E13 0.0 0.0E0
!\Author: WARNING !\Ref: NORTON, T.S ET AL., IJCK.(1991). !\Comment: WARNING
CH2OH+CH3O=CH2O+CH3OH    2.4E13 0.0 0.0E0
!\Author: WARNING !\Ref: TSANG, JPC REF. DATA, 16 !\Comment: WARNING
CH2OH+OH=H2O+CH2O    2.4E13 0.0 0.0E0
!\Author: WARNING !\Ref: TSANG, JPC REF. DATA, 16 !\Comment: WARNING
CH2OH+O=OH+CH2O    4.2E13 0.0 0.0E0
!\Author: WARNING !\Ref: TSANG, JPC REF. DATA, 16 !\Comment: WARNING
2CH2OH=CH2O+CH3OH    3.0E12 0.0 0.0E0
!=============================================================================================================
!\ENDSUBSPECIES: CH2OH
!=============================================================================================================
!=============================================================================================================
!\SUBSPECIES: CH3O
!=============================================================================================================
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: R+R(=)RH+RH
!_____________________________________________________________________________________________________________
!\Author: UB !\Ref: BAULCH ET AL. J. PHYS. CHEM. REF. DATA, 34(2005) 757 !\Comment: WARNING
CH3O+O2=CH2O+HO2    2.17E10 0.0 1.7487E3
!\Author: WARNING !\Ref: HOYERMANN ET AL., 18TH SYMPOSIUM !\Comment: WARNING
CH3O+H=CH2O+H2    2.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
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CH3O+HO2=CH2O+H2O2    3.01E11 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3O+CH3=CH2O+CH4    1.2E13 0.0 0.0E0
!\Author: WARNING !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
2CH3O=CH3OH+CH2O    6.03E13 0.0 0.0E0
!=============================================================================================================
!\ENDSUBSPECIES: CH3O
!=============================================================================================================
!=============================================================================================================
!\SUBSPECIES: HCOH
!=============================================================================================================
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: R+R(=)PRODUCTS
!_____________________________________________________________________________________________________________
!\Author: WARNING !\Ref: MARINOV 1996 !\Comment: WARNING
HCOH+O2=>CO2+H+OH    5.0E12 0.0 0.0E0
!\Author: WARNING !\Ref: MARINOV 1996 !\Comment: WARNING
HCOH+O2=CO2+H2O    3.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: MARINOV 1996 !\Comment: WARNING
HCOH+O=>CO2+2H    5.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: MARINOV 1996 !\Comment: WARNING
HCOH+O=>CO+OH+H    3.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: MARINOV 1996 !\Comment: WARNING
HCOH+H=CH2O+H    2.0E14 0.0 0.0E0
!\Author: WARNING !\Ref: MARINOV 1996 !\Comment: WARNING
HCOH+OH=HCO+H2O    2.0E13 0.0 0.0E0
!=============================================================================================================
!\ENDSUBSPECIES: HCOH
!=============================================================================================================
!-------------------------------------------------------------------------------------------------------------
!\ENDSUBMECH: CH3OH
!-------------------------------------------------------------------------------------------------------------
!-------------------------------------------------------------------------------------------------------------
!\SUBMECH: CH2O
!\MECHCOMMENTS: THE REACTION OCHO+OH(=)HO2CHO SEEMS TO BE A DEAD END OF SORTS, HO2CHO HAS A LIMITED SET OF CONSUMPTION
/ CROSS-REACTIONS(KPS, 28 / 06 / 2015)
!\MECHCOMMENTS: THE REACTION SEQUENCE H+CO2(=)OCHO=)PRODUCTS MEANS THAT THE THE CO / CH2O MECHANISMS ARE INEXTRICABLY
LINKED "IN THEORY". I AM NOT SURE ABOUT "IN PRACTICE".(KPS, 28 / 06 / 2015)
!-------------------------------------------------------------------------------------------------------------
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: RH(=)PRODUCTS
!_____________________________________________________________________________________________________________
!\Author: WARNING !\Ref: LASKIN ET AL. IJCK 32 589-614 2000 !\Comment: WARNING
HCO+H(+M)=CH2O(+M)    1.09E12 0.48 -2.6E2
   LOW/1.35E24 -2.57E0 1.425E3/
   TROE/7.824E-1 2.71E2 2.755E3 6.57E3/
!\Author: WARNING !\Ref: LASKIN ET AL. IJCK 32 589-614 2000 !\Comment: WARNING
CO+H2(+M)=CH2O(+M)    4.3E7 1.5 7.96E4
   LOW/5.07E27 -3.42E0 8.4348E4/
   TROE/9.32E-1 1.97E2 1.54E3 1.03E4/
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: RH+R_ABSTRACTION
!_____________________________________________________________________________________________________________
!\Author: WARNING !\Ref: N. K. SRINIVASAN ET AL.,J. PHYS. CHEM. A 109, 7902-7914(2005) !\Comment: WARNING
CH2O+O2=HCO+HO2    8.07E15 0.0 5.342E4
!\Author: WARNING !\Ref: CURRAN FIT TO NIST DATABASE !\Comment: WARNING
CH2O+O=HCO+OH    6.26E9 1.15 2.26E3
!\Author: UB !\Ref: S.WANG ET AL. J.PHYS.CHEM.A, 118(2014) 10201-10209 !\Comment: RE-FIT TO INCLUDE BRANCHING RATIO TO PROMPT PATHWAY
CH2O+H=HCO+H2    1.0691154E5 2.73093 1.88714E3
!\Author: UB !\Ref: V. VASUDEVAN ET AL. IJCK. 37 !\Comment: RE-FIT TO REMOVE NEGATIVE A-FACTOR BUT RETAIN BRANCHING RATIO TO PROMPT
PATHWAY
CH2O+OH=HCO+H2O    2.185E9 1.1782 -5.7602E2
!\Author: UB/HJC !\Ref: ROBERTSON, S. H.; SEAKINS, P. W.; PILLING, M. J. CHEMICAL KINETICS, IN PILLING, M. J., ED.; ELSEVIER !\Comment: WARNING
CH2O+HO2=HCO+H2O2    7.1E-3 4.517 6.58E3
!\Author: UB !\Ref: NIST FIT TO AVAILABLE EXP. 26-02-2018 !\Comment: WARNING
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CH2O+CH3=HCO+CH4    2.93E-2 4.3 2.831E3
!\Author: WARNING !\Ref: ANALOGY WITH CH3O2+CH2O TSANG / HAMPSON 1986 !\Comment: WARNING
CH2O+O2CHO=HCO+HO2CHO    1.99E12 0.0 1.166E4
!\Author: WARNING !\Ref: FITTSCHEN, C., J. CHIM. PHYS. 95 !\Comment: WARNING
CH2O+CH3O=HCO+CH3OH    6.62E11 0.0 2.294E3
!\Author: WARNING !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
CH2O+CH3O2=HCO+CH3O2H    1.99E12 0.0 1.166E4
!_____________________________________________________________________________________________
!\REACTIONCLASS: PROMPT_ALPHA_SCISSION
!_____________________________________________________________________________________________
!\Author: UB !\Ref: N.J.LABBE, R.SIVARAMAKRISHNAN, C.FRANKLIN-GOLDSMITH, Y.GEORGIEVSKII, J.A.MILLER, S.J.KLIPPENSTEIN,
J.PHYS.CHEM.LETT. 7(2016) 85-89 !\Comme
CH2O+OH=>H+CO+H2O    2.565E11 0.69304 9.3687E3
!\Author: UB !\Ref: N.J.LABBE, R.SIVARAMAKRISHNAN, C.FRANKLIN-GOLDSMITH, Y.GEORGIEVSKII, J.A.MILLER, S.J.KLIPPENSTEIN,
J.PHYS.CHEM.LETT. 7(2016) 85-89 !\Comme
CH2O+H=>H+CO+H2    1.94E7 2.192 1.174029E4
!_____________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ALPHA_SCISSION
!_____________________________________________________________________________________________
!\Author: UB !\Ref: LI ET AL. IJCK 2007 !\Comment: REMOVED X1.2
HCO+M=H+CO+M    4.75E11 0.66 1.487E4
   CO/1.5/
   CH4/2.0/
   H2/2.0/
   CO2/2.0/
   C2H6/3.0/
   H2O/6.0/
!_____________________________________________________________________________________________
!\REACTIONCLASS: R+R(=)RH_RH
!_____________________________________________________________________________________________
!\Author: SP !\Ref: HSU ET AL. !\Comment: WARNING
HCO+O2=CO+HO2    1.2E10 0.807 -7.27E2
!\Author: WARNING !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
HCO+O=CO+OH    3.02E13 0.0 0.0E0
!\Author: UB !\Ref: L.B.HARDING, A.F.WAGNER, PROC. COMBUST. INST. 21(1986) 721-728 !\Comment: WARNING
HCO+H=CO+H2    9.13E12 0.41 -2.155715E2
!\Author: WARNING !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
HCO+OH=CO+H2O    3.011E13 0.0 0.0E0
!\Author: WARNING !\Ref: MULENKO, S.A. REV. ROUM. PHYS. 32, 173(1987) !\Comment: WARNING
HCO+CH3=CO+CH4    2.65E13 0.0 0.0E0
!\Author: UB !\Ref: G.FRIEDRICHS, J.T.HERBON, D.F.DAVIDSON, R.K.HANSON, PHYS. CHEM. CHEM. PHYS. 4(2002) 5778-5788 \COMMENT !\Comment:
WARNING
2HCO=CO+CH2O    2.7E13 0.0 0.0E0
!_____________________________________________________________________________________________
!\REACTIONCLASS: R+R(=)PRODUCTS
!_____________________________________________________________________________________________
!\Author: WARNING !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
HCO+O=CO2+H    3.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
HCO+HO2=>CO2+H+OH    3.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
2HCO=>H2+2CO    3.0E12 0.0 0.0E0
!_____________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONH
!_____________________________________________________________________________________________
!\Author: SP !\Ref: E.E.DAME, D.M.GOLDEN, J. PHYS. CHEM. A, 117(2013) 7686-7696 !\Comment: WARNING
CH2OH(+M)=CH2O+H(+M)    7.37E10 0.811 3.9585E4
   HE/0.67/
   AR/0.85/
   O2/1.0/
   CO/1.5/
   CO2/2.0/
   H2/2.0/
   CH4/2.0/
   CH2O/2.5/
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   CH3OH/3.0/
   C2H6/3.0/
   H2O/6.0/
   LOW/3.5E21 -1.99E0 2.4E4/
   TROE/8.44E-1 9.0E2 1.0E0 3.315E3/
!\Author: UB !\Ref: E.E.DAME, D.M.GOLDEN, J. PHYS. CHEM. A, 117(2013) 7686-7696 !\Comment: WARNING
CH3O(+M)=CH2O+H(+M)    1.13E10 1.21 2.40849E4
   HE/0.67/
   AR/0.85/
   O2/1.0/
   CO/1.5/
   CO2/2.0/
   H2/2.0/
   CH4/2.0/
   CH3OH/3.0/
   C2H6/3.0/
   H2O/6.0/
   LOW/6.022E16 -5.47E-1 1.80239E4/
   TROE/3.41E-1 2.8E1 1.0E3 2.339E3/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+O2(=)RO2
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: CURRAN ESTIMATE !\Comment: WARNING
HCO+O2=O2CHO    1.2E11 0.0 -1.1E3
!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+O2(=)RO2
!_____________________________________________________________________________________________________
!\Author: UB !\Ref: P. MARSHALL, P. GLARBORG, PROC. COMBUST. INST. 35(2015) 153-160 !\Comment: WARNING
OCHO+O2=CO2+HO2    5.0E13 0.0 0.0E0
!=====================================================================================================
!\ENDSUBSPECIES: HOCHO
!=====================================================================================================
!-----------------------------------------------------------------------------------------------------
!\ENDSUBMECH: CH2O
!-----------------------------------------------------------------------------------------------------
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++++++++++++++++++++++++++++++++++++
!\END_KINETICS_MODULE: C1
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++++++++++++++++++++++++++++++++++++
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++++++++++++++++++++++++++++++++++++
!\KINETICS_MODULE: C2
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++++++++++++++++++++++++++++++++++++
!-----------------------------------------------------------------------------------------------------
!\SUBMECH: C2H6
!-----------------------------------------------------------------------------------------------------
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RH(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: WANG ET AL., JPC A 107 !\Comment: WARNING
2CH3(+M)=C2H6(+M)    2.277E15 -0.69 1.749E2
   CO/2.0/
   CO2/3.0/
   H2O/5.0/
   LOW/8.054E31 -3.75E0 9.816E2/
   TROE/0.0E0 5.7E2 1.0E30 1.0E30/
!\Author: WARNING !\Ref: WANG ET AL., JPC A 107 !\Comment: WARNING
C2H5+H(+M)=C2H6(+M)    5.21E17 -0.99 1.58E3
   HE/0.7/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   H2/2.0/
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   CH4/2.0/
   C2H6/3.0/
   H2O/6.0/
   LOW/1.99E41 -7.08E0 6.685E3/
   TROE/8.42E-1 1.25E2 2.219E3 6.882E3/
!\Author: WARNING !\Ref: STEWART ET AL C_F 1989 !\Comment: WARNING
2CH3=H+C2H5    1.032E2 3.23 1.12361E4
   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/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RH+R_ABSTRACTION
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21 !\Comment: WARNING
C2H6+O2=C2H5+HO2    6.03E13 0.0 5.187E4
!\Author: WARNING !\Ref: MIYOSHI,A. ET AL., CHEM. PHYS. LETT. 204, 241-247(1993) !\Comment: WARNING
C2H6+O=C2H5+OH    3.55E6 2.4 5.83E3
!\Author: UB !\Ref: R.SIVARAMAKRISHNAN, J.V.MICHAEL, B.RUSCIC, INT. J. CHEM. KINET. 44(2012) 194-205 !\Comment: WARNING
C2H6+H=C2H5+H2    7.35E3 3.1 5.34E3
   DUP
!\Author: UB !\Ref: R.SIVARAMAKRISHNAN, J.V.MICHAEL, B.RUSCIC, INT. J. CHEM. KINET. 44(2012) 194-205 !\Comment: WARNING
C2H6+H=C2H5+H2    3.26E14 0.0 1.37E4
   DUP
!\Author: UB !\Ref: L.N. KRASNOPEROV, J.V.MICAHEL, J.PHYS.CHEM.A, 108(2004) 5643-5648 !\Comment: WARNING
C2H6+OH=C2H5+H2O    1.6139E6 2.224 7.4123E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H6+HO2=C2H5+H2O2    2.77E1 3.59 1.56E4
!\Author: SP !\Ref: H-H CARSTENSEN, A.M. DEAN, O. DEUTSCHMANN, PROC. COMBUST. INST. 31(2007) 149-157 ! !\Comment: WARNING
C2H6+O2CHO=C2H5+HO2CHO    4.23E3 2.96 1.05E4
!\Author: ANALOGY TO CH3CO2H(=)CH3O+OH(BASED ON BDE) !\Ref: WARNING !\Comment: WARNING
HO2CHO(+M)=OCHO+OH(+M)    4.04972E19 -1.153 4.425049E4
   LOW/3.80285E42 -7.502E0 4.6756097E4/
   TROE/8.375E-1 3.6562E4 4.988E2 9.99E3/
!\Author: WARNING !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
C2H6+CH=C2H5+CH2    1.1E14 0.0 -2.6E2
!\Author: WARNING !\Ref: MECHANISM AND MODELING OF NITROGEN CHEMISTRY IN COMBUSTION, WSS / CI, AUTUMN 1988 !\Comment: WARNING
C2H6+CH2(S)=C2H5+CH3    1.2E14 0.0 0.0E0
!\Author: UB !\Ref: S.L.PEUKERT, N.J.LABBE, R.SIVARAMAKRISHNAN, J.V.MICHAEL, J.PHYS.CHEM.A, 117(2013) 10228-10238 !\Comment: WARNING
C2H6+CH3=C2H5+CH4    3.45E1 3.44 1.0391E4
!\Author: WARNING !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
C2H6+CH3O=C2H5+CH3OH    2.41E11 0.0 7.09E3
!\Author: WARNING !\Ref: CARSTENSEN AND DEAN PROC COMBUST INST 30(2007) 995?003 !\Comment: WARNING
C2H6+CH3O2=C2H5+CH3O2H    4.04E1 3.55 1.69E4
!\Author: WARNING !\Ref: CARSTENSEN AND DEAN PROC COMBUST INST 30(2007) 995?003 !\Comment: WARNING
C2H6+C2H5O2=C2H5+C2H5O2H    5.88E1 3.49 1.71E4
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_BETA_SCISSION
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: MILLER KLIPPENSTEIN PCCP 2004, 6, 1192-1202 !\Comment: WARNING
C2H4+H(+M)=C2H5(+M)    9.569E8 1.463 1.355E3
   AR/0.7/
   CO/1.5/
   H2/2.0/
   CH4/2.0/
   CO2/2.0/
   C2H6/3.0/
   H2O/6.0/
   HE/0.5/
   LOW/1.419E39 -6.642E0 5.769E3/
   TROE/-5.69E-1 2.99E2 -9.147E3 1.524E2/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+R(=)RH+RH
!_____________________________________________________________________________________________________
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!\Author: UB !\Ref: Y.ZHANG, Q.S.LI, S.W.ZHANG, J.MOL.STRUCT.(THEOCHEM) 682(2004) 163-170 !\Comment: WARNING
C2H5+H=C2H4+H2    1.81E11 0.0 0.0E0
!\Author: WARNING !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
2C2H4=C2H5+C2H3    4.82E14 0.0 7.153E4
!\Author: WARNING !\Ref: ZHU, R.S. ET AL.,J. CHEM. PHYS. 120 !\Comment: WARNING
C2H5+CH3=CH4+C2H4    1.18E4 2.45 -2.921E3
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONO
!_____________________________________________________________________________________________________
!\Author: UB !\Ref: L.B.HARDING, S.J.KLIPPENSTEIN, Y.GEORGIEVSHII, PROC.COMBUST.INST, 30(2005) 985-993 !\Comment: WARNING
C2H5+O=C2H5O    3.17E13 0.03 -3.94E2
!\Author: UB !\Ref: L.B.HARDING, S.J.KLIPPENSTEIN, Y.GEORGIEVSHII, PROC.COMBUST.INST, 30(2005) 985-993 !\Comment: WARNING
C2H5+O=C2H4+OH    3.17E12 0.03 -3.94E2
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONOH
!_____________________________________________________________________________________________________
!\Author: UB !\Ref: N.J.LABBE, R.SIVARAMAKRISHNAN, S.J.KLIPPENSTEIN, PROC.COMBUST.INST. 35(2015) 447-455 !\Comment: WARNING
C2H5+OH=C2H4+H2O    4.6961E18 -1.5805 7.9992E3
   PLOG/1.0E-3 1.2926E19 -1.96E0 2.727E2/
   PLOG/1.0E-2 1.2184E19 -1.9533E0 2.388E2/
   PLOG/1.0E-1 4.1052E19 -2.1007E0 6.254E2/
   PLOG/1.0E0 7.9406E22 -2.9892E0 3.8626E3/
   PLOG/1.0E1 2.7926E24 -3.3287E0 7.7488E3/
   PLOG/1.0E2 4.6961E18 -1.5805E0 7.9992E3/
!\Author: UB !\Ref: N.J.LABBE, R.SIVARAMAKRISHNAN, S.J.KLIPPENSTEIN, PROC.COMBUST.INST. 35(2015) 447-455 !\Comment: WARNING
C2H5+OH=CH3+CH2OH    6.5044E22 -2.4427 1.26466E4
   PLOG/1.0E-3 9.2017E17 -1.2994E0 2.5046E3/
   PLOG/1.0E-2 1.0981E18 -1.3206E0 2.5694E3/
   PLOG/1.0E-1 5.7367E18 -1.5182E0 3.1848E3/
   PLOG/1.0E0 6.5278E21 -2.3515E0 6.0227E3/
   PLOG/1.0E1 1.8799E25 -3.2495E0 1.05762E4/
   PLOG/1.0E2 6.5044E22 -2.4427E0 1.26466E4/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONHO2
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H5+HO2=C2H5O+OH    1.0E12 0.269 -6.88E2
!\Author: UB !\Ref: W.LUDWIG, B.BRANDT, G.FRIEDRICHS, F.TEMPS, J.PHYS.CHEM.A, 110(2006) 3330-3337, 80 !\Comment: WARNING
C2H5+HO2=C2H4+H2O2    6.2E12 0.0 0.0E0
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONCH3O2
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: CURRAN. BASED ON CH3+HO2(=)PRODUCTS !\Comment: WARNING
C2H5+CH3O2=C2H5O+CH3O    8.0E12 0.0 -1.0E3
!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+O2(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: UB !\Ref: S.J. KLIPPENSTEIN, PROC. COMBUST. INST. 36(2017) 77-111 !\Comment: WARNING
C2H5+O2=C2H5O2    1.59E30 -5.56 5.909E3
   PLOG/1.0E-4 1.28E42 -1.112E1 5.137E3/
   PLOG/3.0E-4 1.95E43 -1.13E1 5.485E3/
   PLOG/1.0E-3 1.22E44 -1.136E1 5.85E3/
   PLOG/3.0E-3 3.23E44 -1.132E1 6.198E3/
   PLOG/1.0E-2 1.31E45 -1.133E1 6.761E3/
   PLOG/3.0E-2 1.2E45 -1.115E1 7.163E3/
   PLOG/1.0E-1 4.34E44 -1.083E1 7.564E3/
   PLOG/3.0E-1 4.87E43 -1.037E1 7.81E3/
   PLOG/1.0E0 3.98E42 -9.86E0 8.124E3/
   PLOG/3.0E0 1.24E40 -8.95E0 7.857E3/
   PLOG/1.0E1 2.16E37 -7.95E0 7.525E3/
   PLOG/3.0E1 1.59E34 -6.88E0 6.913E3/
   PLOG/1.0E2 1.59E30 -5.56E0 5.909E3/
!\Author: UB !\Ref: S.J. KLIPPENSTEIN, PROC. COMBUST. INST. 36(2017) 77-111 !\Comment: WARNING
C2H5+O2=C2H4+HO2    1.89E11 0.14 6.373E3
   PLOG/1.0E-4 9.1E0 2.87E0 -5.099E3/
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   PLOG/3.0E-4 1.18E1 2.84E0 -5.029E3/
   PLOG/1.0E-3 2.82E1 2.73E0 -4.78E3/
   PLOG/3.0E-3 1.1E2 2.56E0 -4.38E3/
   PLOG/1.0E-2 9.57E2 2.3E0 -3.735E3/
   PLOG/3.0E-2 1.32E4 1.98E0 -2.933E3/
   PLOG/1.0E-1 4.9E5 1.54E0 -1.79E3/
   PLOG/3.0E-1 2.41E7 1.07E0 -4.977E2/
   PLOG/1.0E0 2.47E9 5.1E-1 1.157E3/
   PLOG/3.0E0 1.36E11 4.0E-2 2.789E3/
   PLOG/1.0E1 3.13E12 -3.1E-1 4.501E3/
   PLOG/3.0E1 5.29E12 -3.3E-1 5.728E3/
   PLOG/1.0E2 1.89E11 1.4E-1 6.373E3/
!\Author: SERJIO !\Ref: S.J. KLIPPENSTEIN, PROC. COMBUST. INST. 36(2017) 77-111 !\Comment: WARNING
C2H5O2=C2H4+HO2    1.92E30 -5.71 3.591E4
   PLOG/1.0E-4 1.91E46 -1.185E1 3.644E4/
   PLOG/3.0E-4 4.21E46 -1.188E1 3.682E4/
   PLOG/1.0E-3 3.63E46 -1.177E1 3.71E4/
   PLOG/3.0E-3 1.7E46 -1.158E1 3.733E4/
   PLOG/1.0E-2 4.36E45 -1.128E1 3.757E4/
   PLOG/3.0E-2 8.12E44 -1.094E1 3.778E4/
   PLOG/1.0E-1 4.61E43 -1.043E1 3.791E4/
   PLOG/3.0E-1 8.69E41 -9.77E0 3.786E4/
   PLOG/1.0E0 8.65E39 -9.01E0 3.778E4/
   PLOG/3.0E0 7.24E36 -7.95E0 3.724E4/
   PLOG/1.0E1 4.3E33 -6.84E0 3.666E4/
   PLOG/3.0E1 1.92E30 -5.71E0 3.591E4/
   PLOG/1.0E2 2.37E26 -4.37E0 3.484E4/
!=============================================================================================================
!\SUBSPECIES: C2H5O2H
!=============================================================================================================
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: RH+R_ABSTRACTION
!_____________________________________________________________________________________________________________
!\Author: WARNING !\Ref: TSANG, JPC REF. DATA, 16 !\Comment: WARNING
C2H5O2+HO2=C2H5O2H+O2    1.75E10 0.0 -3.275E3
!\Author: WARNING !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
C2H5O2+CH2O=C2H5O2H+HCO    1.99E12 0.0 1.166E4
!\Author: SP !\Ref: H-H CARSTENSEN, A.M. DEAN, O. DEUTSCHMANN, PROC. COMBUST. INST. 31(2007) 149-157 !\Comment: WARNING
C2H5O2+CH4=C2H5O2H+CH3    1.24E1 3.69 2.13E4
!\Author: WARNING !\Ref: TSANG, JPC REF. DATA, 16 !\Comment: WARNING
C2H5O2+CH3OH=C2H5O2H+CH2OH    1.81E12 0.0 1.371E4
!\Author: WARNING !\Ref: TSANG _ HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986 !\Comment: WARNING
C2H5O2+H2=C2H5O2H+H    1.5E14 0.0 2.603E4
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: KHP_HOMOLYTIC_FISSION
!_____________________________________________________________________________________________________________
!\Author: SP !\Ref: A.W.JASPER, S.J.KLIPPENSTEIN, L.B.HARDING, PROC.COMBUST.INST. 32(2009) 279-286 !\Comment: WARNING
C2H5O2H(+M)=C2H5O+OH(+M)    4.04972E19 -1.153 4.425049E4
   LOW/3.80285E42 -7.502E0 4.6756097E4/
   TROE/8.375E-1 3.6562E4 4.988E2 9.99E3/
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ISOMERISATION
!_____________________________________________________________________________________________________________
!\Author: WARNING !\Ref: BALDWIN ET AL., J. CHEM. SOC. FARADAY TRANS. 1, 80, 435(1984) !\Comment: WARNING
C2H3O1-2=CH3CO    8.5E14 0.0 1.4E4
!\Author: WARNING !\Ref: BALDWIN ET AL., J. CHEM. SOC. FARADAY TRANS. 1, 80, 435(1984) !\Comment: WARNING
C2H3O1-2=CH2CHO    1.0E14 0.0 1.4E4
!=============================================================================================================
!\ENDSUBSPECIES: C2H4O1-2
!=============================================================================================================
!-------------------------------------------------------------------------------------------------------------
!\ENDSUBMECH: C2H6
!-------------------------------------------------------------------------------------------------------------
!-------------------------------------------------------------------------------------------------------------
!\SUBMECH: C2H4
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!_____________________________________________________________________________________________________________________
!\REACTIONCLASS: RH(=)PRODUCTS
!_____________________________________________________________________________________________________________________
!\Author: ABS REFIT_ARAMCO BASIS !\Ref: S.J.KLIPPENSTEIN, L.B.HARDING, PHYS.CHEM.CHEM.PHYS. 1(1999) 989 !\Comment: BASIS FOR THE CHEMICALLY ACTIVATED PATHWAY
C2H3+H=C2H4    1.2495E19 -1.592 1.961089E3
   PLOG/1.0E-3 1.1935E26 -5.021E0 3.089757E3/
   PLOG/1.0E-2 1.0535E27 -5.0E0 3.073364E3/
   PLOG/1.0E-1 2.107E28 -5.085E0 3.485772E3/
   PLOG/1.0E0 8.82E29 -5.236E0 5.080164E3/
   PLOG/1.0E1 3.6239E22 -2.791E0 2.637005E3/
   PLOG/1.0E2 1.2495E19 -1.592E0 1.961089E3/
!_____________________________________________________________________________________________________________________
!\REACTIONCLASS: RH+R_ABSTRACTION
!_____________________________________________________________________________________________________________________
!\Author: UB !\Ref: H.HUA, B.RUSCIC, B.S.WANG, CHEM. PHYS. 311(2005) 335-341 !\Comment: WARNING
C2H4+O2=C2H3+HO2    7.17E13 0.0 6.001E4
!\Author: UB !\Ref: K.P.SOMERS PERSONAL COMMUNICATION WB97XD/CC-PVTZ//QCISD-T !\Comment: WARNING
C2H4+H=C2H3+H2    6.189E6 2.31 1.28299E4
!\Author: UB !\Ref: J.P. SENOSIAIN, S.J. KLIPPENSTEIN, J.A. MILLER, J. PHYS. CHEM. A, 110(2006) 6960-6970 !\Comment: WARNING
C2H4+OH=C2H3+H2O    1.3488E-1 4.1965 -8.6563E2
!\Author: UB !\Ref: C3 NUIG CALCULATION J.M !\Comment: ADDED AS ANALOGY TO ABSTRACTION FROM PROPENE VINYL SITE INCREASED AX2 TO ACCOUNT FOR NO. H-ATOMS
C2H4+HO2=C2H3+H2O2    1.914E3 3.059 2.07986E4
!\Author: WARNING !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
C2H4+CH3O=C2H3+CH3OH    1.2E11 0.0 6.75E3
!\Author: UB !\Ref: ANALOGY TO C2H4+HO2 !\Comment: REDUCED BY FACTOR OF 2.5 RELATIVE TO HO2 'K' SIMILAR TO APPROACH IN C3H6
C2H4+CH3O2=C2H3+CH3O2H    3.828E3 3.059 2.07986E4
!\Author: UB !\Ref: ANALOGY TO C2H4+HO2 !\Comment: REDUCED BY FACTOR OF 2.5 RELATIVE TO HO2 'K' SIMILAR TO APPROACH IN C3H6
C2H4+C2H5O2=C2H3+C2H5O2H    3.828E3 3.059 2.07986E4
!\Author: WARNING !\Ref: BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21 !\Comment: WARNING
C2H4+CH3CO3=C2H3+CH3CO3H    1.13E13 0.0 3.043E4
!\Author: UB !\Ref: J.A. MILLER, S.J. KLIPPENSTEIN, J. PHYS. CHEM. 117(2013) 2718-2727 !\Comment: WARNING
C2H4+CH3=C2H3+CH4    9.75564E2 2.947 1.5148E4
   DUP
!\Author: UB !\Ref: J.A. MILLER, S.J. KLIPPENSTEIN, J. PHYS. CHEM. 117(2013) 2718-2727 !\Comment: WARNING
C2H4+CH3=C2H3+CH4    8.1297E-5 4.417 8.8358E3
   DUP
!\Author: UB !\Ref: J.A. MILLER, S.J. KLIPPENSTEIN, J. PHYS. CHEM. 117(2013) 2718-2727 !\Comment: ANALOGY TO ABSTRACTION BY CH3
C2H4+C2H5=C2H3+C2H6    4.87782E2 2.947 1.5148E4
   DUP
!\Author: UB !\Ref: J.A. MILLER, S.J. KLIPPENSTEIN, J. PHYS. CHEM. 117(2013) 2718-2727 !\Comment: ANALOGY TO ABSTRACTION BY CH3
C2H4+C2H5=C2H3+C2H6    4.06485E-5 4.417 8.8358E3
   DUP
!_____________________________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONO
!_____________________________________________________________________________________________________________________
!\Author: UB !\Ref: X.LI, A.W.JASPER, J.ZADOR, J.A.MILLER, S.J.KLIPPENSTEIN !\Comment: WARNING
C2H4+O=CH3+HCO    5.708E17 -1.713 2.88776E3
!\Author: UB !\Ref: X.LI, A.W.JASPER, J.ZADOR, J.A.MILLER, S.J.KLIPPENSTEIN !\Comment: WARNING
C2H4+O=CH3CO+H    8.414E12 -0.481 1.9525E3
!\Author: UB !\Ref: X.LI, A.W.JASPER, J.ZADOR, J.A.MILLER, S.J.KLIPPENSTEIN !\Comment: WARNING
C2H4+O=CH2CHO+H    3.005E10 0.795 1.95253E3
!\Author: UB !\Ref: X.LI, A.W.JASPER, J.ZADOR, J.A.MILLER, S.J.KLIPPENSTEIN !\Comment: WARNING
C2H4+O=CH2+CH2O    5.775E6 1.991 2.85975E3
!\Author: UB !\Ref: X.LI, A.W.JASPER, J.ZADOR, J.A.MILLER, S.J.KLIPPENSTEIN !\Comment: WARNING
C2H4+O=CH2CO+H2    2.118E16 -1.617 2.85963E3
!_____________________________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONH
!_____________________________________________________________________________________________________________________
!\Author: WARNING !\Ref: BUTLER, FLEMING, GOSS, LIN, ACS SYMP. SER. 134(1980). !\Comment: WARNING
CH+CH4=C2H4+H    6.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: MARINOV ESTIMATE. !\Comment: WARNING
CH2(S)+CH3=C2H4+H    2.0E13 0.0 0.0E0
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!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONOH
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: SJK, J PHYS CHEM 110 2006 6960-6970 !\Comment: WARNING
C2H4+OH=CH3+CH2O    2.76E13 -0.5 1.14551E4
   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/
!\Author: WARNING !\Ref: SJK, J PHYS CHEM 110 2006 6960-6970 !\Comment: WARNING
C2H4+OH=CH3CHO+H    6.8E9 0.81 1.38673E4
   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/
!\Author: WARNING !\Ref: SJK, J PHYS CHEM 110 2006 6960-6970 !\Comment: WARNING
C2H4+OH=C2H3OH+H    8.55E10 0.75 1.14908E4
   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/
!=====================================================================================================
!\SUBSPECIES: C2H3
!=====================================================================================================
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_BETA_SCISSION
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: MILLER KLIPPENSTEIN PCCP 2004, 6, 1192-1202 !\Comment: WARNING
C2H2+H(+M)=C2H3(+M)    1.71E10 1.266 2.709E3
   AR/0.7/
   N2/1.4/
   CO/1.5/
   CO2/2.0/
   H2/2.0/
   CH4/2.0/
   C2H6/3.0/
   H2O/6.0/
   HE/3.0/
   LOW/6.346E31 -4.664E0 3.78E3/
   TROE/7.88E-1 -1.02E4 1.0E-30/
!\Author: UB !\Ref: GOLDSMITH ET AL, J. PHYS. CHEM. A 2015, 119, 7766-7779 !\Comment: WARNING
C2H3+O2=CH2CHO+O    9.27E25 -3.8 1.391E4
   PLOG/1.0E-2 7.16E20 -2.67E0 6.742E3/
   PLOG/1.0E-2 1.24E10 6.2E-1 -2.776E2/
   PLOG/1.0E-1 7.02E20 -2.67E0 6.713E3/
   PLOG/1.0E-1 1.29E10 6.2E-1 -2.477E2/
   PLOG/3.16E-1 8.97E20 -2.7E0 6.724E3/
   PLOG/3.16E-1 1.51E10 6.0E-1 -1.625E2/
   PLOG/1.0E0 6.45E20 -2.65E0 6.489E3/
   PLOG/1.0E0 1.84E10 5.8E-1 3.84E1/
   PLOG/3.16E0 4.09E20 -2.53E0 6.406E3/
   PLOG/3.16E0 8.86E9 6.7E-1 2.48E2/
   PLOG/1.0E1 1.6E23 -3.22E0 8.697E3/
   PLOG/1.0E1 6.67E9 7.2E-1 7.781E2/
   PLOG/3.16E1 2.85E25 -3.77E0 1.153E4/
   PLOG/3.16E1 1.43E9 9.2E-1 1.219E3/
   PLOG/1.0E2 9.27E25 -3.8E0 1.391E4/
   PLOG/1.0E2 7.14E7 1.28E0 1.401E3/
!\Author: WARNING !\Ref: GOLDSMITH ET AL, J. PHYS. CHEM. A 2015, 119, 7766-7779 !\Comment: WARNING
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C2H3+O2=C2H2+HO2    1.06E17 -1.45 1.223E4
   PLOG/1.0E-2 1.08E7 1.28E0 3.322E3/
   PLOG/1.0E-2 4.76E1 2.75E0 -7.964E2/
   PLOG/1.0E-1 7.75E6 1.33E0 3.216E3/
   PLOG/1.0E-1 5.16E1 2.73E0 -7.683E2/
   PLOG/3.16E-1 1.21E7 1.27E0 3.311E3/
   PLOG/3.16E-1 5.55E1 2.73E0 -6.585E2/
   PLOG/1.0E0 2.15E7 1.19E0 3.367E3/
   PLOG/1.0E0 4.6E1 2.76E0 -4.928E2/
   PLOG/3.16E0 1.13E8 1.0E0 3.695E3/
   PLOG/3.16E0 3.75E0 3.07E0 -6.01E2/
   PLOG/1.0E1 1.31E11 1.2E-1 5.872E3/
   PLOG/1.0E1 5.48E0 3.07E0 8.57E1/
   PLOG/3.16E1 1.19E9 8.2E-1 5.617E3/
   PLOG/3.16E1 4.47E8 0.0E0 9.55E2/
   PLOG/1.0E2 1.06E17 -1.45E0 1.223E4/
   PLOG/1.0E2 2.02E1 2.94E0 1.847E3/
!\Author: WARNING !\Ref: GOLDSMITH ET AL, J. PHYS. CHEM. A 2015, 119, 7766-7779 !\Comment: WARNING
C2H3+O2=CH2CO+OH    1.66E10 0.36 1.201E4
   PLOG/1.0E-2 8.66E2 2.41E0 6.061E3/
   PLOG/1.0E-2 1.82E-1 3.12E0 1.331E3/
   PLOG/1.0E-1 8.91E2 2.41E0 6.078E3/
   PLOG/1.0E-1 2.07E-1 3.11E0 1.383E3/
   PLOG/3.16E-1 9.43E2 2.4E0 6.112E3/
   PLOG/3.16E-1 2.71E-1 3.08E0 1.496E3/
   PLOG/1.0E0 1.06E3 2.39E0 6.18E3/
   PLOG/1.0E0 5.26E-1 3.01E0 1.777E3/
   PLOG/3.16E0 1.09E3 2.38E0 6.179E3/
   PLOG/3.16E0 1.37E0 2.9E0 2.225E3/
   PLOG/1.0E1 1.39E3 2.36E0 6.074E3/
   PLOG/1.0E1 4.19E-1 2.93E0 2.052E3/
   PLOG/3.16E1 2.49E6 1.42E0 8.48E3/
   PLOG/3.16E1 1.19E-4 4.21E0 2.043E3/
   PLOG/1.0E2 1.66E10 3.6E-1 1.201E4/
   PLOG/1.0E2 1.3E-3 3.97E0 3.414E3/
!\Author: UB !\Ref: GOLDSMITH ET AL, J. PHYS. CHEM. A 2015, 119, 7766-7779 !\Comment: WARNING
C2H3+O2=CH2O+HCO    3.03E33 -6.28 1.6E4
   PLOG/1.0E-2 2.77E36 -7.6E0 1.264E4/
   PLOG/1.0E-2 5.04E15 -1.28E0 5.153E2/
   PLOG/1.0E-1 2.7E36 -7.6E0 1.261E4/
   PLOG/1.0E-1 5.1E15 -1.28E0 5.13E2/
   PLOG/3.16E-1 2.17E36 -7.57E0 1.249E4/
   PLOG/3.16E-1 5.34E15 -1.29E0 5.206E2/
   PLOG/1.0E0 3.03E35 -7.32E0 1.182E4/
   PLOG/1.0E0 6.76E15 -1.31E0 6.457E2/
   PLOG/3.16E0 1.59E36 -7.47E0 1.246E4/
   PLOG/3.16E0 1.05E16 -1.36E0 1.066E3/
   PLOG/1.0E1 5.76E35 -7.2E0 1.343E4/
   PLOG/1.0E1 2.84E15 -1.18E0 1.429E3/
   PLOG/3.16E1 3.54E20 -2.57E0 5.578E3/
   PLOG/3.16E1 1.14E69 -1.923E1 1.476E4/
   PLOG/1.0E2 3.03E33 -6.28E0 1.6E4/
   PLOG/1.0E2 4.68E10 1.9E-1 8.306E2/
!\Author: UB !\Ref: GOLDSMITH ET AL, J. PHYS. CHEM. A 2015, 119, 7766-7779 !\Comment: WARNING
C2H3+O2=>CH2O+H+CO    7.07E33 -6.28 1.6E4
   PLOG/1.0E-2 6.47E36 -7.6E0 1.264E4/
   PLOG/1.0E-2 1.18E16 -1.28E0 5.153E2/
   PLOG/1.0E-1 6.29E36 -7.6E0 1.261E4/
   PLOG/1.0E-1 1.19E16 -1.28E0 5.13E2/
   PLOG/3.16E-1 5.06E36 -7.57E0 1.249E4/
   PLOG/3.16E-1 1.26E16 -1.29E0 5.206E2/
   PLOG/1.0E0 7.07E35 -7.32E0 1.182E4/
   PLOG/1.0E0 1.58E16 -1.31E0 6.457E2/
   PLOG/3.16E0 3.72E36 -7.47E0 1.246E4/
   PLOG/3.16E0 2.44E16 -1.36E0 1.066E3/
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   PLOG/1.0E1 1.34E36 -7.2E0 1.343E4/
   PLOG/1.0E1 6.64E15 -1.18E0 1.429E3/
   PLOG/3.16E1 8.26E20 -2.57E0 5.578E3/
   PLOG/3.16E1 2.66E69 -1.923E1 1.476E4/
   PLOG/1.0E2 7.07E33 -6.28E0 1.6E4/
   PLOG/1.0E2 1.09E11 1.9E-1 8.306E2/
!\Author: WARNING !\Ref: GOLDSMITH ET AL, J. PHYS. CHEM. A 2015, 119, 7766-7779 !\Comment: WARNING
C2H3+O2=CO+CH3O    5.79E32 -6.45 1.681E4
   PLOG/1.0E-2 8.19E18 -2.66E0 3.201E3/
   PLOG/1.0E-2 1.29E9 1.8E-1 -1.717E3/
   PLOG/1.0E-1 4.06E14 -1.32E0 8.858E2/
   PLOG/1.0E-1 5.99E11 -2.93E0 -9.564E3/
   PLOG/3.16E-1 4.34E14 -1.33E0 9.006E2/
   PLOG/3.16E-1 2.91E11 -2.93E0 -1.012E4/
   PLOG/1.0E0 1.03E11 -3.3E-1 -7.478E2/
   PLOG/1.0E0 5.77E21 -3.54E0 4.772E3/
   PLOG/3.16E0 1.89E12 -3.0E0 -8.995E3/
   PLOG/3.16E0 4.99E15 -1.62E0 1.849E3/
   PLOG/1.0E1 1.93E24 -5.63E0 1.8E0/
   PLOG/1.0E1 9.33E16 -1.96E0 3.324E3/
   PLOG/3.16E1 1.1E18 -2.22E0 5.178E3/
   PLOG/3.16E1 1.02E72 -2.069E1 1.586E4/
   PLOG/1.0E2 5.79E32 -6.45E0 1.681E4/
   PLOG/1.0E2 1.1E9 3.1E-1 1.024E3/
!\Author: WARNING !\Ref: GOLDSMITH ET AL, J. PHYS. CHEM. A 2015, 119, 7766-7779 !\Comment: WARNING
C2H3+O2=CO2+CH3    1.21E32 -6.32 1.619E4
   PLOG/1.0E-2 2.37E35 -7.76E0 1.263E4/
   PLOG/1.0E-2 6.27E13 -1.16E0 4.063E2/
   PLOG/1.0E-1 1.73E35 -7.72E0 1.252E4/
   PLOG/1.0E-1 6.24E13 -1.16E0 4.014E2/
   PLOG/3.16E-1 4.47E34 -7.55E0 1.214E4/
   PLOG/3.16E-1 6.12E13 -1.16E0 3.97E2/
   PLOG/1.0E0 7.25E31 -6.7E0 1.044E4/
   PLOG/1.0E0 5.32E13 -1.14E0 4.467E2/
   PLOG/3.16E0 3.63E35 -7.75E0 1.283E4/
   PLOG/3.16E0 1.45E14 -1.26E0 9.877E2/
   PLOG/1.0E1 2.09E35 -7.53E0 1.405E4/
   PLOG/1.0E1 5.02E13 -1.11E0 1.409E3/
   PLOG/3.16E1 3.84E18 -2.44E0 5.408E3/
   PLOG/3.16E1 1.4E70 -2.011E1 1.543E4/
   PLOG/1.0E2 1.21E32 -6.32E0 1.619E4/
   PLOG/1.0E2 9.21E8 2.5E-1 8.553E2/
!_____________________________________________________________________________________________
!\REACTIONCLASS: R+R(=)RH_RH
!_____________________________________________________________________________________________
!\Author: ABS !\Ref: !MONKS PS NESBITT FL PAYNE WA SCANLON M STIEF LJ SHALLCROSS DE JPC 99 !\Comment: WARNING
C2H3+H=C2H2+H2    4.5E13 0.0 0.0E0
!\Author: UB !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: PRODUCT CHANGED BASED ON G.X.LIU, ET AL. CHEM. J. CHIN.
UNIV. 23(2002) 1147-115
C2H3+OH=C2H3OH    3.011E13 0.0 0.0E0
!\Author: UB !\Ref: A. FAHR ET AL. J. PHYS. CHEM. 95(1991) 3218-3224 !\Comment: WARNING
C2H3+CH3=C2H2+CH4    2.05E13 0.0 0.0E0
!\Author: UB !\Ref: A. FAHR ET AL. J. PHYS. CHEM. 95(1991) 3218-3224 !\Comment: WARNING
2C2H3=C2H2+C2H4    1.45E13 0.0 0.0E0
!\Author: UB !\Ref: W.TSANG, R.F.HAMPSON, J. PHYS. CHEM. REF. DATA, 15(1986) !\Comment: WARNING
C2H3+HO2=>CH2CHO+OH    3.011E13 0.0 0.0E0
!\Author: UB !\Ref: L.B.HARDING, S.J.KLIPPENSTEIN, Y.GEORGIEVSHII, PROC.COMBUST.INST. 30(2005) 985-993 !\Comment: WARNING
C2H3+O=CH2CHO    1.03E13 0.2 -4.27E2
!\Author: UB !\Ref: L.B.HARDING, S.J.KLIPPENSTEIN, Y.GEORGIEVSHII, PROC.COMBUST.INST. 30(2005) 985-993 !\Comment: WARNING
C2H3+O=C2H2+OH    1.03E12 0.2 -4.27E2
!\Author: UB !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
C2H3+HCO=C2H4+CO    9.033E13 0.0 0.0E0
!=============================================================================================
!\ENDSUBSPECIES: CHOCHO
!=============================================================================================
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!-----------------------------------------------------------------------------------------------------------------------
!\ENDSUBMECH: C2H4
!-----------------------------------------------------------------------------------------------------------------------
!-----------------------------------------------------------------------------------------------------------------------
!\SUBMECH: C2H2
!-----------------------------------------------------------------------------------------------------------------------
!_______________________________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONO2
!_______________________________________________________________________________________________________________________
!\Author: UB !\Ref: GIMENEZ-LOPEZ ET AL. INT. J. CHEM. KINET. 48, 11(2016) 724-738 !\Comment: WARNING
C2H2+O2=2HCO    6.1E12 0.0 5.325E4
   DUP
!\Author: UB !\Ref: GIMENEZ-LOPEZ ET AL. INT. J. CHEM. KINET. 48, 11(2016) 724-738 !\Comment: WARNING
C2H2+O2=2HCO    1.7E7 1.67 7.096E4
   DUP
!_______________________________________________________________________________________________________________________
!\REACTIONCLASS: RH+R_ABSTRACTION
!_______________________________________________________________________________________________________________________
!\Author: UB !\Ref: L.B. HARDING ET AL. J. CHEM. PHYS. 76, 10(1982) 5172 !\Comment: WARNING
C2H+H2=H+C2H2    4.1E5 2.39 8.64E2
!\Author: WARNING !\Ref: SJK J. PHYS. CHEM A 2005, 109, 6045-6055 !\Comment: WARNING
C2H2+OH=C2H+H2O    2.632E6 2.14 1.706E4
!_______________________________________________________________________________________________________________________
!\REACTIONCLASS: RH(=)PRODUCTS
!_______________________________________________________________________________________________________________________
!\Author: UB !\Ref: L.B.HARDING, Y.GEORGIEVSKII, S.J.KLIPPENSTEIN, J.PHYS.CHEM.A. 109(2005) 4646-4656 !\Comment: WARNING
C2H+H(+M)=C2H2(+M)    2.25E13 0.32 0.0E0
   HE/0.7/
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   CH4/2.0/
   H2/2.0/
   C2H6/3.0/
   H2O/6.0/
   LOW/3.75E33 -4.8E0 1.9E3/
   TROE/6.46E-1 1.32E2 1.315E3 5.566E3/
!_______________________________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONHCO
!_______________________________________________________________________________________________________________________
!\Author: WARNING !\Ref: GRI 3.0 AND USC II !\Comment: WARNING
C2H2+HCO=C2H3+CO    1.0E7 2.0 6.0E3
!_______________________________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONCH3O2
!_______________________________________________________________________________________________________________________
!\Author: UB !\Ref: K EST. BASED ON TOTAL K FOR C2H2+HO2, P'S BASED ON ADD-ISOM-BETA-S !\Comment: WARNING
C2H2+CH3O2=CH2O+CH2CHO    4.458E-3 4.301 9.04302E3
!\Author: WARNING !\Ref: SJK J. PHYS. CHEM A 2005, 109, 6045-6055 !\Comment: WARNING
C2H2+OH=CH2CO+H    1.457E4 2.45 4.477E3
   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/
!\Author: WARNING !\Ref: SJK J. PHYS. CHEM A 2005, 109, 6045-6055 !\Comment: WARNING
C2H2+OH=CH3+CO    8.25E5 1.77 4.697E3
   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/
!_______________________________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONO
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!_____________________________________________________________________________________________
!\Author: SP !\Ref: NGUYEN ET AL. J.PHYS.CHEM A 2006, 110, 6696-6706 !\Comment: WARNING
C2H2+O=CH2+CO    7.395E8 1.28 2.472E3
!\Author: SP !\Ref: NGUYEN ET AL. J.PHYS.CHEM A 2006, 110, 6696-6706 !\Comment: WARNING
C2H2+O=HCCO+H    2.958E9 1.28 2.472E3
!\Author: UB !\Ref: GIMENEZ-LOPEZ ET AL. INT. J. CHEM. KINET. 48, 11(2016) 724-738 !\Comment: WARNING
C2H2+HO2=CH2CHO+O    5.78E18 -2.09 2.435E4
   PLOG/1.0E-2 5.5E6 1.19E0 1.288E4/
   PLOG/1.0E-2 2.94E-4 4.16E0 7.736E3/
   PLOG/1.0E-1 1.16E8 7.7E-1 1.36E4/
   PLOG/1.0E-1 6.14E-3 3.81E0 8.394E3/
   PLOG/3.16E-1 1.2E7 1.09E0 1.305E4/
   PLOG/3.16E-1 5.44E-4 4.09E0 8.044E3/
   PLOG/1.0E0 3.02E7 9.8E-1 1.331E4/
   PLOG/1.0E0 2.48E-4 4.19E0 8.203E3/
   PLOG/3.16E0 1.98E74 -1.633E1 1.092E5/
   PLOG/3.16E0 6.57E4 1.85E0 1.236E4/
   PLOG/1.0E1 7.5E14 -1.17E0 1.835E4/
   PLOG/1.0E1 2.92E-1 3.38E0 1.059E4/
   PLOG/3.16E1 8.63E18 -2.27E0 2.223E4/
   PLOG/3.16E1 1.95E0 3.17E0 1.174E4/
   PLOG/1.0E2 5.78E18 -2.09E0 2.435E4/
   PLOG/1.0E2 1.1E-1 3.52E0 1.198E4/
!\Author: UB !\Ref: GIMENEZ-LOPEZ ET AL. INT. J. CHEM. KINET. 48, 11(2016) 724-738 !\Comment: WARNING
C2H2+HO2=CH2CO+OH    3.58E3 1.97 2.301E4
   PLOG/1.0E-2 6.25E-7 4.75E0 1.553E4/
   PLOG/1.0E-2 1.31E-14 6.58E0 1.027E4/
   PLOG/1.0E-1 6.7E-7 4.74E0 1.555E4/
   PLOG/1.0E-1 1.29E-14 6.59E0 1.033E4/
   PLOG/3.16E-1 4.18E-7 4.81E0 1.541E4/
   PLOG/3.16E-1 3.99E-14 6.36E0 1.027E4/
   PLOG/1.0E0 5.28E-7 4.78E0 1.546E4/
   PLOG/1.0E0 3.28E-15 6.7E0 1.009E4/
   PLOG/3.16E0 1.04E-6 4.69E0 1.564E4/
   PLOG/3.16E0 8.71E-21 8.3E0 8.107E3/
   PLOG/1.0E1 4.68E-5 4.22E0 1.678E4/
   PLOG/1.0E1 8.36E-22 8.76E0 8.804E3/
   PLOG/3.16E1 8.99E-1 2.97E0 1.973E4/
   PLOG/3.16E1 6.87E-14 6.67E0 1.313E4/
   PLOG/1.0E2 3.58E3 1.97E0 2.301E4/
   PLOG/1.0E2 6.63E-12 6.15E0 1.473E4/
!\Author: UB !\Ref: GIMENEZ-LOPEZ ET AL. INT. J. CHEM. KINET. 48, 11(2016) 724-738 !\Comment: WARNING
C2H2+HO2=CH2O+HCO    2.47E16 -1.7 2.003E4
   PLOG/1.0E-2 3.9E13 -1.17E0 1.375E4/
   PLOG/1.0E-2 8.43E0 2.56E0 7.382E3/
   PLOG/1.0E-1 4.26E0 2.64E0 7.253E3/
   PLOG/1.0E-1 1.56E13 -1.05E0 1.352E4/
   PLOG/3.16E-1 2.59E-6 4.34E0 4.525E3/
   PLOG/3.16E-1 6.9E9 0.0E0 1.172E4/
   PLOG/1.0E0 3.33E102 -2.418E1 1.386E5/
   PLOG/1.0E0 8.07E7 6.0E-1 1.085E4/
   PLOG/3.16E0 5.22E15 -1.75E0 1.518E4/
   PLOG/3.16E0 3.54E0 2.69E0 8.025E3/
   PLOG/1.0E1 7.32E35 -7.77E0 2.697E4/
   PLOG/1.0E1 9.84E6 9.1E-1 1.171E4/
   PLOG/3.16E1 1.78E28 -5.3E0 2.513E4/
   PLOG/3.16E1 1.79E4 1.7E0 1.125E4/
   PLOG/1.0E2 2.47E16 -1.7E0 2.003E4/
   PLOG/1.0E2 4.32E-6 4.31E0 6.829E3/
!\Author: UB !\Ref: GIMENEZ-LOPEZ ET AL. INT. J. CHEM. KINET. 48, 11(2016) 724-738 !\Comment: WARNING
C2H2+HO2=>CH2O+H+CO    5.77E16 -1.7 2.003E4
   PLOG/1.0E-2 9.1E13 -1.17E0 1.375E4/
   PLOG/1.0E-2 1.97E1 2.56E0 7.382E3/
   PLOG/1.0E-1 9.94E0 2.64E0 7.253E3/
   PLOG/1.0E-1 3.63E13 -1.05E0 1.352E4/
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   PLOG/3.16E-1 6.05E-6 4.34E0 4.525E3/
   PLOG/3.16E-1 1.61E10 0.0E0 1.172E4/
   PLOG/1.0E0 7.77E102 -2.418E1 1.386E5/
   PLOG/1.0E0 1.88E8 6.0E-1 1.085E4/
   PLOG/3.16E0 1.22E16 -1.75E0 1.518E4/
   PLOG/3.16E0 8.26E0 2.69E0 8.025E3/
   PLOG/1.0E1 1.71E36 -7.77E0 2.697E4/
   PLOG/1.0E1 2.3E7 9.1E-1 1.171E4/
   PLOG/3.16E1 4.14E28 -5.3E0 2.513E4/
   PLOG/3.16E1 4.19E4 1.7E0 1.125E4/
   PLOG/1.0E2 5.77E16 -1.7E0 2.003E4/
   PLOG/1.0E2 1.01E-5 4.31E0 6.829E3/
!\Author: UB !\Ref: GIMENEZ-LOPEZ ET AL. INT. J. CHEM. KINET. 48, 11(2016) 724-738 !\Comment: WARNING
C2H2+HO2=CO+CH3O    1.17E18 -2.57 2.236E4
   PLOG/1.0E-2 3.54E11 0.0E0 4.951E4/
   PLOG/1.0E-2 2.89E4 1.23E0 9.903E3/
   PLOG/1.0E-1 2.78E8 1.0E-2 1.192E4/
   PLOG/1.0E-1 9.67E-7 4.15E0 5.173E3/
   PLOG/3.16E-1 8.06E7 1.8E-1 1.165E4/
   PLOG/3.16E-1 1.84E-8 4.62E0 4.517E3/
   PLOG/1.0E0 8.94E69 -1.585E1 1.025E5/
   PLOG/1.0E0 5.38E5 8.6E-1 1.07E4/
   PLOG/3.16E0 5.66E12 -1.25E0 1.457E4/
   PLOG/3.16E0 5.37E-4 3.42E0 7.218E3/
   PLOG/1.0E1 3.3E23 -4.45E0 2.121E4/
   PLOG/3.16E1 2.43E22 -3.96E0 2.265E4/
   PLOG/3.16E1 8.11E0 2.3E0 1.056E4/
   PLOG/1.0E2 1.17E18 -2.57E0 2.236E4/
   PLOG/1.0E2 6.86E-4 3.42E0 9.329E3/
!\Author: UB !\Ref: GIMENEZ-LOPEZ ET AL. INT. J. CHEM. KINET. 48, 11(2016) 724-738 !\Comment: WARNING
C2H2+HO2=CO2+CH3    1.71E15 -1.8 2.037E4
   PLOG/1.0E-2 1.15E-7 4.31E0 4.614E3/
   PLOG/1.0E-2 2.01E8 0.0E0 1.179E4/
   PLOG/1.0E-1 1.1E-7 4.32E0 4.622E3/
   PLOG/1.0E-1 2.01E8 0.0E0 1.178E4/
   PLOG/3.16E-1 1.75E142 -3.504E1 1.887E5/
   PLOG/3.16E-1 1.55E5 9.5E-1 1.02E4/
   PLOG/1.0E0 3.96E84 -1.98E1 1.198E5/
   PLOG/1.0E0 1.38E6 6.8E-1 1.081E4/
   PLOG/3.16E0 5.02E13 -1.6E0 1.498E4/
   PLOG/3.16E0 9.29E-3 3.0E0 7.659E3/
   PLOG/1.0E1 8.56E28 -6.15E0 2.403E4/
   PLOG/1.0E1 1.86E4 1.26E0 1.123E4/
   PLOG/3.16E1 1.28E27 -5.42E0 2.538E4/
   PLOG/3.16E1 2.89E2 1.79E0 1.124E4/
   PLOG/1.0E2 1.71E15 -1.8E0 2.037E4/
   PLOG/1.0E2 3.9E-7 4.21E0 7.314E3/
!\Author: UB !\Ref: H. THIESEMANN, C.A. TAATJES, CHEM. PHYS. LETT. 270, 5-6(1997) 580-586 !\Comment: WARNING
C2H+O2=>2CO+H    4.7E13 -0.16 0.0E0
!\Author: WARNING !\Ref: GRI3.0 !\Comment: WARNING
C2H+O=CO+CH    5.0E13 0.0 0.0E0
!\Author: UB !\Ref: B.J. OPANSKY ET AL. J. PHYS. CHEM., 100(1996) 4888-4892 !\Comment: WARNING
C2H+CH4=CH3+C2H2    7.2E12 0.0 9.76E2
!=============================================================================================================
!\ENDSUBSPECIES: C2H2OH
!=============================================================================================================
!-------------------------------------------------------------------------------------------------------------
!\ENDSUBMECH: C2H2
!-------------------------------------------------------------------------------------------------------------
!-------------------------------------------------------------------------------------------------------------
!\SUBMECH: CH3CHO
!-------------------------------------------------------------------------------------------------------------
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: RH(=)PRODUCTS
!_____________________________________________________________________________________________________________
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!\Author: WARNING !\Ref: SIVARAMAKRISHNAN THE JOURNAL OF PHYSICAL CHEMISTRY A 28(2015) 7724-7733. !\Comment: WARNING
CH3CHO(+M)=CH3+HCO(+M)    2.72E22 -1.74 8.6355E4
   LOW/1.144E59 -1.13E1 9.59125E4/
   TROE/1.83E-1 4.62E2 1.6773E5 1.58E6/
!\Author: WARNING !\Ref: SIVARAMAKRISHNAN THE JOURNAL OF PHYSICAL CHEMISTRY A 28(2015) 7724-7733. !\Comment: WARNING
CH3CHO=CH4+CO    1.639E45 -9.1 9.2793E4
   PLOG/5.0E-2 5.124E45 -9.85E0 8.9018E4/
   PLOG/1.0E-1 1.438E45 -9.65E0 8.7925E4/
   PLOG/1.0E0 1.867E45 -9.43E0 8.9415E4/
   PLOG/1.0E1 1.639E45 -9.1E0 9.2793E4/
!\Author: WARNING !\Ref: SIVARAMAKRISHNAN THE JOURNAL OF PHYSICAL CHEMISTRY A 28(2015) 7724-7733. !\Comment: WARNING
CH3CHO=CH2CO+H2    2.219E45 -9.55 9.4879E4
   PLOG/5.0E-2 3.979E44 -1.007E1 8.7428E4/
   PLOG/1.0E-1 7.38E44 -1.005E1 8.8422E4/
   PLOG/1.0E0 8.544E44 -9.77E0 9.0905E4/
   PLOG/1.0E1 2.219E45 -9.55E0 9.4879E4/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RH+R_ABSTRACTION
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CHO+O2=CH3CO+HO2    1.2E5 2.5 3.756E4
!\Author: WARNING !\Ref: CURRAN, FIT TO NIST DATABASE !\Comment: WARNING
CH3CHO+O=CH3CO+OH    5.94E12 0.0 1.868E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CHO+H=CH3CO+H2    6.9E5 2.4 1.905E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CHO+H=CH2CHO+H2    1.05E5 2.5 8.041E3
!\Author: SP !\Ref: S. WANG, D.F. DAVIDSON, R.K. HANSON, PROC. COMBUST. INST. 35(2015) 473-480. !\Comment: WARNING
CH3CHO+OH=CH3CO+H2O    2.8E12 0.0 -7.09E2
!\Author: SP !\Ref: S. WANG, D.F. DAVIDSON, R.K. HANSON, PROC. COMBUST. INST. 35(2015) 473-480. !\Comment: WARNING
CH3CHO+OH=CH2CHO+H2O    8.5E13 0.0 5.313E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CHO+HO2=CH3CO+H2O2    1.7E13 0.0 1.6293E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CHO+HO2=CH2CHO+H2O2    1.1E13 0.0 2.3248E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CHO+CH3=CH3CO+CH4    7.08E-4 4.58 9.66E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CHO+CH3=CH2CHO+CH4    1.437E0 3.7 8.857E3
!\Author: WARNING !\Ref: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325? 3346 !\Comment: WARNING
CH3CHO+C2H3=CH3CO+C2H4    1.65E1 3.17 9.3998E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CHO+CH3O2=CH3CO+CH3O2H    4.83E-1 3.94 9.5E3
   DUP
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CHO+CH3O2=CH3CO+CH3O2H    4.99E-6 4.9756 5.2682E3
   DUP
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CHO+CH3O2=CH2CHO+CH3O2H    8.23E-3 4.2759 1.6817E4
   DUP
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CHO+CH3O2=CH2CHO+CH3O2H    7.08E-9 5.6571 1.1699E4
   DUP
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CHO+CH3CO3=CH2CHO+CH3CO3H    2.54E-3 4.3574 1.3426E4
   DUP
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CHO+CH3CO3=CH2CHO+CH3CO3H    3.6E-11 6.2 7.3508E3
   DUP
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CHO+CH3CO3=CH3CO+CH3CO3H    1.9158E0 3.6426 5.6419E3
   DUP
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CHO+CH3CO3=CH3CO+CH3CO3H    9.81E-4 4.3201 2.6361E3
   DUP
```

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!=============================================================================================================
!\SUBSPECIES: CH3CO
!=============================================================================================================
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ALPHA_SCISSION
!_____________________________________________________________________________________________________________
!\Author: WARNING !\Ref: J. PHYS. CHEM. A 2006, 110, 5772-5781 !\Comment: WARNING
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/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2CO+H=CH3CO    2.3E8 1.61 2.627E3
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: R+R(=)RH_RH
!_____________________________________________________________________________________________________________
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
CH3CO+H=CH2CO+H2    2.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
CH3CO+O=CH2CO+OH    2.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
CH3CO+CH3=CH2CO+CH4    5.0E13 0.0 0.0E0
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: R+O2(=)PRODUCTS
!_____________________________________________________________________________________________________________
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CO+O2=CH3CO3    3.15E59 -15.3 1.46E4
   PLOG/1.0E-1 1.08E95 -2.7336E1 2.5141E4/
   PLOG/1.0E-1 1.21E45 -1.1733E1 5.3583E3/
   PLOG/1.0E0 9.27E68 -1.87E1 1.67E4/
   PLOG/1.0E0 6.18E43 -1.1E1 5.69E3/
   PLOG/1.0E1 3.15E59 -1.53E1 1.46E4/
   PLOG/1.0E1 2.46E45 -1.14E1 6.41E3/
!H2COCO#(=)CH2O+CO                              +1.21000000E+012 +0.00000000E+000 +3.60000000E+004 !\Author: WARNING !\Ref: WARNING !\Comment:
WARNING
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CHO+CH3O=CH3CO+CH3OH    1.69E5 2.0438 2.3532E3
   DUP
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CHO+CH3O=CH3CO+CH3OH    9.62E3 2.5005 1.5895E2
   DUP
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CHO+CH3O=CH2CHO+CH3OH    2.6502E1 3.4519 5.8733E3
   DUP
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CHO+CH3O=CH2CHO+CH3OH    5.64E-6 4.93 6.2769E2
   DUP
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2CHO+HO2=>CO+CH2O+H2O    1.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2CHO+HO2=>HCO+CH2O+OH    1.0E13 0.0 0.0E0
!=============================================================================================================
!\ENDSUBSPECIES: CH3CO
!=============================================================================================================
!=============================================================================================================
!\SUBSPECIES: C2H3OH
!=============================================================================================================
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: RH(=)PRODUCTS
!_____________________________________________________________________________________________________________
!\Author: SP !\Ref: E.E. DAMES, INT. J. CHEM. KINET. 46(2014) 176-188 !\Comment: WARNING
C2H3OH(+M)=CH3CHO(+M)    9.66E23 -3.29 5.998753E4
   LOW/2.87E43 -8.12E0 5.219849E4/
   TROE/5.0E-1 8.63E2 3.2E2 1.0E5/
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: RH+R_ABSTRACTION
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!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: ETHENOL CHEMISTRY FROM CURRAN / YASUNAGA !\Comment: WARNING
C2H3OH+O2=CH2CHO+HO2    5.31E11 0.21 3.983E4
!\Author: WARNING !\Ref: ETHENOL CHEMISTRY FROM CURRAN / YASUNAGA !\Comment: WARNING
C2H3OH+O=CH2CHO+OH    1.875E6 1.9 -8.6E2
!\Author: WARNING !\Ref: ENOL+H RAO |J. PHYS. CHEM. A 2011, 115, 1602-1608, !\Comment: WARNING
C2H3OH+H=CH2CHO+H2    1.48E3 3.077 7.22E3
!\Author: WARNING !\Ref: ETHENOL CHEMISTRY FROM CURRAN / YASUNAGA !\Comment: WARNING
C2H3OH+OH=CH2CHO+H2O    3.33E9 1.1 5.405E2
!\Author: WARNING !\Ref: ETHENOL CHEMISTRY FROM CURRAN / YASUNAGA !\Comment: WARNING
C2H3OH+CH3=CH2CHO+CH4    2.03E-8 5.9 1.052E3
!\Author: WARNING !\Ref: ETHENOL CHEMISTRY FROM CURRAN / YASUNAGA !\Comment: WARNING
C2H3OH+CH3O2=CH2CHO+CH3O2H    3.4E3 2.5 8.922E3
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONHO2
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: DA SILVA BOZZELLI CHEMICAL PHYSICS LETTERS 483(2009) 25-29 !\Comment: WARNING
C2H3OH+HO2=CH3CHO+HO2    1.49E5 1.67 6.81E3
!=====================================================================================================
!\ENDSUBSPECIES: C2H3OH
!=====================================================================================================
!=====================================================================================================
!\SUBSPECIES: CH2CHO
!=====================================================================================================
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_BETA_SCISSION
!_____________________________________________________________________________________________________
!\Author: UB !\Ref: J.P. SENOSIAIN, ET AL. J. PHYS. CHEM. A, 110(2006) 5772-5781 !\Comment: WARNING
CH2CHO=H+CH2CO    1.18E36 -6.48 5.5171E4
   PLOG/1.0E-2 2.39E25 -4.8E0 4.3424E4/
   PLOG/2.5E-2 2.48E27 -5.23E0 4.4304E4/
   PLOG/1.0E-1 2.37E30 -5.86E0 4.6114E4/
   PLOG/1.0E0 1.32E34 -6.57E0 4.9454E4/
   PLOG/1.0E1 3.46E36 -6.92E0 5.2979E4/
   PLOG/1.0E2 1.18E36 -6.48E0 5.5171E4/
!\Author: UB !\Ref: J.P. SENOSIAIN, ET AL. J. PHYS. CHEM. A, 110(2006) 5772-5781 !\Comment: WARNING
CH2CHO=CH3+CO    2.23E33 -5.97 5.0448E4
   PLOG/1.0E-2 1.16E30 -6.07E0 4.1332E4/
   PLOG/2.5E-2 1.54E31 -6.27E0 4.2478E4/
   PLOG/1.0E-1 6.37E32 -6.57E0 4.4282E4/
   PLOG/1.0E0 6.51E34 -6.87E0 4.7191E4/
   PLOG/1.0E1 2.15E35 -6.67E0 4.9548E4/
   PLOG/1.0E2 2.23E33 -5.97E0 5.0448E4/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+H(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: UB !\Ref: N.J. LABBE, ET AL. PROC. COMBUST. INST. 35(2015) 447-455 !\Comment: WARNING
CH2CHO+H=CH3+HCO    7.4673E20 -1.693 1.34293E4
   PLOG/1.0E-3 1.4865E17 -9.03E-1 3.0235E3/
   PLOG/1.0E-2 1.9331E17 -9.35E-1 3.1198E3/
   PLOG/1.0E-1 2.5358E18 -1.243E0 4.0618E3/
   PLOG/1.0E0 1.9282E22 -2.3E0 7.6927E3/
   PLOG/1.0E1 2.7876E25 -3.1E0 1.24544E4/
   PLOG/1.0E2 7.4673E20 -1.693E0 1.34293E4/
!\Author: UB !\Ref: N.J. LABBE, ET AL. PROC. COMBUST. INST. 35(2015) 447-455 !\Comment: WARNING
CH2CHO+H=H+CH3CO    8.07038E19 -1.50969 1.5533928E4
   PLOG/1.0E-3 3.60192E13 5.139E-2 4.30182E3/
   PLOG/1.0E-2 4.63879E13 2.101E-2 4.392213E3/
   PLOG/1.0E-1 3.37344E14 -2.1686E-1 5.1131929E3/
   PLOG/1.0E0 9.20824E17 -1.15762E0 8.19254E3/
   PLOG/1.0E1 1.58439E22 -2.27331E0 1.3260714E4/
   PLOG/1.0E2 8.07038E19 -1.50969E0 1.5533928E4/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+OH(=)PRODUCTS
!_____________________________________________________________________________________________________
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!\Author: UB !\Ref: C.J. POPE, J.A. MILLER, PROC. COMBUST. INST. 28(2000) 1518-1529 !\Comment: WARNING
CH2CHO+OH=CH2CO+H2O    2.0E13 0.0 0.0E0
!\Author: UB !\Ref: C.J. POPE, J.A. MILLER, PROC. COMBUST. INST. 28(2000) 1518-1529 !\Comment: WARNING
CH2CHO+OH=CH2OH+HCO    1.0E13 0.0 0.0E0
!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+O(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: UB !\Ref: C.J. POPE, J.A. MILLER, PROC. COMBUST. INST. 28(2000) 1518-1529 !\Comment: WARNING
CH2CHO+O=CH2O+HCO    5.0E13 0.0 0.0E0
!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+O2(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: J. LEE, AND J.W. BOZZELLI. J. PHYS. CHEM. A, 2003, 107(19), 3778-3791 !\Comment: WARNING
CH2CHO+O2=O2CH2CHO    3.05E50 -12.2 1.563E4
   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/
!\Author: WARNING !\Ref: J. LEE, AND J.W. BOZZELLI. J. PHYS. CHEM. A, 2003, 107(19), 3778-3791 !\Comment: WARNING
CH2CHO+O2=CH2CO+HO2    7.05E7 1.63 2.529E4
   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/
!\Author: WARNING !\Ref: J. LEE, AND J.W. BOZZELLI. J. PHYS. CHEM. A, 2003, 107(19), 3778-3791 !\Comment: WARNING
CH2CHO+O2=>CH2O+CO+OH    8.953E13 -0.6 1.012E4
   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/
!\Author: WARNING !\Ref: J. LEE, AND J.W. BOZZELLI. J. PHYS. CHEM. A, 2003, 107(19), 3778-3791 !\Comment: WARNING
CH2CHO+O2=HO2CH2CO    4.8E38 -12.14 1.496E4
   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/
!\Author: WARNING !\Ref: J. LEE, AND J.W. BOZZELLI. J. PHYS. CHEM. A, 2003, 107(19), 3778-3791 !\Comment: WARNING
O2CH2CHO=HO2CH2CO    1.43E16 -1.67 2.121E4
   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/
!\Author: WARNING !\Ref: J. LEE, AND J.W. BOZZELLI. J. PHYS. CHEM. A, 2003, 107(19), 3778-3791 !\Comment: WARNING
O2CH2CHO=CH2CO+HO2    1.12E61 -16.04 6.001E4
   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/
!\Author: WARNING !\Ref: J. LEE, AND J.W. BOZZELLI. J. PHYS. CHEM. A, 2003, 107(19), 3778-3791 !\Comment: WARNING
HO2CH2CO=>CO+CH2O+OH    4.16E20 -3.02 8.24E3
   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/
!\Author: WARNING !\Ref: J. LEE, AND J.W. BOZZELLI. J. PHYS. CHEM. A, 2003, 107(19), 3778-3791 !\Comment: WARNING
HO2CH2CO=CH2CO+HO2    2.09E9 -3.55 2.122E4
   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/
!=====================================================================================================
!\ENDSUBSPECIES: CH2CHO
!=====================================================================================================
!=====================================================================================================
!\SUBSPECIES: CH3CO3H
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!=============================================================================================================
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: RH(=)PRODUCTS
!_____________________________________________________________________________________________________________
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CO3H(+M)=CH3CO2+OH(+M)    1.82237E20 -1.153 4.425049E4
   LOW/1.71128E43 -7.502E0 4.6756097E4/
   TROE/8.375E-1 3.6562E4 4.988E2 9.99E3/
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: RH+R_ABSTRACTION
!_____________________________________________________________________________________________________________
!\Author: WARNING !\Ref: ANALOGY TO CH3O2+CH2O !\Comment: WARNING
CH3CO3+CH2O=CH3CO3H+HCO    1.99E12 0.0 1.166E4
!\Author: WARNING !\Ref: ANALOGY TO CH3O2+CH2O !\Comment: WARNING
CH3CO3+C2H6=CH3CO3H+C2H5    1.01E2 3.37 9.64E3
!\Author: WARNING !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
CH3CO3+HO2=CH3CO3H+O2    1.75E10 0.0 -3.275E3
!\Author: WARNING !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
CH3CO3+H2O2=CH3CO3H+HO2    2.41E12 0.0 9.936E3
!\Author: SP !\Ref: H-H CARSTENSEN, A.M. DEAN, O. DEUTSCHMANN, PROC. COMBUST. INST. 31(2007) 149-157 !\Comment: WARNING
CH3CO3+CH4=CH3CO3H+CH3    7.26E1 3.6 1.42E4
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ALPHA_SCISSION
!_____________________________________________________________________________________________________________
!\Author: WARNING !\Ref: ANALOGY TO CH3CO(=)CH3+CO !\Comment: WARNING
CH3CO2+M=CH3+CO2+M    4.4E15 0.0 1.05E4
!=============================================================================================================
!\ENDSUBSPECIES: CH3CO3H
!=============================================================================================================
!-------------------------------------------------------------------------------------------------------------
!\ENDSUBMECH: CH3CHO
!-------------------------------------------------------------------------------------------------------------
!-------------------------------------------------------------------------------------------------------------
!\SUBMECH: CH2CO
!-------------------------------------------------------------------------------------------------------------
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: RH(=)PRODUCTS
!_____________________________________________________________________________________________________________
!\Author: UB !\Ref: LASKIN ET AL. IJCK 32 589-614 2000 !\Comment: HPL CORRECTED TO USCII VALUE
CH2+CO(+M)=CH2CO(+M)    8.1E11 0.5 4.51E3
   AR/0.7/
   HE/0.7/
   CO/1.5/
   H2/2.0/
   CH4/2.0/
   CO2/2.0/
   C2H6/3.0/
   H2O/6.0/
   LOW/2.69E33 -5.11E0 7.095E3/
   TROE/5.907E-1 2.75E2 1.226E3 5.185E3/
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: RH+R_ABSTRACTION
!_____________________________________________________________________________________________________________
!\Author: WARNING !\Ref: WKM(SEE COMMENTS AT BEGINNING OF FILE 15 / 09 / 2011 !\Comment: WARNING
CH2CO+H=HCCO+H2    1.401E15 -0.171 8.7832E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2CO+OH=>HCCO+H2O    3.93E4 2.45 4.524E3
   DUP
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2CO+OH=>HCCO+H2O    2.6E2 2.7 1.279E3
   DUP
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2CO+OH=CH2OH+CO    3.5E7 1.41 -1.249E3
   DUP
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
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CH2CO+OH=CH2OH+CO    4.09E6 1.76 2.088E3
   DUP
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2CO+OH=>CH3+CO2    9.59E21 -2.66 1.667E4
   PLOG/1.0E-4 1.17E12 -1.1E-1 3.67E1/
   PLOG/1.0E-4 3.61E-15 -1.554E1 -9.058E4/
   PLOG/1.0E-3 1.17E12 -1.1E-1 3.64E1/
   PLOG/1.0E-3 2.81E-7 -8.0E-1 -2.658E4/
   PLOG/1.0E-2 1.54E12 -1.5E-1 1.334E2/
   PLOG/1.0E-2 1.34E-8 -6.2E-1 -2.788E4/
   PLOG/1.0E0 2.7E25 -3.95E0 9.988E3/
   PLOG/1.0E0 3.06E8 9.1E-1 3.748E2/
   PLOG/1.0E1 4.64E23 -3.26E0 1.29E4/
   PLOG/1.0E1 3.92E5 1.68E0 4.316E2/
   PLOG/2.0E1 4.58E22 -2.93E0 1.361E4/
   PLOG/2.0E1 4.22E4 1.93E0 3.485E2/
   PLOG/5.0E1 1.7E22 -2.76E0 1.525E4/
   PLOG/5.0E1 9.9E2 2.38E0 1.964E2/
   PLOG/1.0E2 9.59E21 -2.66E0 1.667E4/
   PLOG/1.0E2 2.67E1 2.83E0 3.0E0/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONH
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2CO+H=CH3+CO    7.8E8 1.45 2.78E3
!\Author: WARNING !\Ref: REG 2.11 !\Comment: WARNING
CH+CH2O=H+CH2CO    9.46E13 0.0 -5.15E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
O2+CH2CO=>CO2+CH2O    1.0E14 0.0 3.7E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
O2+CH2CO=>OH+CO+HCO    3.0E14 0.0 4.0E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
O2+CH2CO=>HO2+HCCO    1.36E7 2.0 5.452643E4
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONO
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: WKM ESTIMATE, LLNL !\Comment: WARNING
CH2CO+O=HCCO+OH    1.0E13 0.0 8.0E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2CO+O=CO2+CH2    1.8E12 0.0 1.35E3
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONMISC
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: WKM CALCULATION !\Comment: CHEMICALLY ACTIVATED, APPEARS PRESSURE INDEPENDANT
CH2CO+CH2(S)=C2H4+CO    1.6E14 0.0 0.0E0
!\Author: WARNING !\Ref: WKM CALCULATION !\Comment: CHEMICALLY ACTIVATED, APPEARS PRESSURE INDEPENDANT
CH2CO+CH3=C2H5+CO    4.769E4 2.312 9.468E3
!=====================================================================================================
!\SUBSPECIES: HCCO
!=====================================================================================================
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ALPHA_SCISSION
!_____________________________________________________________________________________________________
!\Author: UB !\Ref: GRI3.0 !\Comment: WARNING
CH+CO(+M)=HCCO(+M)    5.0E13 0.0 0.0E0
   AR/0.7/
   CO/1.5/
   CH4/2.0/
   H2/2.0/
   CO2/2.0/
   C2H6/3.0/
   H2O/6.0/
   LOW/2.69E28 -3.74E0 1.936E3/
   TROE/5.757E-1 2.37E2 1.652E3 5.069E3/
!_____________________________________________________________________________________________________
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!\REACTIONCLASS: RADICAL_ADDITIONO2
!_____________________________________________________________________________________________________
!\Author: UB !\Ref: S.J. KLIPPENSTEIN ET AL. PROC. COMBUST. INST. 29(2002) 1209-1217 !\Comment: WARNING
HCCO+O2=>OH+2CO    1.91E11 -0.02 1.02E3
!\Author: UB !\Ref: S.J. KLIPPENSTEIN ET AL. PROC. COMBUST. INST. 29(2002) 1209-1217 !\Comment: WARNING
HCCO+O2=>CO2+CO+H    4.78E12 -0.142 1.15E3
!\Author: UB !\Ref: S.J. KLIPPENSTEIN ET AL. PROC. COMBUST. INST. 29(2002) 1209-1217 !\Comment: WARNING
HCCO+O2=>HCO+CO+O    2.18E2 2.692 3.541E3
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONOH
!_____________________________________________________________________________________________________
!\Author: UB !\Ref: REFIT OF XIONG ET AL COMBUST. FLAME, 161(2014) 885-897 !\Comment: WARNING
HCCO+OH=CO+HCOH    1.5E14 -0.0575 2.6077E2
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONMISC
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: WKM CALCULATION !\Comment: CHEMICALLY ACTIVATED, APPEARS PRESSURE INDEPENDANT
HCCO+O=>H+2CO    8.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: GRI3.0 !\Comment: WARNING
HCCO+CH=CO+C2H2    1.0E13 0.0 0.0E0
!\Author: UB !\Ref: GIMENEZ-LOPEZ ET AL. INT. J. CHEM. KINET. 48, 11(2016) 724-738 !\Comment: WARNING
HCCO+CH2=C2H3+CO    1.0E13 0.0 0.0E0
!\Author: UB !\Ref: GLASS ET AL. J.PHYS.CHEM.A, 104(2000) 8360-8367 !\Comment: WARNING
HCCO+H=CH2(S)+CO    1.02E14 0.0 0.0E0
!\Author: UB !\Ref: GIMENEZ-LOPEZ ET AL. INT. J. CHEM. KINET. 48, 11(2016) 724-738 !\Comment: WARNING
2HCCO=>C2H2+2CO    1.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: HARDING J. PHYS. CHEM., VOL. 114, NO. 2, 2010 !\Comment: WARNING
CH3CHO+H=C2H5O    4.61E7 1.71 7.09E3
!\Author: SP !\Ref: E.E. DAMES, INT. J. CHEM. KINET. 46(2014) 176-188 !\Comment: WARNING
C2H5O(+M)=CH3+CH2O(+M)    6.3E10 0.93 1.7098E4
   LOW/4.7E25 -3.0E0 1.6532E4/
   TROE/4.26E-1 3.0E-1 2.278E3 1.0E5/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+O2(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: HARTMANN ET AL. 1990 !\Comment: WARNING
C2H5O+O2=CH3CHO+HO2    4.28E10 0.0 1.097E3
!\Author: WARNING !\Ref: FRIEDRICHS, G.; DAVIDSON, D. F.; HANSON, R. K. INT J. CHEM. KINET. 2004, 36, 157. !\Comment: ULTAN ADDED 21 / 08 / 15
CH3O+HCO=CH3OH+CO    9.0E13 0.0 0.0E0
!-----------------------------------------------------------------------------------------------------------
!\ENDSUBMECH: CH3OCHO
!-----------------------------------------------------------------------------------------------------------
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++++++++++++++++++++++++++++++++++++
!\END_KINETICS_MODULE: C2
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
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!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++++++++++++++++++++++++++++++++++++++
!\KINETICS_MODULE: C3
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++++++++++++++++++++++++++++++++++++++
!-----------------------------------------------------------------------------------------------------------
!\SUBMECH: C3H8
!-----------------------------------------------------------------------------------------------------------
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RH(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: SP !\Ref: SIVARAMAKRISHNAN ET AL., DX.DOI.ORG / 10.1021 / JP2006205 / / J. PHYS. CHEM. A 2011, 115, 3366-3379, !\Comment: WARNING
C3H8(+M)=C2H5+CH3(+M)    1.55E24 -2.034 9.0388E4
   N2/1.5/
   H2/2.0/
   CO/2.0/
   CO2/3.0/
   H2O/5.0/
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   LOW/4.77E77 -1.667E1 1.001E5/
   TROE/8.1E-1 3.091E3 1.28E2 8.829E3/
!\Author: SP !\Ref: TSANG, W. J.PHYS.CHEM.REF.DATA 1988, 17, 887 !\Comment: WARNING
NC3H7+H(+M)=C3H8(+M)    3.6E13 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/3.01E48 -9.32E0 5.8336E3/
   TROE/4.98E-1 1.314E3 1.314E3 5.0E4/
!\Author: SP !\Ref: HARDING ET AL., J. PHYS. CHEM. A, 2005, 109(21), PP 4646-4656 !\Comment: WARNING
IC3H7+H=C3H8    1.66E13 0.22 0.0E0
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RO2+RO2(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: ESTIMATE !\Ref: WARNING !\Comment: WARNING
NC3H7O2+CH3O2=>NC3H7O+CH3O+O2    1.4E16 -1.61 1.86E3
!\Author: ESTIMATE !\Ref: WARNING !\Comment: WARNING
NC3H7O2+C2H5O2=>NC3H7O+C2H5O+O2    1.4E16 -1.61 1.86E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
2NC3H7O2=>2NC3H7O+O2    7.0E16 -1.61 1.86E3
!\Author: SP !\Ref: JOHNSON, D.; PRICE, D.W.; MARSTON, G.; ATMOS. ENVIRON. 38(2004) 1447 - 1458 !\Comment: WARNING
NC3H7O2+IC3H7O2=>NC3H7O+IC3H7O+O2    4.0E9 0.0 0.0E0
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
NC3H7O2+CH3CO3=>NC3H7O+CH3CO2+O2    1.4E16 -1.61 1.86E3
!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+RO2(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
NC3H7O2+CH3=NC3H7O+CH3O    7.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
NC3H7O2+C2H5=NC3H7O+C2H5O    7.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
NC3H7O2+IC3H7=NC3H7O+IC3H7O    7.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
NC3H7O2+NC3H7=2NC3H7O    7.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
NC3H7O2+C3H5-A=NC3H7O+C3H5O    2.6E13 0.0 -1.0E3
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RH+R_ABSTRACTION
!_____________________________________________________________________________________________________
!\Author: SP !\Ref: TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887(1988) !\Comment: WARNING
C3H8+IC3H7=NC3H7+C3H8    8.44E-3 4.2 8.724E3
!\Author: SP !\Ref: TSANG 1988 !\Comment: WARNING
C3H8+O2=NC3H7+HO2    3.97E13 0.0 5.09E4
!\Author: SP WARNING !\Ref: SIVARAMAKRISHNAN ET AL., INT. J. CHEMICAL KINETIC 44.3(2012) !\Comment: WARNING
C3H8+H=NC3H7+H2    1.29E4 2.93 5.24568E3
   DUP
!\Author: SP WARNING !\Ref: SIVARAMAKRISHNAN ET AL., INT. J. CHEMICAL KINETIC 44.3(2012) !\Comment: WARNING
C3H8+H=NC3H7+H2    1.47E10 1.31 1.03E4
   DUP
!\Author: SP WARNING !\Ref: SIVARAMAKRISHNAN ET AL., INT. J. CHEMICAL KINETIC 44.3(2012) !\Comment: WARNING
C3H8+H=IC3H7+H2    3.06E4 2.8 3.473276E3
   DUP
!\Author: SP WARNING !\Ref: SIVARAMAKRISHNAN ET AL., INT. J. CHEMICAL KINETIC 44.3(2012) !\Comment: WARNING
C3H8+H=IC3H7+H2    5.73E13 0.1 1.06E4
   DUP
!\Author: WARNING !\Ref: COHEN, N.; WESTBERG, K.R., THE USE OF TRANSITION-STATE THEORY TO EXTRAPOLATE RATE COEFFICIENTS FOR REACTIONS OF O ATOMS WITH ALKANES,
C3H8+O=NC3H7+OH    3.71E6 2.4 5.505E3
!\Author: SP !\Ref: FAROOQ ET AL., SITE-SPECIFIC RATE CONSTANT MEASUREMENTS FOR PRIMARY AND SECONDARY H-ABSTRACTION BY OH RADICALS !\Comment: WARNING
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C3H8+OH=NC3H7+H2O 6.86508E6 2.0 6.7730869E2
!\Author: SP !\Ref: NEW FIT !\Comment: WARNING
C3H8+OH=IC3H7+H2O 3.73838198E5 2.30514 -5.6132233E2
!\Author: SP !\Ref: 60% OF NEW FIT !\Comment: WARNING
C3H8+HO2=NC3H7+H2O2 2.08E1 3.59 1.56E4
!\Author: WARNING !\Ref: J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A(2008) 112(30) !\Comment: WARNING
C3H8+HO2=IC3H7+H2O2 6.32E1 3.37 1.372E4
!\Author: WARNING !\Ref: FIT TO NIST DATABASE !\Comment: WARNING
C3H8+CH3=IC3H7+CH4 1.51E0 3.46 5.48E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H8+CH3=NC3H7+CH4 3.45E1 3.44 1.04E4
!\Author: SP !\Ref: RAMAN, CARSTENSEN, INT J CHEM KINET 44.5(2012) !\Comment: WARNING
C3H8+C2H3=NC3H7+C2H4 8.4E2 3.05 6.0E3
!\Author: SP !\Ref: RATKIEWICZ, HUYNH, PHAM, TRUONG, THEOR CHEM ACC(2013) 132 !\Comment: WARNING
C3H8+C2H5=NC3H7+C2H6 3.132E-1 3.76 9.5858E3
!\Author: WARNING !\Ref: DAGAUT ET AL., CST 71, 111(1990) !\Comment: WARNING
C3H8+C3H5-A=NC3H7+C3H6 7.94E11 0.0 2.05E4
!\Author: WARNING !\Ref: DRYER ESTIMATE !\Comment: WARNING
C3H8+CH3O=NC3H7+CH3OH 3.0E11 0.0 7.0E3
!\Author: SP !\Ref: H-H CARSTENSEN, A.M. DEAN, O. DEUTSCHMANN, PROC. COMBUST. INST. 31(2007) 149-157 !\Comment: WARNING
C3H8+CH3O2=NC3H7+CH3O2H 6.71E0 3.72 1.69E4
!\Author: SP !\Ref: H-H CARSTENSEN, A.M. DEAN, O. DEUTSCHMANN, PROC. COMBUST. INST. 31(2007) 149-157 !\Comment: WARNING
C3H8+C2H5O2=NC3H7+C2H5O2H 7.14E0 3.65 1.71E4
!\Author: WARNING !\Ref: ANALOGY TO C2H6+C2H5O2 !\Comment: WARNING
C3H8+NC3H7O2=NC3H7+NC3H7O2H 7.14E0 3.65 1.71E4
!\Author: WARNING !\Ref: ANALOGY TO C2H6+C2H5O2 !\Comment: WARNING
C3H8+IC3H7O2=NC3H7+IC3H7O2H 7.14E0 3.65 1.71E4
!\Author: WARNING !\Ref: ANALOGY TO C2H6+HO2 !\Comment: WARNING
C3H8+CH3CO3=NC3H7+CH3CO3H 2.08E1 3.59 1.56E4
!\Author: SP !\Ref: HO2 !\Comment: WARNING
C3H8+O2CHO=NC3H7+HO2CHO 2.08E1 3.59 1.56E4
!\Author: SP ! !\Ref: TSANG 1988 !\Comment: WARNING
C3H8+O2=IC3H7+HO2 3.97E13 0.0 4.77E4
!\Author: WARNING !\Ref: COHEN, N.; WESTBERG, K.R. INT. J. CHEM. KINET., 99-140(1986) !\Comment: WARNING
C3H8+O=IC3H7+OH 5.49E5 2.5 3.14E3
!\Author: SP !\Ref: RAMAN, CARSTENSEN, INT J CHEM KINET 44.5(2012) !\Comment: WARNING
C3H8+C2H3=IC3H7+C2H4 1.02E3 2.92 4.2E3
!\Author: SP !\Ref: RATKIEWICZ, HUYNH, PHAM, TRUONG, THEOR CHEM ACC(2013) 132 !\Comment: WARNING
C3H8+C2H5=IC3H7+C2H6 1.566E-1 3.71 6.5554E3
!\Author: WARNING !\Ref: DAGAUT ET AL., CST 71, 111(1990) !\Comment: WARNING
C3H8+C3H5-A=IC3H7+C3H6 7.94E11 0.0 1.62E4
!\Author: WARNING !\Ref: DRYER ESTIMATE !\Comment: WARNING
C3H8+CH3O=IC3H7+CH3OH 3.0E11 0.0 7.0E3
!\Author: SP !\Ref: H-H CARSTENSEN, A.M. DEAN, O. DEUTSCHMANN, PROC. COMBUST. INST. 31(2007) 149-157 !\Comment: WARNING
C3H8+C2H5O2=IC3H7+C2H5O2H 4.02E1 3.41 1.41E4
!\Author: SP !\Ref: C2H5O2 !\Comment: WARNING
C3H8+CH3O2=IC3H7+CH3O2H 4.02E1 3.41 1.41E4
!\Author: WARNING !\Ref: WALKER, R. W., REACTION KINETICS, VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975 !\Comment: WARNING
C3H8+NC3H7O2=IC3H7+NC3H7O2H 2.0E12 0.0 1.7E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H8+CH3CO3=IC3H7+CH3CO3H 6.32E1 3.37 1.372E4
!\Author: HO2 !\Ref: WARNING !\Comment: WARNING
C3H8+O2CHO=IC3H7+HO2CHO 6.32E1 3.37 1.372E4
!\Author: WARNING !\Ref: WALKER, R. W., REACTION KINETICS, VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975 !\Comment: WARNING
C3H8+IC3H7O2=IC3H7+IC3H7O2H 2.0E12 0.0 1.7E4
!_____
!\REACTIONCLASS: R+R(=)PRODUCTS
!_____
!\Author: WARNING !\Ref: GLAUDE,P.A. ET AL,PROC. COMBUST. INST !\Comment: WARNING
IC3H7+H=C2H5+CH3 2.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887(1988) !\Comment: WARNING
IC3H7+OH=C3H6+H2O 2.41E13 0.0 0.0E0
!\Author: SP !\Ref: HOYERMANN, ET AL PCI 33, 283-291(2011) !\Comment: WARNING
IC3H7+O=CH3COCH3+H 4.1E13 0.0 0.0E0
!\Author: SP !\Ref: HOYERMANN, ET AL PCI 33, 283-291(2011) !\Comment: WARNING

IC3H7+O=CH3CHO+CH3 4.56E13 0.0 0.0E0
!\Author: SP !\Ref: HOYERMANN, ET AL PCI 33, 283-291(2011) !\Comment: WARNING
IC3H7+O=C3H6+OH 2.74E13 0.0 0.0E0
!_____
!\REACTIONCLASS: R+RO2(=)PRODUCTS
!_____
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NC3H7+HO2=NC3H7O+OH 2.58E16 -1.178 1.148E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NC3H7+CH3O2=NC3H7O+CH3O 2.58E16 -1.178 1.148E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC3H7+HO2=IC3H7O+OH 2.58E16 -1.178 1.148E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC3H7+CH3O2=IC3H7O+CH3O 2.58E16 -1.178 1.148E2
!_____
!\REACTIONCLASS: R+O2(=)PRODUCTS
!_____
!\Author: UB !\Ref: C. FRANKLIN GOLDSMITH, W.H. GREEN, S.J. KLIPPENSTEIN, J. PHYS. CHEM. A. 116, 2012, 3325-3346 !\Comment: WARNING
O2+NC3H7=HO2+C3H6 7.37E2 2.71 5.49647E3
  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/
!\Author: UB !\Ref: C. FRANKLIN GOLDSMITH, W.H. GREEN, S.J. KLIPPENSTEIN, J. PHYS. CHEM. A. 116, 2012, 3325-3346 !\Comment: WARNING
O2+IC3H7=HO2+C3H6 9.84E7 1.34 5.37912E3
  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/
!\Author: UB !\Ref: C. FRANKLIN GOLDSMITH, W.H. GREEN, S.J. KLIPPENSTEIN, J. PHYS. CHEM. A. 116, 2012, 3325-3346 !\Comment: WARNING
O2+NC3H7=C3H6OOH1-3 6.58E-15 7.8 -3.43101E3
  PLOG/1.0E-2 3.09E146 -4.59E1 3.12822E4/
  PLOG/1.0E-2 6.19E8 8.78E-1 1.11866E4/
  PLOG/1.0E-1 1.26E47 -1.24E1 8.20313E3/
  PLOG/1.0E-1 1.12E14 -5.31E-1 1.38975E4/
  PLOG/1.0E0 1.3E23 -4.03E0 5.08867E3/
  PLOG/1.0E0 2.07E14 -4.0E-1 1.51581E4/
  PLOG/1.0E1 3.94E-18 8.88E0 -6.1997E3/
  PLOG/1.0E1 1.02E21 -2.26E0 1.8554E4/
  PLOG/1.0E2 6.58E-15 7.8E0 -3.43101E3/
  PLOG/1.0E2 1.05E15 -4.86E-1 1.58767E4/
!_____
!\REACTIONCLASS: R+O2(=)RO2
!_____
!\Author: UB !\Ref: C. FRANKLIN GOLDSMITH, W.H. GREEN, S.J. KLIPPENSTEIN, J. PHYS. CHEM. A. 116, 2012, 3325-3346 !\Comment: WARNING
O2+NC3H7=NC3H7O2 2.07001E16 -1.3 8.03419E2
  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/
!\Author: UB !\Ref: C. FRANKLIN GOLDSMITH, W.H. GREEN, S.J. KLIPPENSTEIN, J. PHYS. CHEM. A. 116, 2012, 3325-3346 !\Comment: WARNING
O2+IC3H7=IC3H7O2 1.67E29 -5.15 5.03645E3
  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/
!_____
!\REACTIONCLASS: RO2(=)ALKENE_HO2
!_____
!\Author: UB !\Ref: C. FRANKLIN GOLDSMITH, W.H. GREEN, S.J. KLIPPENSTEIN, J. PHYS. CHEM. A. 116, 2012, 3325-3346 !\Comment: WARNING
NC3H7O2=HO2+C3H6 2.26E32 -6.22 3.79482E4

PLOG/1.0E-2 4.3E53 -1.4E1 3.9526E4/
PLOG/1.0E-1 9.52E57 -1.5E1 4.26843E4/
PLOG/1.0E0 7.9E33 -7.03E0 3.65435E4/
PLOG/1.0E1 2.55E16 -1.22E0 3.24803E4/
PLOG/1.0E2 2.26E32 -6.22E0 3.79482E4/
!\Author: UB !\Ref: C. FRANKLIN GOLDSMITH, W.H. GREEN, S.J. KLIPPENSTEIN, J. PHYS. CHEM. A. 116, 2012, 3325-3346 !\Comment: WARNING
IC3H7O2=C3H6+HO2 6.4E25 -4.02 3.49139E4
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/
!\Author: UB !\Ref: C. FRANKLIN GOLDSMITH, W.H. GREEN, S.J. KLIPPENSTEIN, J. PHYS. CHEM. A. 116, 2012, 3325-3346 !\Comment: REFIT BY SJK 03 / 05 / 17
NC3H7O2=C3H6OOH1-3 7.15E0 3.12 1.934E4
PLOG/1.0E-2 6.38E6 7.5E-1 1.955E4/
PLOG/1.0E-1 3.85E6 1.07E0 2.024E4/
PLOG/1.0E0 1.5E3 2.32E0 1.98E4/
PLOG/1.0E1 1.44E4 2.06E0 2.02E4/
PLOG/1.0E2 7.87E0 3.12E0 1.93E4/
!\Author: UB !\Ref: C. FRANKLIN GOLDSMITH, W.H. GREEN, S.J. KLIPPENSTEIN, J. PHYS. CHEM. A. 116, 2012, 3325-3346 !\Comment: WARNING
C3H6OOH1-3=HO2+C3H6 3.45E17 -2.82 2.15791E4
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/
!_____
!\REACTIONCLASS: QOOH+O2(=)O2QOOH
!_____
!\Author: UB !\Ref: C. FRANKLIN GOLDSMITH, W.H. GREEN, S.J. KLIPPENSTEIN, J. PHYS. CHEM. A. 116, 2012, 3325-3346 !\Comment: WARNING
O2+C3H6OOH1-3=C3H6OOH1-3O2 1.46E18 -1.85 1.00584E3
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/
!_____
!\REACTIONCLASS: QOOH+O2(=)PRODUCTS
!_____
!\Author: SP !\Ref: C. FRANKLIN GOLDSMITH, W.H. GREEN, S.J. KLIPPENSTEIN, J. PHYS. CHEM. A. 116, 2012, 3325-3346 !\Comment: WARNING
O2+C3H6OOH1-3=>2OH+OCHCH2CH2O 6.32E0 3.02 1.62507E3
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/
!\Author: UB !\Ref: C. FRANKLIN GOLDSMITH, W.H. GREEN, S.J. KLIPPENSTEIN, J. PHYS. CHEM. A. 116, 2012, 3325-3346 !\Comment: WARNING
O2+C3H6OOH1-3=HO2+AC3H5OOH 6.76E-4 4.57 4.46375E3
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/
!_____
!\REACTIONCLASS: O2QOOH(=)PRODUCTS
!_____
!\Author: UB !\Ref: C. FRANKLIN GOLDSMITH, W.H. GREEN, S.J. KLIPPENSTEIN, J. PHYS. CHEM. A. 116, 2012, 3325-3346 !\Comment: WARNING
C3H6OOH1-3O2=C3KET13+OH 1.67E5 1.48 1.62379E4
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/
!\Author: UB !\Ref: C. FRANKLIN GOLDSMITH, W.H. GREEN, S.J. KLIPPENSTEIN, J. PHYS. CHEM. A. 116, 2012, 3325-3346 !\Comment: WARNING

C3H6OOH1-3O2=HO2+AC3H5OOH 1.96E16 -1.27 3.09174E4
  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/
!_____
!\REACTIONCLASS: KHP_HOMOLYTIC_FISSION
!_____
!\Author: SP !\Ref: C. FRANKLIN GOLDSMITH, W.H. GREEN, S.J. KLIPPENSTEIN, J. PHYS. CHEM. A. 116, 2012, 3325-3346 !\Comment: INCREASED EA
C3KET13=OCHCH2CH2O+OH 4.06E33 -5.54 4.95254E4
  PLOG/1.0E-2 3.41E64 -1.59E1 5.70614E4/
  PLOG/1.0E-1 1.97E61 -1.46E1 5.73115E4/
  PLOG/1.0E0 1.07E54 -1.21E1 5.58628E4/
  PLOG/1.0E1 5.29E43 -8.74E0 5.28685E4/
  PLOG/1.0E2 4.06E33 -5.54E0 4.95254E4/
!\Author: UB !\Ref: C. FRANKLIN GOLDSMITH, W.H. GREEN, S.J. KLIPPENSTEIN, J. PHYS. CHEM. A. 116, 2012, 3325-3346 !\Comment: ESTIMATED AS
PROD_4(=)FRAG_4+OH
C3KET21=CH3COCH2O+OH 1.03E31 -4.76 4.89219E4
  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 5.55804E4/
  PLOG/1.0E1 1.56E41 -7.97E0 5.2321E4/
  PLOG/1.0E2 1.03E31 -4.76E0 4.89219E4/
!\Author: SP !\Ref: C. FRANKLIN GOLDSMITH, W.H. GREEN, S.J. KLIPPENSTEIN, J. PHYS. CHEM. A. 116, 2012, 3325-3346 !\Comment: WARNING
OCHCH2CH2O=CH2O+CH2CHO 4.94E10 0.857 5.8092E3
!\Author: SP !\Ref: C. FRANKLIN GOLDSMITH, W.H. GREEN, S.J. KLIPPENSTEIN, J. PHYS. CHEM. A. 116, 2012, 3325-3346 !\Comment: WARNING
CH3COCH2O=CH3CO+CH2O 5.73E13 -0.0247 4.47348E3
!\Author: SP !\Ref: TSANG 1988 !\Comment: WARNING
NC3H7+H=C3H6+H2 1.81E12 0.0 0.0E0
!\Author: SP !\Ref: TSANG 1988 !\Comment: WARNING
NC3H7+OH=C3H6+H2O 2.4E13 0.0 0.0E0
!\Author: SP !\Ref: TSANG 1988 !\Comment: WARNING
NC3H7+CH3=CH4+C3H6 1.1E13 0.0 0.0E0
!===
!\ENDSUBSPECIES: NC3H7
!===
!===
!\SUBSPECIES: IC3H7
!===
!_____
!\REACTIONCLASS: KHP_HOMOLYTIC_FISSION
!_____
!\Author: SP !\Ref: TSANG 1988 !\Comment: WARNING
IC3H7+H=C3H6+H2 3.61E12 0.0 0.0E0
!\Author: SP !\Ref: TSANG 1988 !\Comment: WARNING
IC3H7+C3H5-A=C3H8+C3H4-A 4.58E12 -0.35 -1.31E2
!\Author: SP !\Ref: NIST !\Comment: WARNING
IC3H7+C2H4=C3H6+C2H5 2.65E10 0.0 6.598E3
!===
!\ENDSUBSPECIES: IC3H7
!===
!===
!\SUBSPECIES: NC3H7O2H
!===
!_____
!\REACTIONCLASS: RH(=)PRODUCTS
!_____
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
NC3H7O2H=NC3H7O+OH 1.05E19 -1.09 4.44E4
!_____
!\REACTIONCLASS: RH+R_ABSTRACTION
!_____
!\Author: WARNING !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
NC3H7O2+H2=NC3H7O2H+H 3.01E13 0.0 2.603E4

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!\Author: WARNING !\Ref: TSANG, JPC REF. DATA, 16 !\Comment: WARNING
NC3H7O2+HO2=NC3H7O2H+O2    1.75E10 0.0 -3.275E3
!\Author: WARNING !\Ref: ANALOGY TO CH2O+HO2 !\Comment: WARNING
NC3H7O2+CH2O=NC3H7O2H+HCO    5.6E12 0.0 1.36E4
!\Author: SP\REF !\Ref: WARNING !\Comment: WARNING
NC3H7O2+CH4=NC3H7O2H+CH3    7.0E-1 3.95 2.14E4
!\Author: WARNING !\Ref: ANALOGY TO CH3OH+HO2 !\Comment: WARNING
NC3H7O2+CH3OH=NC3H7O2H+CH2OH    6.3E12 0.0 1.936E4
!\Author: WARNING !\Ref: HALF OF CH2O+HO2 !\Comment: WARNING
NC3H7O2+CH3CHO=NC3H7O2H+CH3CO    2.8E12 0.0 1.36E4
!\Author: WARNING !\Ref: ANALOGY TO C2H4+HO2 !\Comment: WARNING
NC3H7O2+C2H4=NC3H7O2H+C2H3    1.13E13 0.0 3.043E4
!\Author: SP !\Ref: H-H CARSTENSEN, A.M. DEAN, O. DEUTSCHMANN, PROC. COMBUST. INST. 31(2007) 149-157 !\Comment: WARNING
NC3H7O2+C2H6=NC3H7O2H+C2H5    2.7E0 3.81 1.72E4
!\Author: WARNING !\Ref: HALF OF CH2O+HO2 !\Comment: WARNING
NC3H7O2+C2H3CHO=NC3H7O2H+C2H3CO    2.8E12 0.0 1.36E4
!=============================================================================================================
!\ENDSUBSPECIES: NC3H7O2H
!=============================================================================================================
!=============================================================================================================
!\SUBSPECIES: IC3H7O2H
!=============================================================================================================
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: RH(=)PRODUCTS
!_____________________________________________________________________________________________________________
!\Author: WARNING !\Ref: PITZ ESTIMATE !\Comment: WARNING
IC3H7O+OH=IC3H7O2H    1.0E15 -0.8 0.0E0
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: RH+R_ABSTRACTION
!_____________________________________________________________________________________________________________
!\Author: WARNING !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
IC3H7O2+H2=IC3H7O2H+H    3.01E13 0.0 2.603E4
!\Author: WARNING !\Ref: TSANG, JPC REF. DATA, 16 !\Comment: WARNING
IC3H7O2+HO2=IC3H7O2H+O2    1.75E10 0.0 -3.275E3
!\Author: WARNING !\Ref: ANALOGY TO CH2O+HO2 !\Comment: WARNING
IC3H7O2+CH2O=IC3H7O2H+HCO    5.6E12 0.0 1.36E4
!\Author: SP !\Ref: H-H CARSTENSEN, A.M. DEAN, O. DEUTSCHMANN, PROC. COMBUST. INST. 31(2007) 149-157 !\Comment: WARNING
IC3H7O2+CH4=IC3H7O2H+CH3    3.06E0 3.87 2.18E4
!\Author: WARNING !\Ref: HALF OF CH2O+HO2 !\Comment: WARNING
IC3H7O2+CH3CHO=IC3H7O2H+CH3CO    2.8E12 0.0 1.36E4
!\Author: WARNING !\Ref: ANALOGY TO C2H4+HO2 !\Comment: WARNING
IC3H7O2+C2H4=IC3H7O2H+C2H3    1.13E13 0.0 3.043E4
!\Author: WARNING !\Ref: ANALOGY TO CH3OH+HO2 !\Comment: WARNING
IC3H7O2+CH3OH=IC3H7O2H+CH2OH    6.3E12 0.0 1.936E4
!\Author: SP !\Ref: H-H CARSTENSEN, A.M. DEAN, O. DEUTSCHMANN, PROC. COMBUST. INST. 31(2007) 149-157 !\Comment: WARNING
IC3H7O2+C2H6=IC3H7O2H+C2H5    1.06E1 3.69 1.75E4
!\Author: WARNING !\Ref: HALF OF CH2O+HO2 !\Comment: WARNING
IC3H7O2+C2H3CHO=IC3H7O2H+C2H3CO    2.8E12 0.0 1.36E4
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: RO2+RO2(=)PRODUCTS
!_____________________________________________________________________________________________________________
!\Author: SP !\Ref: JOHNSON, D.; PRICE, D.W.; MARSTON, G.; ATMOS. ENVIRON. 38(2004) 1447 - 1458 !\Comment: WARNING
IC3H7O2+CH3O2=>IC3H7O+CH3O+O2    6.2E9 0.0 0.0E0
!\Author: SP !\Ref: JOHNSON, D.; PRICE, D.W.; MARSTON, G.; ATMOS. ENVIRON. 38(2004) 1447 - 1458 !\Comment: WARNING
IC3H7O2+CH3O2=>CH3COCH3+CH3OH+O2    6.2E9 0.0 0.0E0
!\Author: SP !\Ref: JOHNSON, D.; PRICE, D.W.; MARSTON, G.; ATMOS. ENVIRON. 38(2004) 1447 - 1458 !\Comment: WARNING
IC3H7O2+C2H5O2=>IC3H7O+C2H5O+O2    1.02E9 0.0 0.0E0
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
2IC3H7O2=>2IC3H7O+O2    1.4E16 -1.61 1.86E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
IC3H7O2+CH3CO3=>IC3H7O+CH3CO2+O2    1.4E16 -1.61 1.86E3
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: R+RO2(=)PRODUCTS
!_____________________________________________________________________________________________________________
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
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IC3H7O2+CH3=IC3H7O+CH3O 7.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
IC3H7O2+C2H5=IC3H7O+C2H5O 7.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
IC3H7O2+IC3H7=2IC3H7O 7.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
IC3H7O2+NC3H7=IC3H7O+NC3H7O 7.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2CHO+H=CH3CHO 1.0E14 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CO+H=CH3CHO 1.0E14 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2(S)+C2H4=C3H6 6.07E47 -9.85 2.21E4
   PLOG/1.0E-2 4.82E57 -1.43E1 1.71E4/
   PLOG/1.0E-2 1.15E45 -1.11E1 6.1452E3/
   PLOG/1.0E-1 3.84E59 -1.44E1 1.84E4/
   PLOG/1.0E-1 1.83E45 -1.07E1 6.6385E3/
   PLOG/1.0E0 2.13E58 -1.35E1 2.04E4/
   PLOG/1.0E0 1.3E40 -8.77E0 5.8638E3/
   PLOG/1.0E1 8.48E52 -1.16E1 2.07E4/
   PLOG/1.0E1 2.27E32 -6.14E0 4.3179E3/
   PLOG/1.0E2 6.07E47 -9.85E0 2.21E4/
   PLOG/1.0E2 1.28E24 -3.49E0 2.5299E3/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2(S)+C2H4=C3H5-A+H 6.51E26 -3.58 1.89E4
   PLOG/1.0E-2 8.2E19 -2.06E0 1.15E3/
   PLOG/1.0E-2 1.08E7 1.62E0 -3.1746E3/
   PLOG/1.0E-1 2.27E21 -2.44E0 2.65E3/
   PLOG/1.0E-1 1.37E5 2.15E0 -3.7992E3/
   PLOG/1.0E0 4.44E35 -6.55E0 1.39E4/
   PLOG/1.0E0 3.89E14 -4.2E-1 1.2376E3/
   PLOG/1.0E1 1.18E28 -4.09E0 1.4E4/
   PLOG/1.0E1 2.45E10 6.7E-1 7.5093E2/
   PLOG/1.0E2 6.51E26 -3.58E0 1.89E4/
   PLOG/1.0E2 1.81E2 2.97E0 -7.4603E2/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2(S)+C2H4=C2H3+CH3 7.36E29 -4.28 2.38E4
   PLOG/1.0E-2 1.77E19 -1.94E0 6.79E3/
   PLOG/1.0E-2 4.3E12 1.9E-1 -1.1041E2/
   PLOG/1.0E-1 1.68E19 -1.8E0 4.31E3/
   PLOG/1.0E-1 2.26E11 5.4E-1 4.781E1/
   PLOG/1.0E0 4.16E24 -3.19E0 9.76E3/
   PLOG/1.0E0 4.92E9 1.02E0 5.9977E2/
   PLOG/1.0E1 7.89E24 -3.07E0 1.39E4/
   PLOG/1.0E1 1.47E8 1.33E0 1.2284E3/
   PLOG/1.0E2 7.36E29 -4.28E0 2.38E4/
   PLOG/1.0E2 8.11E10 5.5E-1 5.5065E3/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H3+CH3=C3H5-A+H 5.16E28 -4.03 2.38E4
   PLOG/1.0E-2 4.12E29 -4.95E0 8.0E3/
   PLOG/1.0E-2 5.73E15 -7.7E-1 1.1959E3/
   PLOG/1.0E-1 4.86E30 -5.03E0 1.13E4/
   PLOG/1.0E-1 2.06E13 -7.4E-2 1.4287E3/
   PLOG/1.0E0 5.3E29 -4.57E0 1.44E4/
   PLOG/1.0E0 4.48E10 6.0E-1 1.4216E3/
   PLOG/1.0E1 1.32E30 -4.54E0 1.93E4/
   PLOG/1.0E1 4.1E6 1.71E0 1.0569E3/
   PLOG/1.0E2 5.16E28 -4.03E0 2.38E4/
   PLOG/1.0E2 1.37E-1 3.91E0 -3.5355E2/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H6=C2H3+CH3 2.15E64 -13.4 1.35E5
   PLOG/1.0E-2 1.88E78 -1.87E1 1.3E5/
   PLOG/1.0E-2 1.69E59 -1.36E1 1.1329E5/
   PLOG/1.0E-1 8.73E76 -1.79E1 1.32E5/
   PLOG/1.0E-1 2.0E60 -1.37E1 1.1489E5/

PLOG/1.0E0 5.8E75 -1.72E1 1.34E5/
PLOG/1.0E0 6.7E54 -1.18E1 1.1384E5/
PLOG/1.0E1 8.12E71 -1.58E1 1.36E5/
PLOG/1.0E1 1.06E47 -9.27E0 1.1151E5/
PLOG/1.0E2 2.15E64 -1.34E1 1.35E5/
PLOG/1.0E2 7.29E38 -6.7E0 1.0874E5/
!\Author: WARNING !\Ref: YE, GEORGIEVSKII, KLIPPENSTEIN, PROC. COMBUST. 35(2015) 223-230 !\Comment: WARNING
C3H6=C3H5-A+H 8.05E56 -11.5 1.22E5
PLOG/1.0E-2 9.16E74 -1.76E1 1.2E5/
PLOG/1.0E-2 2.98E54 -1.23E1 1.012E5/
PLOG/1.0E-1 1.73E70 -1.6E1 1.2E5/
PLOG/1.0E-1 1.37E43 -8.87E0 9.6365E4/
PLOG/1.0E0 1.08E71 -1.59E1 1.2486E5/
PLOG/1.0E0 6.28E42 -8.51E0 9.8004E4/
PLOG/1.0E1 6.4E65 -1.42E1 1.25E5/
PLOG/1.0E1 4.73E35 -6.26E0 9.5644E4/
PLOG/1.0E2 8.05E56 -1.15E1 1.22E5/
PLOG/1.0E2 4.34E28 -4.06E0 9.3114E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H5-T+H=C3H6 1.15E50 -10.4 2.33E4
PLOG/1.0E-2 4.96E60 -1.52E1 1.8E4/
PLOG/1.0E-2 1.49E48 -1.2E1 7.2033E3/
PLOG/1.0E-1 3.2E62 -1.51E1 2.01E4/
PLOG/1.0E-1 6.76E46 -1.11E1 7.6299E3/
PLOG/1.0E0 2.31E60 -1.4E1 2.19E4/
PLOG/1.0E0 1.09E40 -8.66E0 6.4478E3/
PLOG/1.0E1 3.69E54 -1.2E1 2.21E4/
PLOG/1.0E1 2.38E31 -5.73E0 4.506E3/
PLOG/1.0E2 1.15E50 -1.04E1 2.33E4/
PLOG/1.0E2 5.69E25 -3.83E0 3.2504E3/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H5-T+H=C3H5-A+H 2.28E29 -4.12 2.09E4
PLOG/1.0E-2 2.11E17 -1.08E0 1.29E3/
PLOG/1.0E-2 6.41E3 2.61E0 -3.7784E3/
PLOG/1.0E-1 9.05E29 -4.91E0 8.54E3/
PLOG/1.0E-1 5.19E14 -3.0E-1 1.0904E3/
PLOG/1.0E0 2.98E30 -4.79E0 1.2E4/
PLOG/1.0E0 8.17E11 4.9E-1 1.1846E3/
PLOG/1.0E1 8.22E28 -4.14E0 1.54E4/
PLOG/1.0E1 2.79E9 1.09E0 1.1875E3/
PLOG/1.0E2 2.28E29 -4.12E0 2.09E4/
PLOG/1.0E2 6.75E3 2.7E0 3.738E2/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H5-T+H=C2H3+CH3 3.15E32 -4.83 2.6E4
PLOG/1.0E-2 3.31E16 -6.9E-1 5.2E3/
PLOG/1.0E-2 8.04E13 -1.4E-1 1.15E3/
PLOG/1.0E-1 9.04E16 -8.1E-1 4.8E3/
PLOG/1.0E-1 7.17E10 6.7E-1 6.738E2/
PLOG/1.0E0 2.01E24 -2.86E0 1.09E4/
PLOG/1.0E0 9.97E8 1.36E0 1.5964E3/
PLOG/1.0E1 2.75E26 -3.31E0 1.58E4/
PLOG/1.0E1 7.41E7 1.57E0 2.1088E3/
PLOG/1.0E2 3.15E32 -4.83E0 2.6E4/
PLOG/1.0E2 2.7E12 3.2E-1 6.7918E3/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H5-S+H=C3H6 1.42E14 -0.06 2.4E1
PLOG/1.0E-2 5.82E56 -1.428E1 1.6407E4/
PLOG/1.0E-2 1.95E45 -1.14E1 6.309E3/
PLOG/1.0E-1 1.24E62 -1.522E1 1.9112E4/
PLOG/1.0E-1 2.65E48 -1.175E1 7.584E3/
PLOG/1.0E0 3.77E60 -1.424E1 2.0603E4/
PLOG/1.0E0 4.28E42 -9.54E0 6.789E3/
PLOG/1.0E1 9.1E56 -1.274E1 2.2284E4/
PLOG/1.0E1 4.44E34 -6.79E0 5.17E3/
PLOG/1.0E2 6.39E49 -1.035E1 2.1902E4/

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   PLOG/1.0E2 5.11E26 -4.13E0 3.313E3/
   PLOG/1.0E3 1.42E14 -6.0E-2 2.4E1/
   PLOG/1.0E3 4.42E11 6.5E-1 -3.06E2/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H5-S+H=C3H5-A+H    3.74E28 -3.92 1.8561E4
   PLOG/1.0E-2 3.47E16 -8.4E-1 7.11E2/
   PLOG/1.0E-2 4.53E2 2.94E0 -4.342E3/
   PLOG/1.0E-1 1.47E21 -2.26E0 3.18E3/
   PLOG/1.0E-1 3.31E11 5.9E-1 -7.49E2/
   PLOG/1.0E0 1.75E30 -4.82E0 1.0284E4/
   PLOG/1.0E0 1.59E13 1.6E-1 9.63E2/
   PLOG/1.0E1 7.23E28 -4.17E0 1.3614E4/
   PLOG/1.0E1 1.24E10 9.8E-1 8.42E2/
   PLOG/1.0E2 3.74E28 -3.92E0 1.8561E4/
   PLOG/1.0E2 1.36E6 2.06E0 4.47E2/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H5-S+H=C2H3+CH3    9.72E30 -4.44 2.2834E4
   PLOG/1.0E-2 1.43E16 -5.9E-1 4.573E3/
   PLOG/1.0E-2 4.31E13 -1.0E-2 4.35E2/
   PLOG/1.0E-1 1.76E15 -3.14E-1 3.087E3/
   PLOG/1.0E-1 9.21E13 -2.2E-1 7.82E2/
   PLOG/1.0E0 2.09E22 -2.34E0 8.157E3/
   PLOG/1.0E0 9.24E9 1.12E0 8.44E2/
   PLOG/1.0E1 1.76E25 -3.01E0 1.3177E4/
   PLOG/1.0E1 4.4E8 1.41E0 1.351E3/
   PLOG/1.0E2 9.72E30 -4.44E0 2.2834E4/
   PLOG/1.0E2 6.46E12 2.2E-1 5.469E3/
!_____
!\REACTIONCLASS: RH+R_ABSTRACTION
!_____
!\Author: WARNING !\Ref: J.A.MILLER, S.J.KLIPPENSTEIN, J.PHYS.CHEM.A, 117(2013) 2718-2727 !\Comment: REFIT TO REMOVE NEGATIVE A-FACTOR
C3H6+H=C3H5-A+H2    3.644E5 2.455 4.3612E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H6+O2=C3H5-A+HO2    6.62E17 -1.16 4.51E4
!\Author: SP !\Ref: BEDJANIAN, MORIN, J. PHYS. CHEM. A 2017, 121, 1553-1562 !\Comment: WARNING
C3H6+O=C3H5-A+OH    9.68E-3 4.54 -2.4684E3
!\Author: SP !\Ref: WARNING !\Comment: WARNING
C3H6+OH=C3H5-A+H2O    2.1E7 1.77 2.71E2
!\Author: SP !\Ref: ZADOR, KLIPPENSTEIN, AND MILLER - J. PHYS. CHEM. A, 2011, 115(36), PP 10218-10225 !\Comment: WARNING
C3H6+HO2=C3H5-A+H2O2    7.71E-2 4.4 1.3547E4
!\Author: WARNING !\Ref: TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887(1988) !\Comment: ADDED FROM LLNL PAH
C3H6+CH3=C3H5-A+CH4    5.52E1 3.27 7.15E3
!\Author: WARNING !\Ref: BILL !\Comment: WARNING
C3H6+CH3O=C3H5-A+CH3OH    8.4E10 0.0 2.6E3
!\Author: WARNING !\Ref: ANALOGY TO C3H6+HO2 !\Comment: WARNING
C3H6+CH3O2=C3H5-A+CH3O2H    7.71E-2 4.4 1.45E4
C3H6+C2H5O2=C3H5-A+C2H5O2H    7.68E-2 4.4 1.55E4
!\Author: WARNING !\Ref: ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523(1980) !\Comment: WARNING !C3H6+C2H5O2(=)C3H5-
A+C2H5O2H +7.68000000E-002 +
C3H6+C2H5=C3H5-A+C2H6    1.0E11 0.0 9.8E3
!\Author: WARNING !\Ref: ANALOGY TO C3H6+HO2 !\Comment: WARNING
C3H6+CH3CO3=C3H5-A+CH3CO3H    7.68E-2 4.403 1.35472E4
C3H6+IC3H7O2=C3H5-A+IC3H7O2H    7.68E-2 4.4 1.65E4
C3H6+NC3H7O2=C3H5-A+NC3H7O2H    7.68E-2 4.4 1.65E4
!\Author: WARNING !\Ref: J.A.MILLER, S.J.KLIPPENSTEIN, J.PHYS.CHEM.A, 117(2013) 2718-2727 !\Comment: WARNING
C3H6+H=C3H5-T+H2    1.498E2 3.381 8.9095E3
!\Author: WARNING !\Ref: ANALOGY WITH C2H4 !\Comment: WARNING
C3H6+O=C3H5-T+OH    6.03E10 0.7 7.632E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H6+OH=C3H5-T+H2O    8.37E12 0.0 4.51049E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H6+OH=C3H5-S+H2O    4.34E12 0.0 4.534334E3
!\Author: WARNING !\Ref: C3 NUIG CALCULATION J.M !\Comment: WARNING
C3H6+HO2=C3H5-T+H2O2    1.56E4 2.82 2.44279E4
!\Author: WARNING !\Ref: ESTIMATE C3 NUIG S. M. BURKE !\Comment: WARNING
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C3H6+O2=C3H5-T+HO2    1.0E13 0.0 5.877E4
!\Author: WARNING !\Ref: TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887(1988) !\Comment: ADDED FROM LLNL PAH
C3H6+CH3=C3H5-T+CH4    8.9E1 3.29 1.46E4
!\Author: WARNING !\Ref: J.A.MILLER, S.J.KLIPPENSTEIN, J.PHYS.CHEM.A, 117(2013) 2718-2727 !\Comment: WARNING
C3H6+H=C3H5-S+H2    5.101E2 3.234 1.2357E4
   DUP
!\Author: WARNING !\Ref: J.A.MILLER, S.J.KLIPPENSTEIN, J.PHYS.CHEM.A, 117(2013) 2718-2727 !\Comment: WARNING
C3H6+H=C3H5-S+H2    3.969E2 3.252 1.2007E4
   DUP
!\Author: WARNING !\Ref: ESTIMATE C3 NUIG S. M. BURKE !\Comment: WARNING
C3H6+O2=C3H5-S+HO2    2.0E13 0.0 6.227E4
!\Author: WARNING !\Ref: ANALOGY WITH C2H4 !\Comment: WARNING
C3H6+O=C3H5-S+OH    1.2E11 0.7 8.9591E3
!\Author: WARNING !\Ref: C3 NUIG CALCULATION J.M !\Comment: WARNING
C3H6+HO2=C3H5-S+H2O2    9.57E2 3.059 2.07986E4
!\Author: SP !\Ref: KUN, CBS-QB3 03.2014 !\Comment: WARNING
C3H6+CH3=C3H5-S+CH4    7.19E2 2.938 1.3913E4
!\Author: WARNING !\Ref: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325? 3346 !\Comment: WARNING
C3H5-S+CH2O=C3H6+HCO    1.65E1 3.17 9.3998E3
!\Author: SP !\Ref: RAMAN, CARSTENSEN, INT J CHEM KINET 44.5(2012) !\Comment: WARNING
C3H6+C2H3=C3H5-S+C2H4    9.4E1 3.13 8.3E3
!\Author: SP !\Ref: RAMAN, CARSTENSEN, INT J CHEM KINET 44.5(2012) !\Comment: WARNING
C3H6+C2H3=C3H5-T+C2H4    2.9E2 3.03 6.2E3
!\Author: SP !\Ref: RAMAN, CARSTENSEN, INT J CHEM KINET 44.5(2012) !\Comment: WARNING
C3H6+C2H3=C3H5-A+C2H4    5.4E1 3.34 3.0E3
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONO
!_____________________________________________________________________________________________________
!\Author: SP !\Ref: BEDJANIAN, MORIN, J. PHYS. CHEM. A 2017, 121, 1553-1562 !\Comment: WARNING
C3H6+O=CH3CHCHO+H    1.17E-3 4.94 -2.4228E3
!\Author: SP !\Ref: BEDJANIAN, MORIN, J. PHYS. CHEM. A 2017, 121, 1553-1562 !\Comment: WARNING
C3H6+O=CH3COCH2+H    1.17E-3 4.94 -2.4228E3
!\Author: SP !\Ref: BEDJANIAN, MORIN, J. PHYS. CHEM. A 2017, 121, 1553-1562 !\Comment: WARNING
C3H6+O=CH2CHO+CH3    9.24E8 1.2 -2.383E2
!\Author: SP !\Ref: BEDJANIAN, MORIN, J. PHYS. CHEM. A 2017, 121, 1553-1562 !\Comment: WARNING
C3H6+O=C2H5+HCO    6.23E9 0.79 -1.47E2
!\Author: SP !\Ref: BEDJANIAN, MORIN, J. PHYS. CHEM. A 2017, 121, 1553-1562 !\Comment: WARNING
C3H6+O=C2H4+CH2O    1.46E5 2.365 -8.321E2
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONH
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: J.A.MILLER, S.J.KLIPPENSTEIN, J.PHYS.CHEM.A 117(2013) 2718-2727 !\Comment: WARNING
C3H6+H=NC3H7    4.22E27 -4.39 9.3458E3
   PLOG/1.3E-3 7.99E81 -2.3161E1 2.2239E4/
   PLOG/1.3E-3 1.85E26 -5.83E0 3.8658E3/
   PLOG/4.0E-2 4.24E68 -1.8427E1 1.9665E4/
   PLOG/4.0E-2 2.82E30 -6.49E0 5.4708E3/
   PLOG/1.0E0 1.04E49 -1.15E1 1.5359E4/
   PLOG/1.0E0 3.78E28 -5.57E0 5.6251E3/
   PLOG/1.0E1 6.2E41 -8.892E0 1.4637E4/
   PLOG/1.0E1 1.46E25 -4.28E0 5.2478E3/
   PLOG/1.0E2 4.22E27 -4.39E0 9.3458E3/
   PLOG/1.0E2 1.0E-10 0.0E0 0.0E0/
!\Author: WARNING !\Ref: J.A.MILLER, S.J.KLIPPENSTEIN, J.PHYS.CHEM.A 117(2013) 2718-2727 !\Comment: WARNING
C3H6+H=C2H4+CH3    1.32E23 -2.42 1.65E4
   PLOG/1.3E-3 1.54E9 1.35E0 2.542E3/
   PLOG/1.3E-3 1.0E-10 0.0E0 0.0E0/
   PLOG/4.0E-2 7.88E10 8.7E-1 3.5996E3/
   PLOG/4.0E-2 1.0E-10 0.0E0 0.0E0/
   PLOG/1.0E0 2.67E12 4.7E-1 5.4311E3/
   PLOG/1.0E0 1.0E-10 0.0E0 0.0E0/
   PLOG/1.0E1 9.25E22 -2.6E0 1.2898E4/
   PLOG/1.0E1 1.24E5 2.52E0 3.6791E3/
   PLOG/1.0E2 1.32E23 -2.42E0 1.65E4/
   PLOG/1.0E2 2.51E3 2.91E0 3.9809E3/
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!\Author: WARNING !\Ref: J.A.MILLER, S.J.KLIPPENSTEIN, J.PHYS.CHEM.A 117(2013) 2718-2727 !\Comment: WARNING
C3H6+H=IC3H7    1.11E50 -10.8 2.0202E4
   PLOG/1.3E-3 1.35E44 -1.068E1 8.1964E3/
   PLOG/1.3E-3 2.17E130 -3.258E1 1.3614E5/
   PLOG/4.0E-2 2.11E57 -1.423E1 1.5147E4/
   PLOG/4.0E-2 2.25E29 -5.84E0 4.2419E3/
   PLOG/1.0E0 3.26E61 -1.494E1 2.0161E4/
   PLOG/1.0E0 1.06E30 -5.63E0 5.6134E3/
   PLOG/1.0E1 5.3E56 -1.312E1 2.0667E4/
   PLOG/1.0E1 6.11E26 -4.44E0 5.1823E3/
   PLOG/1.0E2 1.11E50 -1.08E1 2.0202E4/
   PLOG/1.0E2 2.73E23 -3.26E0 4.597E3/
!\Author: WARNING !\Ref: J.A.MILLER, S.J.KLIPPENSTEIN, J.PHYS.CHEM.A 117(2013) 2718-2727 !\Comment: WARNING
C2H4+CH3=NC3H7    2.04E40 -8.25 2.4214E4
   PLOG/1.3E-3 8.67E48 -1.254E1 1.8206E4/
   PLOG/1.3E-3 1.12E43 -1.13E1 1.308E4/
   PLOG/4.0E-2 1.06E49 -1.204E1 2.0001E4/
   PLOG/4.0E-2 7.28E39 -9.88E0 1.3164E4/
   PLOG/1.0E0 7.67E47 -1.117E1 2.2366E4/
   PLOG/1.0E0 2.6E33 -7.46E0 1.2416E4/
   PLOG/1.0E1 1.81E45 -1.003E1 2.3769E4/
   PLOG/1.0E1 3.85E27 -5.38E0 1.1455E4/
   PLOG/1.0E2 2.04E40 -8.25E0 2.4214E4/
   PLOG/1.0E2 1.66E21 -3.17E0 1.0241E4/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+R(=)RH+RH
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: KLIPPENSTEIN _ HARDING 2007 !\Comment: WARNING
C3H5-A+H=C3H4-A+H2    1.232E3 3.035 2.582E3
!\Author: WARNING !\Ref: TSANG, W. J.PHYS.CHEM.REF.DATA 1991, 20, 221. !\Comment: WARNING
C3H5-A+OH=C3H4-A+H2O    6.0E12 0.0 0.0E0
!\Author: WARNING !\Ref: LASKIN ET AL. IJCK 32 589-614 2000 !\Comment: WARNING
C3H5-A+CH3=C3H4-A+CH4    3.0E12 -0.32 -1.31E2
!\Author: WARNING !\Ref: DAGAUT, P. ET AL., CST 71, 111(1990). !\Comment: WARNING
C3H5-A+C2H5=C3H4-A+C2H6    4.0E11 0.0 0.0E0
!\Author: WARNING !\Ref: DAGAUT, P. ET AL., CST 71, 111(1990). !\Comment: WARNING
C3H5-A+C2H3=C3H4-A+C2H4    1.0E12 0.0 0.0E0
!\Author: WARNING !\Ref: ZIEGLER ET AL. J. ANAL.APPLY.PYROLYSIS 73 212-230(2005) !\Comment: WARNING
2C3H4-A=C3H5-A+C3H3    5.0E14 0.0 6.47467E4
!\Author: WARNING !\Ref: DAGAUT, P. ET AL., CST 71, 111(1990). !\Comment: WARNING
C3H5-S+CH3=C3H4-A+CH4    1.0E11 0.0 0.0E0
!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+R(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: FRIDLYAND ET AL. J. PHYS. CHEM. A, 2013, 117, 4762-4776 !\Comment: WARNING
2C3H5-A=C3H4-A+C3H6    1.46E28 -5.5 7.41E3
   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/
!\Author: WARNING !\Ref: DAGAUT, P. ET AL., CST 71, 111(1990). !\Comment: WARNING
C3H5-A+C2H5=C2H4+C3H6    4.0E11 0.0 0.0E0
!\Author: WARNING !\Ref: LASKIN ET AL. IJCK 32 589-614 2000 !\Comment: WARNING
C3H5-A+HCO=C3H6+CO    6.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: LASKIN ET AL. IJCK 32 589-614 2000 !\Comment: WARNING
C3H5-S+HCO=C3H6+CO    9.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: LASKIN ET AL. IJCK 32 589-614 2000 !\Comment: WARNING
C3H5-S+O=C2H4+HCO    6.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: LASKIN ET AL. IJCK 32 589-614 2000 !\Comment: WARNING
C3H5-S+OH=>C2H4+HCO+H    5.0E12 0.0 0.0E0
!\Author: WARNING !\Ref: LASKIN ET AL. IJCK 32 589-614 2000 !\Comment: WARNING
C3H5-S+HO2=>C2H4+HCO+OH    2.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: LASKIN ET AL. IJCK 32 589-614 2000 !\Comment: WARNING
C3H5-T+O=CH3+CH2CO    6.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: LASKIN ET AL. IJCK 32 589-614 2000 !\Comment: WARNING
C3H5-T+OH=>CH3+CH2CO+H    5.0E12 0.0 0.0E0
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!\Author: WARNING !\Ref: LASKIN ET AL. IJCK 32 589-614 2000 !\Comment: WARNING
C3H5-T+HO2=>CH3+CH2CO+OH    2.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: LASKIN ET AL. IJCK 32 589-614 2000 !\Comment: WARNING
C3H5-T+HCO=C3H6+CO    9.0E13 0.0 0.0E0
!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+O(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: TSANG, W. J.PHYS.CHEM.REF.DATA 1991, 20, 221. !\Comment: WARNING
C3H5-A+O=C2H3CHO+H    6.0E13 0.0 0.0E0
!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+OH(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: TSANG, W. J.PHYS.CHEM.REF.DATA 1991, 20, 221. !\Comment: WARNING
C3H5-A+OH=>C2H3CHO+2H    1.6E20 -1.56 2.633E4
   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/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+O2(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: LASKIN ET AL. IJCK 32 589-614 2000 !\Comment: WARNING
C3H5-A+O2=C3H4-A+HO2    2.18E21 -2.85 3.0755E4
   PLOG/1.0E0 4.99E15 -1.4E0 2.2428E4/
   PLOG/1.0E1 2.18E21 -2.85E0 3.0755E4/
!\Author: WARNING !\Ref: LASKIN ET AL. IJCK 32 589-614 2000 !\Comment: WARNING
C3H5-A+O2=CH3CO+CH2O    7.14E15 -1.21 2.1046E4
   PLOG/1.0E0 1.19E15 -1.01E0 2.0128E4/
   PLOG/1.0E1 7.14E15 -1.21E0 2.1046E4/
!\Author: WARNING !\Ref: LASKIN ET AL. IJCK 32 589-614 2000 !\Comment: WARNING
C3H5-A+O2=C2H3CHO+OH    2.47E13 -0.45 2.3017E4
   PLOG/1.0E0 1.82E13 -4.1E-1 2.2859E4/
   PLOG/1.0E1 2.47E13 -4.5E-1 2.3017E4/
!\Author: SP WARNING !\Ref: X. CHEN AND F. GOLDSMITH(2017) !\Comment: WARNING
C3H5-S+O2=SC3H5OO    8.1E29 -5.32 6.909E3
   PLOG/1.0E-2 4.71E26 -6.57E0 6.937E3/
   PLOG/1.0E-1 2.51E34 -8.4E0 4.828E3/
   PLOG/3.16E-1 9.99E37 -9.13E0 5.553E3/
   PLOG/1.0E0 1.28E40 -9.39E0 6.832E3/
   PLOG/3.16E0 8.2E39 -8.99E0 7.829E3/
   PLOG/1.0E1 4.15E37 -8.01E0 8.148E3/
   PLOG/3.16E1 8.57E33 -6.68E0 7.744E3/
   PLOG/1.0E2 8.1E29 -5.32E0 6.909E3/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H5-S+O2=CH3CHCHO+O    3.47E13 -0.24 8.639E3
   PLOG/1.0E-2 1.84E9 8.3E-1 1.963E3/
   PLOG/1.0E-1 2.34E9 8.1E-1 2.049E3/
   PLOG/3.16E-1 4.1E9 7.4E-1 2.25E3/
   PLOG/1.0E0 1.91E10 5.5E-1 2.807E3/
   PLOG/3.16E0 4.47E11 1.8E-1 4.014E3/
   PLOG/1.0E1 2.99E13 -3.1E-1 5.862E3/
   PLOG/3.16E1 3.85E14 -5.9E-1 7.713E3/
   PLOG/1.0E2 3.47E13 -2.4E-1 8.639E3/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H5-S+O2=C2H3CHO+OH    8.16E16 -1.34 7.005E3
   PLOG/1.0E-2 4.51E14 -8.5E-1 1.319E3/
   PLOG/1.0E-1 4.73E14 -8.5E-1 1.337E3/
   PLOG/3.16E-1 6.2E14 -8.9E-1 1.43E3/
   PLOG/1.0E0 2.46E15 -1.05E0 1.912E3/
   PLOG/3.16E0 7.29E16 -1.46E0 3.194E3/
   PLOG/1.0E1 4.24E18 -1.93E0 5.094E3/
   PLOG/3.16E1 1.18E19 -2.01E0 6.666E3/
   PLOG/1.0E2 8.16E16 -1.34E0 7.005E3/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H5-S+O2=CH2O+CH3CO    1.11E16 -1.48 6.906E3
   PLOG/1.0E-2 8.0E14 -1.31E0 1.709E3/
```

```
   PLOG/1.0E-1 8.24E14 -1.31E0 1.718E3/
   PLOG/3.16E-1 1.05E15 -1.34E0 1.797E3/
   PLOG/1.0E0 4.18E15 -1.51E0 2.274E3/
   PLOG/3.16E0 2.3E18 -2.27E0 4.429E3/
   PLOG/1.0E1 3.06E17 -2.0E0 4.528E3/
   PLOG/3.16E1 4.91E18 -2.29E0 6.709E3/
   PLOG/1.0E2 1.11E16 -1.48E0 6.906E3/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H5-S+O2=CH3CHO+HCO    1.32E21 -2.49 8.439E3
   PLOG/1.0E-2 3.03E18 -1.9E0 2.187E3/
   PLOG/1.0E-1 3.05E18 -1.9E0 2.186E3/
   PLOG/3.16E-1 3.73E18 -1.93E0 2.246E3/
   PLOG/1.0E0 1.5E19 -2.1E0 2.712E3/
   PLOG/3.16E0 5.19E20 -2.52E0 4.032E3/
   PLOG/1.0E1 1.49E22 -2.9E0 5.752E3/
   PLOG/3.16E1 1.56E23 -3.14E0 7.824E3/
   PLOG/1.0E2 1.32E21 -2.49E0 8.439E3/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H5-S+O2=CO2+C2H5    9.18E18 -2.39 8.508E3
   PLOG/1.0E-2 1.66E16 -1.77E0 2.16E3/
   PLOG/1.0E-1 1.69E16 -1.77E0 2.164E3/
   PLOG/3.16E-1 2.12E16 -1.8E0 2.236E3/
   PLOG/1.0E0 8.51E16 -1.97E0 2.709E3/
   PLOG/3.16E0 2.85E18 -2.39E0 4.025E3/
   PLOG/1.0E1 1.2E20 -2.81E0 5.858E3/
   PLOG/3.16E1 6.93E20 -2.98E0 7.748E3/
   PLOG/1.0E2 9.18E18 -2.39E0 8.508E3/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H5-S+O2=CH2OH+CH2CO    6.81E7 0.63 3.59E3
   PLOG/1.0E-2 9.08E9 -1.3E-1 6.34E2/
   PLOG/1.0E-1 9.69E9 -1.3E-1 6.584E2/
   PLOG/3.16E-1 1.31E10 -1.7E-1 7.658E2/
   PLOG/1.0E0 5.31E10 -3.4E-1 1.261E3/
   PLOG/3.16E0 3.72E12 -8.5E-1 2.82E3/
   PLOG/1.0E1 3.19E7 6.0E-1 -2.62E1/
   PLOG/3.16E1 3.09E11 -4.7E-1 4.106E3/
   PLOG/1.0E2 6.81E7 6.3E-1 3.59E3/
!\Author: WARNING !\Ref: GOLDSMITH ET AL, J. PHYS. CHEM. A 2015, 119, 7766-7779 !\Comment: WARNING
C3H5-T+O2=TC3H5OO    3.41E39 -8.04 1.436E4
   PLOG/1.0E-2 1.55E24 -5.45E0 9.662E3/
   PLOG/1.0E-2 1.78E-9 4.15E0 -4.707E3/
   PLOG/1.0E-1 3.48E56 -1.501E1 1.916E4/
   PLOG/1.0E-1 2.36E22 -4.52E0 2.839E3/
   PLOG/3.16E-1 1.25E64 -1.697E1 2.129E4/
   PLOG/3.16E-1 2.0E26 -5.43E0 2.725E3/
   PLOG/1.0E0 3.34E61 -1.579E1 2.015E4/
   PLOG/1.0E0 6.13E28 -5.89E0 3.154E3/
   PLOG/3.16E0 7.34E53 -1.311E1 1.73E4/
   PLOG/3.16E0 2.14E29 -5.8E0 3.52E3/
   PLOG/1.0E1 4.16E48 -1.121E1 1.6E4/
   PLOG/1.0E1 3.48E28 -5.37E0 3.636E3/
   PLOG/3.16E1 2.33E43 -9.38E0 1.481E4/
   PLOG/3.16E1 3.32E27 -4.95E0 3.61E3/
   PLOG/1.0E2 3.41E39 -8.04E0 1.436E4/
   PLOG/1.0E2 1.03E27 -4.72E0 3.68E3/
!\Author: UB !\Ref: GOLDSMITH ET AL, J. PHYS. CHEM. A 2015, 119, 7766-7779 !\Comment: WARNING
C3H5-T+O2=CH3COCH2+O    9.27E25 -3.8 1.391E4
   PLOG/1.0E-2 7.16E20 -2.67E0 6.742E3/
   PLOG/1.0E-2 1.24E10 6.2E-1 -2.776E2/
   PLOG/1.0E-1 7.02E20 -2.67E0 6.713E3/
   PLOG/1.0E-1 1.29E10 6.2E-1 -2.477E2/
   PLOG/3.16E-1 8.97E20 -2.7E0 6.724E3/
   PLOG/3.16E-1 1.51E10 6.0E-1 -1.625E2/
   PLOG/1.0E0 6.45E20 -2.65E0 6.489E3/
   PLOG/1.0E0 1.84E10 5.8E-1 3.84E1/
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   PLOG/3.16E0 4.09E20 -2.53E0 6.406E3/
   PLOG/3.16E0 8.86E9 6.7E-1 2.48E2/
   PLOG/1.0E1 1.6E23 -3.22E0 8.697E3/
   PLOG/1.0E1 6.67E9 7.2E-1 7.781E2/
   PLOG/3.16E1 2.85E25 -3.77E0 1.153E4/
   PLOG/3.16E1 1.43E9 9.2E-1 1.219E3/
   PLOG/1.0E2 9.27E25 -3.8E0 1.391E4/
   PLOG/1.0E2 7.14E7 1.28E0 1.401E3/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H5-T+O2=C3H4-A+HO2    1.83E8 1.11 1.024E4
   PLOG/1.0E-2 1.48E7 1.28E0 4.732E3/
   PLOG/1.0E-1 1.05E7 1.33E0 4.929E3/
   PLOG/3.16E-1 4.15E6 1.45E0 4.916E3/
   PLOG/1.0E0 2.55E6 1.53E0 5.139E3/
   PLOG/3.16E0 6.14E6 1.43E0 5.931E3/
   PLOG/1.0E1 4.39E7 1.22E0 7.305E3/
   PLOG/3.16E1 3.59E8 9.9E-1 8.997E3/
   PLOG/1.0E2 1.83E8 1.11E0 1.024E4/
!\Author: UB !\Ref: GOLDSMITH ET AL, J. PHYS. CHEM. A 2015, 119, 7766-7779 !\Comment: WARNING
C3H5-T+O2=CH2O+CH3CO    3.03E33 -6.28 1.6E4
   PLOG/1.0E-2 2.77E36 -7.6E0 1.264E4/
   PLOG/1.0E-2 5.04E15 -1.28E0 5.153E2/
   PLOG/1.0E-1 2.7E36 -7.6E0 1.261E4/
   PLOG/1.0E-1 5.1E15 -1.28E0 5.13E2/
   PLOG/3.16E-1 2.17E36 -7.57E0 1.249E4/
   PLOG/3.16E-1 5.34E15 -1.29E0 5.206E2/
   PLOG/1.0E0 3.03E35 -7.32E0 1.182E4/
   PLOG/1.0E0 6.76E15 -1.31E0 6.457E2/
   PLOG/3.16E0 1.59E36 -7.47E0 1.246E4/
   PLOG/3.16E0 1.05E16 -1.36E0 1.066E3/
   PLOG/1.0E1 5.76E35 -7.2E0 1.343E4/
   PLOG/1.0E1 2.84E15 -1.18E0 1.429E3/
   PLOG/3.16E1 3.54E20 -2.57E0 5.578E3/
   PLOG/3.16E1 1.14E69 -1.923E1 1.476E4/
   PLOG/1.0E2 3.03E33 -6.28E0 1.6E4/
   PLOG/1.0E2 4.68E10 1.9E-1 8.306E2/
!\Author: UB !\Ref: GOLDSMITH ET AL, J. PHYS. CHEM. A 2015, 119, 7766-7779 !\Comment: WARNING
C3H5-T+O2=>CH2O+CH3+CO    7.07E33 -6.28 1.6E4
   PLOG/1.0E-2 6.47E36 -7.6E0 1.264E4/
   PLOG/1.0E-2 1.18E16 -1.28E0 5.153E2/
   PLOG/1.0E-1 6.29E36 -7.6E0 1.261E4/
   PLOG/1.0E-1 1.19E16 -1.28E0 5.13E2/
   PLOG/3.16E-1 5.06E36 -7.57E0 1.249E4/
   PLOG/3.16E-1 1.26E16 -1.29E0 5.206E2/
   PLOG/1.0E0 7.07E35 -7.32E0 1.182E4/
   PLOG/1.0E0 1.58E16 -1.31E0 6.457E2/
   PLOG/3.16E0 3.72E36 -7.47E0 1.246E4/
   PLOG/3.16E0 2.44E16 -1.36E0 1.066E3/
   PLOG/1.0E1 1.34E36 -7.2E0 1.343E4/
   PLOG/1.0E1 6.64E15 -1.18E0 1.429E3/
   PLOG/3.16E1 8.26E20 -2.57E0 5.578E3/
   PLOG/3.16E1 2.66E69 -1.923E1 1.476E4/
   PLOG/1.0E2 7.07E33 -6.28E0 1.6E4/
   PLOG/1.0E2 1.09E11 1.9E-1 8.306E2/
!\Author: WARNING !\Ref: GOLDSMITH ET AL, J. PHYS. CHEM. A 2015, 119, 7766-7779 !\Comment: WARNING
C3H5-T+O2=C2H5+CO2    1.21E32 -6.32 1.619E4
   PLOG/1.0E-2 2.37E35 -7.76E0 1.263E4/
   PLOG/1.0E-2 6.27E13 -1.16E0 4.063E2/
   PLOG/1.0E-1 1.73E35 -7.72E0 1.252E4/
   PLOG/1.0E-1 6.24E13 -1.16E0 4.014E2/
   PLOG/3.16E-1 4.47E34 -7.55E0 1.214E4/
   PLOG/3.16E-1 6.12E13 -1.16E0 3.97E2/
   PLOG/1.0E0 7.25E31 -6.7E0 1.044E4/
   PLOG/1.0E0 5.32E13 -1.14E0 4.467E2/
   PLOG/3.16E0 3.63E35 -7.75E0 1.283E4/
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   PLOG/3.16E0 1.45E14 -1.26E0 9.877E2/
   PLOG/1.0E1 2.09E35 -7.53E0 1.405E4/
   PLOG/1.0E1 5.02E13 -1.11E0 1.409E3/
   PLOG/3.16E1 3.84E18 -2.44E0 5.408E3/
   PLOG/3.16E1 1.4E70 -2.011E1 1.543E4/
   PLOG/1.0E2 1.21E32 -6.32E0 1.619E4/
   PLOG/1.0E2 9.21E8 2.5E-1 8.553E2/
!\Author: SP !\Ref: ANALOGY TO C2H3OO(=)CH2CHO+O !\Comment: WARNING
TC3H5OO=CH3COCH2+O    4.3E48 -10.31 5.609E4
   PLOG/1.0E-2 2.7E180 -4.819E1 1.693E5/
   PLOG/1.0E-2 1.47E30 -6.64E0 4.111E4/
   PLOG/1.0E-1 3.9E38 -8.69E0 4.277E4/
   PLOG/1.0E-1 9.65E-12 5.96E0 2.289E4/
   PLOG/3.16E-1 4.57E47 -1.121E1 4.705E4/
   PLOG/3.16E-1 3.95E22 -3.71E0 3.627E4/
   PLOG/1.0E0 7.62E81 -2.128E1 6.508E4/
   PLOG/1.0E0 2.39E33 -6.62E0 4.128E4/
   PLOG/3.16E0 1.86E68 -1.683E1 6.068E4/
   PLOG/3.16E0 6.37E31 -5.96E0 4.126E4/
   PLOG/1.0E1 2.02E55 -1.269E1 5.584E4/
   PLOG/1.0E1 2.13E29 -5.1E0 4.071E4/
   PLOG/3.16E1 1.11E53 -1.179E1 5.669E4/
   PLOG/3.16E1 4.66E27 -4.5E0 4.053E4/
   PLOG/1.0E2 4.3E48 -1.031E1 5.609E4/
   PLOG/1.0E2 5.99E25 -3.85E0 4.012E4/
!\Author: SP !\Ref: ANALOGY TO C2H3OO(=)CO2+CH3 !\Comment: WARNING
TC3H5OO=C2H5+CO2    7.01E37 -8.06 4.22E4
   PLOG/1.0E-1 1.21E118 -3.313E1 7.379E4/
   PLOG/1.0E-1 1.96E29 -6.29E0 3.092E4/
   PLOG/3.16E-1 8.56E32 -7.21E0 3.355E4/
   PLOG/3.16E-1 5.1E-66 2.137E1 -1.111E4/
   PLOG/1.0E0 3.27E33 -7.22E0 3.499E4/
   PLOG/1.0E0 1.76E-47 1.585E1 -5.283E3/
   PLOG/1.0E1 8.16E32 -6.76E0 3.727E4/
   PLOG/1.0E1 4.62E0 2.1E0 1.717E4/
   PLOG/3.16E1 7.01E37 -8.06E0 4.22E4/
   PLOG/3.16E1 3.49E14 -1.58E0 2.647E4/
!\Author: SP !\Ref: ANALOGY TO C2H3OO(=)CH2O+HCO !\Comment: WARNING
TC3H5OO=CH2O+CH3CO    5.7E29 -5.19 3.68E4
   PLOG/1.0E-2 1.66E174 -5.552E1 6.032E4/
   PLOG/1.0E-2 2.27E35 -7.97E0 3.128E4/
   PLOG/1.0E-1 9.03E66 -1.725E1 4.812E4/
   PLOG/1.0E-1 2.08E26 -4.96E0 2.878E4/
   PLOG/3.16E-1 1.82E43 -9.87E0 3.796E4/
   PLOG/3.16E-1 1.45E20 -3.08E0 2.663E4/
   PLOG/1.0E0 8.64E33 -6.88E0 3.437E4/
   PLOG/1.0E0 1.06E130 -3.938E1 5.47E4/
   PLOG/3.16E0 7.29E171 -4.353E1 1.919E5/
   PLOG/3.16E0 2.35E34 -6.87E0 3.57E4/
   PLOG/1.0E1 1.03E32 -6.06E0 3.55E4/
   PLOG/1.0E1 2.18E175 -5.378E1 6.85E4/
   PLOG/3.16E1 1.85E34 -6.57E0 3.851E4/
   PLOG/3.16E1 1.07E185 -5.422E1 8.899E4/
   PLOG/1.0E2 5.7E29 -5.19E0 3.68E4/
   PLOG/1.0E2 4.68E2 1.81E0 1.81E4/
!\Author: SP !\Ref: C2H3OO=)CH2O+H+CO GOLDSMITH ET AL, J. PHYS. CHEM. A 2015, 119, 7766-7779 !\Comment: WARNING
TC3H5OO=>CH2O+CH3+CO    1.33E30 -5.19 3.68E4
   PLOG/1.0E-2 3.88E174 -5.552E1 6.032E4/
   PLOG/1.0E-2 5.29E35 -7.97E0 3.128E4/
   PLOG/1.0E-1 2.11E67 -1.725E1 4.812E4/
   PLOG/1.0E-1 4.85E26 -4.96E0 2.878E4/
   PLOG/3.16E-1 4.26E43 -9.87E0 3.796E4/
   PLOG/3.16E-1 3.37E20 -3.08E0 2.663E4/
   PLOG/1.0E0 2.02E34 -6.88E0 3.437E4/
   PLOG/1.0E0 2.46E130 -3.938E1 5.47E4/
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PLOG/3.16E0 1.7E172 -4.353E1 1.919E5/
PLOG/3.16E0 5.49E34 -6.87E0 3.57E4/
PLOG/1.0E1 2.4E32 -6.06E0 3.55E4/
PLOG/1.0E1 5.09E175 -5.378E1 6.85E4/
PLOG/3.16E1 4.32E34 -6.57E0 3.851E4/
PLOG/3.16E1 2.49E185 -5.422E1 8.899E4/
PLOG/1.0E2 1.33E30 -5.19E0 3.68E4/
PLOG/1.0E2 1.09E3 1.81E0 1.81E4/
!\Author: SP !\Ref: ANALOGY TO C2H3OO(=)CH2CHO+O !\Comment: WARNING
SC3H5OO=CH3CHCHO+O 4.3E48 -10.31 5.609E4
PLOG/1.0E-2 2.7E180 -4.819E1 1.693E5/
PLOG/1.0E-2 1.47E30 -6.64E0 4.111E4/
PLOG/1.0E-1 3.9E38 -8.69E0 4.277E4/
PLOG/1.0E-1 9.65E-12 5.96E0 2.289E4/
PLOG/3.16E-1 4.57E47 -1.121E1 4.705E4/
PLOG/3.16E-1 3.95E22 -3.71E0 3.627E4/
PLOG/1.0E0 7.62E81 -2.128E1 6.508E4/
PLOG/1.0E0 2.39E33 -6.62E0 4.128E4/
PLOG/3.16E0 1.86E68 -1.683E1 6.068E4/
PLOG/3.16E0 6.37E31 -5.96E0 4.126E4/
PLOG/1.0E1 2.02E55 -1.269E1 5.584E4/
PLOG/1.0E1 2.13E29 -5.1E0 4.071E4/
PLOG/3.16E1 1.11E53 -1.179E1 5.669E4/
PLOG/3.16E1 4.66E27 -4.5E0 4.053E4/
PLOG/1.0E2 4.3E48 -1.031E1 5.609E4/
PLOG/1.0E2 5.99E25 -3.85E0 4.012E4/
!\Author: SP !\Ref: ANALOGY TO C2H3OO(=)CH2O+HCO !\Comment: WARNING
SC3H5OO=CH2O+CH3CO 5.7E29 -5.19 3.68E4
PLOG/1.0E-2 1.66E174 -5.552E1 6.032E4/
PLOG/1.0E-2 2.27E35 -7.97E0 3.128E4/
PLOG/1.0E-1 9.03E66 -1.725E1 4.812E4/
PLOG/1.0E-1 2.08E26 -4.96E0 2.878E4/
PLOG/3.16E-1 1.82E43 -9.87E0 3.796E4/
PLOG/3.16E-1 1.45E20 -3.08E0 2.663E4/
PLOG/1.0E0 8.64E33 -6.88E0 3.437E4/
PLOG/1.0E0 1.06E130 -3.938E1 5.47E4/
PLOG/3.16E0 7.29E171 -4.353E1 1.919E5/
PLOG/3.16E0 2.35E34 -6.87E0 3.57E4/
PLOG/1.0E1 1.03E32 -6.06E0 3.55E4/
PLOG/1.0E1 2.18E175 -5.378E1 6.85E4/
PLOG/3.16E1 1.85E34 -6.57E0 3.851E4/
PLOG/3.16E1 1.07E185 -5.422E1 8.899E4/
PLOG/1.0E2 5.7E29 -5.19E0 3.68E4/
PLOG/1.0E2 4.68E2 1.81E0 1.81E4/
!\Author: SP !\Ref: C2H3OO=)CH2O+H+CO GOLDSMITH ET AL, J. PHYS. CHEM. A 2015, 119, 7766-7779 !\Comment: WARNING
SC3H5OO=>CH2O+CH3+CO 1.33E30 -5.19 3.68E4
PLOG/1.0E-2 3.88E174 -5.552E1 6.032E4/
PLOG/1.0E-2 5.29E35 -7.97E0 3.128E4/
PLOG/1.0E-1 2.11E67 -1.725E1 4.812E4/
PLOG/1.0E-1 4.85E26 -4.96E0 2.878E4/
PLOG/3.16E-1 4.26E43 -9.87E0 3.796E4/
PLOG/3.16E-1 3.37E20 -3.08E0 2.663E4/
PLOG/1.0E0 2.02E34 -6.88E0 3.437E4/
PLOG/1.0E0 2.46E130 -3.938E1 5.47E4/
PLOG/3.16E0 1.7E172 -4.353E1 1.919E5/
PLOG/3.16E0 5.49E34 -6.87E0 3.57E4/
PLOG/1.0E1 2.4E32 -6.06E0 3.55E4/
PLOG/1.0E1 5.09E175 -5.378E1 6.85E4/
PLOG/3.16E1 4.32E34 -6.57E0 3.851E4/
PLOG/3.16E1 2.49E185 -5.422E1 8.899E4/
PLOG/1.0E2 1.33E30 -5.19E0 3.68E4/
PLOG/1.0E2 1.09E3 1.81E0 1.81E4/
!_____
!\REACTIONCLASS: R+HO2(=)PRODUCTS
!_____

!\Author: WARNING !\Ref: FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325?346 \COMMENT !\Comment: WARNING
C3H5-A+HO2=C3H5O+OH 1.64E4 2.74 1.1444E3
  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/
!\Author: WARNING !\Ref: FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325?346 \COMMENT !\Comment: WARNING
C3H5-A+HO2=AC3H5OOH 1.44E32 -6.01 6.0536E3
  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/
!\Author: WARNING !\Ref: FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325?346 \COMMENT !\Comment: WARNING
C3H5-A+HO2=C2H3CHO+H2O 5.07E-5 4.59 9.275E2
  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/
!\Author: WARNING !\Ref: FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325?346 \COMMENT !\Comment: WARNING
AC3H5OOH=C2H3CHO+H2O 1.48E16 -1.12 4.59493E4
  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/
!\Author: WARNING !\Ref: FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325?346 \COMMENT !\Comment: DECOMP BELONGS TO THE
ALLYL+HO2 MECHANISM.
AC3H5OOH=C3H5O+OH 1.28E27 -3.61 4.63331E4
  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/
!\Author: WARNING !\Ref: FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325?346 \COMMENT !\Comment: WARNING
C3H5O=C2H3+CH2O 8.52E25 -3.61 2.78634E4
  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/
!\Author: WARNING !\Ref: FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325?346 \COMMENT !\Comment: WARNING
C3H5O=CH2CH2CHO 1.67E21 -2.74 2.03377E4
  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/
!\Author: WARNING !\Ref: FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325?346 \COMMENT !\Comment: WARNING
C3H5O=C2H3CHO+H 2.57E20 -2.06 2.20401E4
  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/
!\Author: WARNING !\Ref: FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325?346 \COMMENT !\Comment: WARNING
C3H5O=C2H4+HCO 4.75E8 1.14 2.09225E4

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/
!\Author: WARNING !\Ref: FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325?346 \COMMENT !\Comment: WARNING
CH2CH2CHO=C2H3+CH2O 1.93E19 -1.94 4.844E4
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/
!\Author: WARNING !\Ref: FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325?346 \COMMENT !\Comment: WARNING
CH2CH2CHO=C2H3CHO+H 4.52E12 0.214 3.45705E4
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/
!\Author: WARNING !\Ref: FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325?346 \COMMENT !\Comment: WARNING
CH2CH2CHO=C2H4+HCO 1.59E13 0.063 2.40863E4
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/
!\Author: WARNING !\Ref: FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325?346 \COMMENT !\Comment: WARNING
C2H3+CH2O=C2H3CHO+H 6.01E5 2.09 7.8956E3
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/
!\Author: WARNING !\Ref: FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325?346 \COMMENT !\Comment: WARNING
C2H3+CH2O=C2H4+HCO 1.65E1 3.17 9.3998E3
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/
!\Author: SP !\Ref: ZADOR AND MILLER, PROCEEDINGS OF THE COMBUSTION INSTITUTE 35(2015) 181-188 \COMMENT !\Comment: WARNING
CH3CHCHO=CH2CH2CHO 1.11E20 -2.19 4.278E4
PLOG/9.869E-4 1.23E65 -1.801E1 5.15E4/
PLOG/9.869E-4 9.43E16 -3.28E0 3.195E4/
PLOG/9.869E-3 2.43E27 -5.88E0 3.811E4/
PLOG/9.869E-3 5.64E2 -7.68E0 -2.367E3/
PLOG/9.869E-2 3.53E21 -3.61E0 3.788E4/
PLOG/9.869E-2 3.42E-1 -8.98E0 -1.124E4/
PLOG/9.869E-1 1.44E12 -5.3E-1 3.529E4/
PLOG/9.869E-1 1.44E12 -5.3E-1 3.529E4/
PLOG/9.869E0 1.36E34 -6.67E0 4.741E4/
PLOG/9.869E0 1.68E1 2.48E0 2.988E4/
PLOG/9.869E1 1.11E20 -2.19E0 4.278E4/

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   PLOG/9.869E1 6.7E-8 5.27E0 2.782E4/
!\Author: SP !\Ref: ZADOR AND MILLER, PROCEEDINGS OF THE COMBUSTION INSTITUTE 35(2015) 181-188 \COMMENT !\Comment: WARNING
CH3CHCHO=C2H5+CO    1.7E28 -4.59 5.16E4
   PLOG/9.869E-4 1.19E24 -4.69E0 4.161E4/
   PLOG/9.869E-4 0.0E0 0.0E0 0.0E0/
   PLOG/9.869E-3 2.15E48 -1.16E1 5.447E4/
   PLOG/9.869E-3 9.02E17 -3.22E0 3.814E4/
   PLOG/9.869E-2 4.35E47 -1.106E1 5.584E4/
   PLOG/9.869E-2 1.23E17 -2.75E0 3.855E4/
   PLOG/9.869E-1 7.95E43 -9.64E0 5.604E4/
   PLOG/9.869E-1 9.89E13 -1.61E0 3.818E4/
   PLOG/9.869E0 5.14E23 -3.52E0 4.687E4/
   PLOG/9.869E0 9.51E0 -7.24E0 1.184E3/
   PLOG/9.869E1 1.7E28 -4.59E0 5.16E4/
   PLOG/9.869E1 3.95E5 1.31E0 3.659E4/
!\Author: SP !\Ref: ZADOR AND MILLER, PROCEEDINGS OF THE COMBUSTION INSTITUTE 35(2015) 181-188 \COMMENT !\Comment: WARNING
CH3CHCHO=C2H4+HCO    1.08E46 -9.23 6.703E4
   PLOG/9.869E-4 4.29E53 -1.316E1 5.313E4/
   PLOG/9.869E-4 3.11E35 -8.14E0 4.25E4/
   PLOG/9.869E-3 3.44E53 -1.282E1 5.482E4/
   PLOG/9.869E-3 1.21E36 -8.06E0 4.405E4/
   PLOG/9.869E-2 1.18E53 -1.237E1 5.688E4/
   PLOG/9.869E-2 2.69E32 -6.63E0 4.476E4/
   PLOG/9.869E-1 6.35E49 -1.106E1 5.833E4/
   PLOG/9.869E-1 2.18E29 -5.57E0 4.531E4/
   PLOG/9.869E0 1.25E47 -9.92E0 6.126E4/
   PLOG/9.869E0 5.08E21 -3.11E0 4.454E4/
   PLOG/9.869E1 1.08E46 -9.23E0 6.703E4/
   PLOG/9.869E1 8.62E10 3.4E-1 4.291E4/
!\Author: SP !\Ref: ZADOR AND MILLER, PROCEEDINGS OF THE COMBUSTION INSTITUTE 35(2015) 181-188 !\Comment: WARNING
CH3CHCHO=C2H3CHO+H    2.82E42 -8.17 6.072E4
   PLOG/9.869E-4 1.84E57 -1.412E1 5.678E4/
   PLOG/9.869E-4 4.76E41 -9.85E0 4.739E4/
   PLOG/9.869E-3 3.14E55 -1.324E1 5.746E4/
   PLOG/9.869E-3 3.72E39 -8.95E0 4.73E4/
   PLOG/9.869E-2 3.54E55 -1.293E1 5.934E4/
   PLOG/9.869E-2 1.45E32 -6.32E0 4.603E4/
   PLOG/9.869E-1 6.49E51 -1.147E1 5.996E4/
   PLOG/9.869E-1 3.03E28 -5.01E0 4.54E4/
   PLOG/9.869E0 4.14E47 -9.93E0 6.064E4/
   PLOG/9.869E0 5.82E24 -3.71E0 4.474E4/
   PLOG/9.869E1 2.82E42 -8.17E0 6.072E4/
   PLOG/9.869E1 4.19E19 -1.96E0 4.363E4/
!\AUTHOR: SP !\REF: ZADOR AND MILLER, PROCEEDINGS OF THE COMBUSTION INSTITUTE 35 (2015) 181-188!\COMMENT: WARNING
! FIT BTW. 300 AND 900 K WITH MAE OF 81.7%, 291.5%
! FIT BTW. 300 AND 1000 K WITH MAE OF 14.2%, 38.9%
! FIT BTW. 300 AND 1000 K WITH MAE OF 38.6%, 105.1%
! FIT BTW. 500 AND 1200 K WITH MAE OF 20.0%
! FIT BTW. 300 AND 1200 K WITH MAE OF 2.6%, 4.3%
! FIT BTW. 500 AND 1000 K WITH MAE OF 20%
CH2CH2CHO=C2H5+CO    2.07E-25 10.82 1.618E4
   PLOG/9.87E-4 1.33E155 -4.833E1 6.065E4/
   PLOG/9.87E-4 2.47E130 -3.717E1 8.775E4/
   PLOG/9.87E-3 1.45E14 -2.75E0 2.394E4/
   PLOG/9.87E-3 1.15E-18 -1.636E1 -6.734E4/
   PLOG/9.87E-2 6.48E27 -6.45E0 3.078E4/
   PLOG/9.87E-2 2.21E-16 -1.502E1 -5.98E4/
   PLOG/9.87E-1 3.82E8 6.0E-2 2.657712E4/
   PLOG/9.87E-1 3.04E-30 1.22E1 2.984E4/
   PLOG/9.87E0 9.16E-23 8.8E0 1.244E4/
   PLOG/9.87E0 2.43E28 -5.45E0 3.775E4/
   PLOG/9.87E1 2.3E9 3.85E-1 3.007712E4/
   PLOG/9.87E1 4.004E-29 1.218E1 1.884E4/
!_____
!\REACTIONCLASS: R+CH3O2(=)PRODUCTS
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!_____________________________________________________________________________________________
!\Author: WARNING !\Ref: ANOLOGY WITH C3H5-A+HO2 !\Comment: WARNING
C3H5-A+CH3O2=C3H5O+CH3O    1.64E4 2.74 1.1444E3
   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/
!\Author: WARNING !\Ref: ZADOR PHYS. CHEM. CHEM. PHYS., 2009, 11, 11040?1053 !\Comment: WARNING
C3H6+OH=C2H3OH+CH3    3.3E-1 3.7 3.665E3
   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/
!\Author: WARNING !\Ref: ZADOR PHYS. CHEM. CHEM. PHYS., 2009, 11, 11040?1053 !\Comment: WARNING
C3H6+OH=CH3CHO+CH3    5.45E-5 4.22 1.141E3
   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/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H6OH1-2=C3H6+OH    3.75E23 -3.22 3.06E4
   PLOG/5.26E-3 1.48E28 -5.71E0 2.63E4/
   PLOG/1.0E-1 2.32E32 -6.53E0 3.02E4/
   PLOG/1.0E0 1.51E33 -6.46E0 3.24E4/
   PLOG/1.0E1 1.1E30 -5.28E0 3.26E4/
   PLOG/1.0E2 3.75E23 -3.22E0 3.06E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H6OH2-1=C3H6+OH    4.49E26 -4.08 3.21E4
   PLOG/5.26E-3 8.0E28 -5.92E0 2.66E4/
   PLOG/1.0E-1 3.17E33 -6.86E0 3.05E4/
   PLOG/1.0E0 1.29E35 -7.02E0 3.31E4/
   PLOG/1.0E1 6.99E32 -6.09E0 3.37E4/
   PLOG/1.0E2 4.49E26 -4.08E0 3.21E4/
!\Author: UB !\Ref: GIMENEZ-LOPEZ ET AL. INT. J. CHEM. KINET. 48, 11(2016) 724-738 !\Comment: WARNING
C3H4-A+HO2=CH3COCH2+O    5.78E18 -2.09 2.435E4
   PLOG/1.0E-2 5.5E6 1.19E0 1.288E4/
   PLOG/1.0E-2 2.94E-4 4.16E0 7.736E3/
   PLOG/1.0E-1 1.16E8 7.7E-1 1.36E4/
   PLOG/1.0E-1 6.14E-3 3.81E0 8.394E3/
   PLOG/3.16E-1 1.2E7 1.09E0 1.305E4/
   PLOG/3.16E-1 5.44E-4 4.09E0 8.044E3/
   PLOG/1.0E0 3.02E7 9.8E-1 1.331E4/
   PLOG/1.0E0 2.48E-4 4.19E0 8.203E3/
   PLOG/3.16E0 1.98E74 -1.633E1 1.092E5/
   PLOG/3.16E0 6.57E4 1.85E0 1.236E4/
   PLOG/1.0E1 7.5E14 -1.17E0 1.835E4/
   PLOG/1.0E1 2.92E-1 3.38E0 1.059E4/
   PLOG/3.16E1 8.63E18 -2.27E0 2.223E4/
   PLOG/3.16E1 1.95E0 3.17E0 1.174E4/
   PLOG/1.0E2 5.78E18 -2.09E0 2.435E4/
   PLOG/1.0E2 1.1E-1 3.52E0 1.198E4/
!\Author: UB !\Ref: GIMENEZ-LOPEZ ET AL. INT. J. CHEM. KINET. 48, 11(2016) 724-738 !\Comment: WARNING
C3H4-A+HO2=TC3H5OO    2.53E35 -7.26 2.639E4
   PLOG/1.0E-2 4.99E6 -1.02E0 9.152E3/
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   PLOG/1.0E-2 1.88E26 -8.34E0 9.249E3/
   PLOG/1.0E-1 6.02E17 -3.82E0 1.079E4/
   PLOG/1.0E-1 5.26E129 -4.174E1 3.593E4/
   PLOG/3.16E-1 2.47E48 -1.282E1 2.522E4/
   PLOG/3.16E-1 1.96E18 -3.67E0 1.048E4/
   PLOG/1.0E0 4.06E50 -1.307E1 2.722E4/
   PLOG/1.0E0 4.93E21 -4.37E0 1.222E4/
   PLOG/3.16E0 9.08E46 -1.157E1 2.688E4/
   PLOG/3.16E0 1.92E22 -4.28E0 1.308E4/
   PLOG/1.0E1 4.6E43 -1.024E1 2.693E4/
   PLOG/1.0E1 2.11E21 -3.78E0 1.338E4/
   PLOG/3.16E1 5.61E38 -8.49E0 2.621E4/
   PLOG/3.16E1 1.39E20 -3.3E0 1.341E4/
   PLOG/1.0E2 2.53E35 -7.26E0 2.639E4/
   PLOG/1.0E2 1.42E19 -2.91E0 1.342E4/
!\Author: UB !\Ref: GIMENEZ-LOPEZ ET AL. INT. J. CHEM. KINET. 48, 11(2016) 724-738 !\Comment: WARNING
C3H4-A+HO2=CH2O+CH3CO    2.47E16 -1.7 2.003E4
   PLOG/1.0E-2 3.9E13 -1.17E0 1.375E4/
   PLOG/1.0E-2 8.43E0 2.56E0 7.382E3/
   PLOG/1.0E-1 4.26E0 2.64E0 7.253E3/
   PLOG/1.0E-1 1.56E13 -1.05E0 1.352E4/
   PLOG/3.16E-1 2.59E-6 4.34E0 4.525E3/
   PLOG/3.16E-1 6.9E9 0.0E0 1.172E4/
   PLOG/1.0E0 3.33E102 -2.418E1 1.386E5/
   PLOG/1.0E0 8.07E7 6.0E-1 1.085E4/
   PLOG/3.16E0 5.22E15 -1.75E0 1.518E4/
   PLOG/3.16E0 3.54E0 2.69E0 8.025E3/
   PLOG/1.0E1 7.32E35 -7.77E0 2.697E4/
   PLOG/1.0E1 9.84E6 9.1E-1 1.171E4/
   PLOG/3.16E1 1.78E28 -5.3E0 2.513E4/
   PLOG/3.16E1 1.79E4 1.7E0 1.125E4/
   PLOG/1.0E2 2.47E16 -1.7E0 2.003E4/
   PLOG/1.0E2 4.32E-6 4.31E0 6.829E3/
!\Author: UB !\Ref: GIMENEZ-LOPEZ ET AL. INT. J. CHEM. KINET. 48, 11(2016) 724-738 !\Comment: WARNING
C3H4-A+HO2=>CH2O+CH3+CO    5.77E16 -1.7 2.003E4
   PLOG/1.0E-2 9.1E13 -1.17E0 1.375E4/
   PLOG/1.0E-2 1.97E1 2.56E0 7.382E3/
   PLOG/1.0E-1 9.94E0 2.64E0 7.253E3/
   PLOG/1.0E-1 3.63E13 -1.05E0 1.352E4/
   PLOG/3.16E-1 6.05E-6 4.34E0 4.525E3/
   PLOG/3.16E-1 1.61E10 0.0E0 1.172E4/
   PLOG/1.0E0 7.77E102 -2.418E1 1.386E5/
   PLOG/1.0E0 1.88E8 6.0E-1 1.085E4/
   PLOG/3.16E0 1.22E16 -1.75E0 1.518E4/
   PLOG/3.16E0 8.26E0 2.69E0 8.025E3/
   PLOG/1.0E1 1.71E36 -7.77E0 2.697E4/
   PLOG/1.0E1 2.3E7 9.1E-1 1.171E4/
   PLOG/3.16E1 4.14E28 -5.3E0 2.513E4/
   PLOG/3.16E1 4.19E4 1.7E0 1.125E4/
   PLOG/1.0E2 5.77E16 -1.7E0 2.003E4/
   PLOG/1.0E2 1.01E-5 4.31E0 6.829E3/
!\Author: SP !\Ref: MILLER AND KLIPPENSTEIN, J. PHYS. CHEM. A 2003, 107, 2680-2692 !\Comment: WARNING !SP_
C3H3+H=C3H4-A    4.35E23 -3.2 3.255E3
   PLOG/3.95E-2 1.7E36 -7.41E0 6.337E3/
   PLOG/1.0E0 1.58E29 -5.0E0 4.711E3/
   PLOG/1.0E1 4.35E23 -3.2E0 3.255E3/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONCH2
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: LASKIN ET AL. IJCK 32 589-614 2000 !\Comment: WARNING
C3H4-A+C2H=C2H2+C3H3    1.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: ANALOGY WITH CURRAN 2006 ALKYL DECOMP !\Comment: WARNING
C3H4-A+O2=C3H3+HO2    4.0E13 0.0 4.132E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
O2+C3H4-A=>CH2O+CH2CO    5.0E13 0.0 4.1E4
```

!\Author: SP !\Ref: ANALOGHY TO C3H6+HO2 !\Comment: WARNING
C3H4-A+HO2=C3H3+H2O2 7.7E-2 4.403 1.35472E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H4-A+CH3=C3H3+CH4 4.4E1 3.24 7.761E3
!\Author: SP !\Ref: MILLER ET AL., J. PHYS. CHEM. A, VOL. 112, NO. 39, 2008 !\Comment: WARNING
C3H4-A+H=C3H3+H2 6.625E3 3.095 5.522E3
!\Author: SP !\Ref: ZADOR AND MILLER, PROCEEDINGS OF THE COMBUSTION INSTITUTE 35(2015) 181-188 !\Comment: WARNING
C3H4-A+OH=C3H3+H2O 5.05E5 2.36 2.879E3
  DUP
!\Author: SP !\Ref: ZADOR AND MILLER, PROCEEDINGS OF THE COMBUSTION INSTITUTE 35(2015) 181-188 !\Comment: WARNING
C3H4-A+OH=C3H3+H2O 5.95E4 2.5 6.611E2
  DUP
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H4-A+CH3=C2H3+C2H4 2.69E38 -7.298 4.2739E4
  PLOG/1.0E-3 1.17E14 -7.48E-1 1.7356E4/
  PLOG/1.0E-2 3.48E12 -3.13E-1 1.6527E4/
  PLOG/1.0E-1 2.73E17 -1.698E0 1.9791E4/
  PLOG/1.0E0 3.93E25 -3.975E0 2.6034E4/
  PLOG/1.0E1 4.04E33 -6.14E0 3.4023E4/
  PLOG/1.0E2 2.69E38 -7.298E0 4.2739E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H4-A+CH3O2=C3H3+CH3O2H 7.7E-2 4.4 1.38E4
!\Author: SP !\Ref: LLNL, RATE MODIFIED, USED RATE FROM C4H8-1+C3H5-A AND REDICED IT BY FACTOR OF 8 !\Comment: WARNING
C3H4-A+C3H5-A=C3H3+C3H6 8.4E2 3.224 1.7402E4
!\Author: WARNING !\Ref: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438 !\Comment: WARNING
C3H4-A+H=C3H5-A 4.23E43 -8.61 2.2522E4
  PLOG/1.0E-3 2.21E61 -1.525E1 2.0076E4/
  PLOG/1.0E-3 2.8E38 -8.67E0 8.035E3/
  PLOG/3.9E-2 1.24E52 -1.202E1 1.7839E4/
  PLOG/3.9E-2 9.33E36 -8.19E0 7.462E3/
  PLOG/1.0E0 4.67E51 -1.145E1 2.134E4/
  PLOG/1.0E0 3.32E30 -5.78E0 6.913E3/
  PLOG/1.0E1 3.75E48 -1.027E1 2.2511E4/
  PLOG/1.0E1 2.29E26 -4.32E0 6.163E3/
  PLOG/1.0E2 4.23E43 -8.61E0 2.2522E4/
  PLOG/1.0E2 4.38E21 -2.71E0 5.187E3/
!\Author: WARNING !\Ref: DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589 !\Comment: WARNING
C3H4-A+H=C3H5-S 3.2E31 -5.88 2.15E4
  PLOG/1.0E-1 1.1E30 -6.52E0 1.52E4/
  PLOG/1.0E0 5.4E29 -6.09E0 1.63E4/
  PLOG/1.0E1 2.6E31 -6.23E0 1.87E4/
  PLOG/1.0E2 3.2E31 -5.88E0 2.15E4/
!\Author: WARNING !\Ref: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438 !\Comment: WARNING
C3H4-A+H=C3H5-T 4.22E52 -11.64 2.2262E4
  PLOG/1.0E-3 6.44E102 -2.751E1 5.1768E4/
  PLOG/1.0E-3 1.1E54 -1.429E1 1.0809E4/
  PLOG/3.9E-2 1.55E53 -1.31E1 1.4472E4/
  PLOG/3.9E-2 9.88E44 -1.121E1 8.212E3/
  PLOG/1.0E0 1.9E53 -1.259E1 1.6726E4/
  PLOG/1.0E0 2.82E40 -9.42E0 7.85E3/
  PLOG/1.0E1 7.96E51 -1.182E1 1.8286E4/
  PLOG/1.0E1 2.6E35 -7.57E0 7.147E3/
  PLOG/1.0E2 4.22E52 -1.164E1 2.2262E4/
  PLOG/1.0E2 9.88E29 -5.53E0 6.581E3/
!\Author: WARNING !\Ref: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438 !\Comment: WARNING
C3H4-A+H=CH3+C2H2 1.37E17 -0.79 1.7603E4
  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/1.0E0 1.23E4 2.68E0 6.335E3/
  PLOG/1.0E1 1.68E16 -6.0E-1 1.4754E4/
  PLOG/1.0E1 3.31E8 1.14E0 8.886E3/
  PLOG/1.0E2 1.37E17 -7.9E-1 1.7603E4/
  PLOG/1.0E2 1.28E6 1.71E0 9.774E3/
!\Author: WARNING !\Ref: DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589 !\Comment: WARNING

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C3H5-A=C3H5-T    2.8E43 -9.27 7.4E4
   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/
!\Author: WARNING !\Ref: DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589 !\Comment: WARNING
C3H5-A=C3H5-S    4.86E44 -9.84 7.34E4
   PLOG/1.0E-1 1.3E55 -1.453E1 7.38E4/
   PLOG/1.0E0 5.0E51 -1.302E1 7.33E4/
   PLOG/1.0E1 9.7E48 -1.173E1 7.37E4/
   PLOG/1.0E2 4.86E44 -9.84E0 7.34E4/
!\Author: WARNING !\Ref: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438 !\Comment: WARNING
C2H2+CH3=C3H5-T    3.8E36 -7.58 3.13E4
   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/
!\Author: WARNING !\Ref: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438 !\Comment: WARNING
C3H5-T=C3H5-S    5.8E51 -12.43 5.92E4
   PLOG/1.0E-1 1.6E44 -1.216E1 5.22E4/
   PLOG/1.0E0 1.5E48 -1.271E1 5.39E4/
   PLOG/1.0E1 5.1E52 -1.337E1 5.72E4/
   PLOG/1.0E2 5.8E51 -1.243E1 5.92E4/
!\Author: WARNING !\Ref: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438 !\Comment: WARNING
C2H2+CH3=C3H5-A    3.8E44 -9.63 3.76E4
   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/
!\Author: WARNING !\Ref: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438 !\Comment: WARNING
CH3+C2H2=C3H5-S    1.42E42 -8.91 2.2235E4
   PLOG/1.0E-3 1.78E42 -1.04E1 1.3647E4/
   PLOG/3.9E-2 4.32E37 -8.79E0 1.3594E4/
   PLOG/1.0E0 1.19E44 -1.019E1 1.8728E4/
   PLOG/1.0E0 8.49E35 -8.43E0 1.2356E4/
   PLOG/1.0E1 6.02E43 -9.74E0 2.0561E4/
   PLOG/1.0E1 3.04E32 -7.01E0 1.2357E4/
   PLOG/1.0E2 1.42E42 -8.91E0 2.2235E4/
   PLOG/1.0E2 1.69E27 -5.07E0 1.169E4/
!\Author: SP !\Ref: LLNL !\Comment: OLD RATE IN ARAMCO2.0 IS MIGHT HIGHER THAN C4H8-1+C3H5-A
C3H4-A+O=C3H3+OH    5.24E11 0.7 5.88E3
!\Author: SP !\Ref: LLNL !\Comment: BASED ON INFROMATION FROM VANUZZO ET AL., AND NGUYEN( J. PHYS. CHEM. A, VOL. 110, NO. 44, 2006)
C3H4-A+O=C2H4+CO    6.24E6 2.05 1.8E2
!\Author: WARNING !\Ref: GRI 3.0 AND USC II !\Comment: C2H2+HCO(=)C2H3+CO
C3H4-A+HCO=C3H5-A+CO    1.0E7 2.0 6.0E3
!\Author: SP !\Ref: ZADOR AND MILLER, PROCEEDINGS OF THE COMBUSTION INSTITUTE 35(2015) 181-188 !\Comment: WARNING
C3H4-A+OH=CH2CO+CH3    7.91E12 0.32 1.998E4
   PLOG/9.869E-4 3.03E22 -3.01E0 6.341E3/
   PLOG/9.869E-4 8.33E8 1.01E0 2.68E1/
   PLOG/9.869E-3 3.46E26 -4.03E0 1.086E4/
   PLOG/9.869E-3 4.23E7 1.4E0 7.651E2/
   PLOG/9.869E-2 4.27E25 -3.56E0 1.398E4/
   PLOG/9.869E-2 7.9E5 1.78E0 1.082E3/
   PLOG/1.313E-1 2.06E25 -3.45E0 1.432E4/
   PLOG/1.313E-1 3.45E6 1.55E0 1.33E3/
   PLOG/9.869E-1 4.07E25 -3.41E0 1.837E4/
   PLOG/9.869E-1 1.51E4 2.2E0 1.759E3/
   PLOG/9.869E0 4.47E20 -1.9E0 2.004E4/
   PLOG/9.869E0 1.29E-3 4.35E0 1.625E3/
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   PLOG/9.869E1 7.91E12 3.2E-1 1.998E4/
   PLOG/9.869E1 3.1E-12 6.76E0 6.564E2/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+R(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: LASKIN ET AL. IJCK 32 589-614 2000 !\Comment: WARNING
C3H3+O=CH2O+C2H    2.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: LASKIN ET AL. IJCK 32 589-614 2000 !\Comment: WARNING
C3H3+HCO=C3H4-A+CO    2.5E13 0.0 0.0E0
!\Author: WARNING !\Ref: TSANG, W.; HAMPSON, R.F., J. PHYS. CHEM. REF. DATA 15, 1087(1986) !\Comment: WARNING
C2H5+C2H=C3H3+CH3    1.81E13 0.0 0.0E0
!\Author: SP !\Ref: DAVID K. HAHN,FARADAY DISCUSS., 2002, 119, 79-100 !\Comment: WARNING
C3H3+O2=CH2CO+HCO    1.7E5 1.7 1.5E3
!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+OH(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: SP !\Ref: VANUZZO, BALUCANI, LEONORI, STRANGES, FALCINELLI, BERGEAT, CASAVECCHIA, GIMONDI, CAVALLOTTI, J. PHYS. CHEM. LETT.
2016, 7, 1010-1015 !\Com
C3H3+OH=C2H3+HCO    2.29E36 -6.25 2.41E4
   PLOG/1.0E-1 1.07088E19 -1.65E0 4.47E3/
   PLOG/1.0E0 1.09582E19 -1.65E0 4.628E3/
   PLOG/1.0E1 4.56815E25 -3.41E0 1.209E4/
   PLOG/3.0E1 2.29E36 -6.25E0 2.41E4/
!\Author: SP !\Ref: VANUZZO, BALUCANI, LEONORI, STRANGES, FALCINELLI, BERGEAT, CASAVECCHIA, GIMONDI, CAVALLOTTI, J. PHYS. CHEM. LETT.
2016, 7, 1010-1015 !\Com
C3H3+OH=>H2+C2H2+CO    5.49E18 -1.8 2.757E3
   PLOG/1.0E-1 9.77E17 -1.6E0 1.85E3/
   PLOG/1.0E0 1.51E20 -2.2E0 3.992E3/
   PLOG/1.0E1 1.78E29 -4.61E0 1.3931E4/
   PLOG/3.0E1 5.49E18 -1.8E0 2.757E3/
!\Author: SP !\Ref: VANUZZO, BALUCANI, LEONORI, STRANGES, FALCINELLI, BERGEAT, CASAVECCHIA, GIMONDI, CAVALLOTTI, J. PHYS. CHEM. LETT.
2016, 7, 1010-1015 !\Com
C3H3+OH=C2H4+CO    1.77722E35 -6.86 6.225E3
   PLOG/1.0E-1 1.25817E23 -3.46E0 3.95E2/
   PLOG/1.0E0 3.30934E29 -5.24E0 5.051E3/
   PLOG/1.0E1 3.79963E13 -1.01E0 -1.416E4/
   PLOG/3.0E1 1.77722E35 -6.86E0 6.225E3/
!\Author: SP !\Ref: !ZADOR AND MILLER, PROC. COMBUST. 34(2013) 519-526 !\Comment: WARNING
NC3H7O=C2H5+CH2O    9.11E23 -3.44 1.77E4
   PLOG/5.26E-3 1.22E32 -7.45E0 1.7E4/
   PLOG/1.0E-1 1.19E35 -7.95E0 1.84E4/
   PLOG/1.0E0 2.46E35 -7.69E0 1.92E4/
   PLOG/1.0E1 5.18E31 -6.18E0 1.91E4/
   PLOG/1.0E2 9.11E23 -3.44E0 1.77E4/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+O2(=)RO2
!_____________________________________________________________________________________________________
!\Author: JB !\Ref: A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\Comment: ASSUMED TO BE THE SAME AS REGULAR ALKYL RADICAL
C3H6OH1-2+O2=TQJC3H6OH    3.487E14 -0.816 -5.365E2
!\Author: SP !\Ref: LIZARDO-HUERTA, J. C., ET AL. PHYSICAL CHEMISTRY CHEMICAL PHYSICS 18.17(2016) !\Comment: WARNING
TQJC3H6OH=>TQC3H6OI    2.61E10 0.29 2.0378E4
!\Author: SP !\Ref: LIZARDO-HUERTA, J. C., ET AL. PHYSICAL CHEMISTRY CHEMICAL PHYSICS 18.17(2016) !\Comment: WARNING
TQJC3H6OH=>QC3H5OHP    1.35E-3 4.55 2.6985E4
!\Author: SP !\Ref: LIZARDO-HUERTA, J. C., ET AL. PHYSICAL CHEMISTRY CHEMICAL PHYSICS 18.17(2016) !\Comment: WARNING
TQC3H6OI=>CH3CHO+CH2O+OH    1.99E19 -1.5 1.082E4
!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+O2(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: ACETALDEHYDE ANALOG !\Comment: WARNING
C3H5O+O2=C2H3CHO+HO2    1.0E12 0.0 6.0E3
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_BETA_SCISSION
!_____________________________________________________________________________________________________
!\Author: SP !\Ref: ZADOR AND MILLER, PROC. COMBUST. 34(2013) 519-526 !\Comment: WARNING
C3H6OH2-1=C2H3OH+CH3    2.72E32 -5.66 4.04E4
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PLOG/5.26E-3 2.81E15 -2.39E0 2.33E4/
PLOG/1.0E-1 1.72E26 -4.99E0 3.0E4/
PLOG/1.0E0 2.27E33 -6.63E0 3.58E4/
PLOG/1.0E1 2.83E36 -7.14E0 4.01E4/
PLOG/1.0E2 2.72E32 -5.66E0 4.04E4/
!\Author: WARNING !\Ref: ZADOR AND MILLER, PROC. COMBUST. 34(2013) 519-526 !\Comment: WARNING
IC3H7O=CH3CHO+CH3 6.42E27 -4.63 1.84E4
PLOG/5.26E-3 1.76E31 -7.2E0 1.64E4/
PLOG/1.0E-1 1.18E35 -7.97E0 1.8E4/
PLOG/1.0E0 8.1E35 -7.88E0 1.89E4/
PLOG/1.0E1 1.09E34 -6.93E0 1.92E4/
PLOG/1.0E2 6.42E27 -4.63E0 1.84E4/
!\Author: WARNING !\Ref: ZADOR AND MILLER, PROC. COMBUST. 34(2013) 519-526 !\Comment: WARNING
IC3H7O=CH3COCH3+H 1.37E34 -7.02 2.28E4
PLOG/5.26E-3 4.26E4 1.5E-1 8.99E3/
PLOG/1.0E-1 2.91E14 -2.31E0 1.3E4/
PLOG/1.0E0 9.13E21 -4.18E0 1.6E4/
PLOG/1.0E1 4.64E28 -5.79E0 1.92E4/
PLOG/1.0E2 1.37E34 -7.02E0 2.28E4/
!_____
!\REACTIONCLASS: R+O2(=)PRODUCTS
!_____
!\Author: SP !\Ref: A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\Comment: ASSUMED TO BE THE SAME AS REGULAR ALKYL RADICAL
C3H6OH2-1+O2=IQJC3H6OH 6.863E16 -1.627 1.99E2
!\AUTHOR: SP !\REF: Lizardo-Huerta, J. C., et al. Physical Chemistry Chemical Physics 18.17 (2016): 12231-12251.!\COMMENT:
IQJC3H6OH=IQC3H6OT 1.18E10 0.39 2.0322E4
!\Author: SP !\Ref: LIZARDO-HUERTA, J. C., ET AL. PHYSICAL CHEMISTRY CHEMICAL PHYSICS 18.17(2016) !\Comment:
PQC4H8OS=)C2H5CHO+CH2O+OH
IQC3H6OT=>CH3CHO+CH2O+OH 8.69E21 -2.37 1.2629E4
!_____
!\REACTIONCLASS: RO2(=)ALKENE+HO2
!_____
!\Author: WARNING !\Ref: BALLA ET AL., CHEM. PHYSICS, 99, 323(1985) !\Comment: WARNING
IC3H7O+O2=CH3COCH3+HO2 9.09E9 0.0 3.9E2
!----------
!\ENDSUBMECH: IC3H7OH
!----------
!----------
!\SUBMECH: CH3COCH3
!\MECHCOMMENTS: ACETONE HAS NOLOW-TEMPERATURE CHEMISTRY
!----------
!_____
!\REACTIONCLASS: RH(=)PRODUCTS
!_____
!\Author: WARNING !\Ref: SAXENA ET AL. PROCEEDINGS. 32 123-130(2009) !\Comment: WARNING
CH3COCH3=CH3CO+CH3 9.4E28 -3.669 8.90228E4
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/
!\Author: WARNING !\Ref: WJP !\Comment: WARNING
CH3COCH2+H=CH3COCH3 1.0E13 0.0 0.0E0
!_____
!\REACTIONCLASS: RH+R_ABSTRACTION
!_____
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
CH3COCH3+OH=CH3COCH2+H2O 1.25E5 2.483 4.45E2
!\Author: WARNING !\Ref: CURRAN ESTIMATE !\Comment: WARNING
CH3COCH3+H=CH3COCH2+H2 9.8E5 2.43 5.16E3
!\Author: WARNING !\Ref: FIT TO DATA ON NIST STANDARD REFERENCE DATABASE 17 -2Q98 !\Comment: WARNING
CH3COCH3+O=CH3COCH2+OH 5.13E11 0.211 4.89E3
!\Author: WARNING !\Ref: S. PICHON, COMBUSTION AND FLAME(2009) 156(2) 494?04. !\Comment: WARNING
CH3COCH3+CH3=CH3COCH2+CH4 3.96E11 0.0 9.784E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING

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CH3COCH3+CH3O=CH3COCH2+CH3OH    4.34E11 0.0 6.46E3
!\Author: WARNING !\Ref: A-FACTOR BY ANALOGY WITH C2H6+O2 AND EA FROM DHRXN !\Comment: WARNING
CH3COCH3+O2=CH3COCH2+HO2    6.03E13 0.0 4.85E4
!\Author: WARNING !\Ref: ANALOGY TO ETHANE !\Comment: WARNING
CH3COCH3+HO2=CH3COCH2+H2O2    1.7E13 0.0 2.046E4
!\Author: WARNING !\Ref: ANALOGY TO ETHANE !\Comment: WARNING
CH3COCH3+CH3O2=CH3COCH2+CH3O2H    1.7E13 0.0 2.046E4
!\Author: WARNING !\Ref: WESTBROOK ESTIMATE !\Comment: WARNING
CH3COCH3+CH3COCH2O2=CH3COCH2+C3KET21    1.0E11 0.0 5.0E3
!_____
!\REACTIONCLASS: RADICAL_BETA_SCISSION
!_____
!\Author: SP !\Ref: ZADOR AND MILLER, PROCEEDINGS OF THE COMBUSTION INSTITUTE 35(2015) 181-188 !\Comment: WARNING
CH3COCH2=CH2CO+CH3    7.04E36 -6.61 5.55E4
   PLOG/9.869E-4 5.41E58 -1.454E1 5.567E4/
   PLOG/9.869E-4 1.04E46 -1.116E1 4.747E4/
   PLOG/9.869E-3 5.78E57 -1.389E1 5.688E4/
   PLOG/9.869E-3 1.55E42 -9.7E0 4.71E4/
   PLOG/9.869E-2 4.72E55 -1.292E1 5.801E4/
   PLOG/9.869E-2 7.49E36 -7.81E0 4.622E4/
   PLOG/1.313E-1 2.02E55 -1.277E1 5.812E4/
   PLOG/1.313E-1 1.23E36 -7.53E0 4.607E4/
   PLOG/9.869E-1 1.28E52 -1.154E1 5.875E4/
   PLOG/9.869E-1 3.99E30 -5.63E0 4.501E4/
   PLOG/9.869E0 1.74E46 -9.54E0 5.837E4/
   PLOG/9.869E0 3.96E24 -3.58E0 4.374E4/
   PLOG/9.869E1 7.04E36 -6.61E0 5.55E4/
   PLOG/9.869E1 3.5E19 -1.89E0 4.258E4/
!_____
!\REACTIONCLASS: R+HO2(=)PRODUCTS
!_____
!\Author: SP !\Ref: FROM C3H5-A+HO2=C3H5O+OH ! !KUKKADAPU1@LLNL.GOV !\Comment: WARNING
CH3COCH2+HO2=CH3COCH2O+OH    8.05E17 -1.503 4.82E3
!\Author: SP !\Ref: FROM C3H5-A+HO2, 10 ATM RATE KUKKADAPU1.LLNL.GOV !\Comment: WARNING
CH3COCH2+HO2=C3KET21    1.82E40 -8.906 8.12E3
!\Author: WARNING !\Ref: WJP !\Comment: WARNING
CH3COCH2+CH3O2=CH3COCH2O+CH3O    1.205E13 0.0 0.0E0
!_____
!\REACTIONCLASS: R+O2(=)RO2
!_____
!\Author: WARNING !\Ref: CURRAN ESTIMATE !\Comment: WARNING
CH3COCH2+O2=CH3COCH2O2    1.2E11 0.0 -1.1E3
!\Author: WARNING !\Ref: WESTBROOK ESTIMATE !\Comment: WARNING
CH2O+CH3COCH2O2=HCO+C3KET21    1.288E11 0.0 9.0E3
!\Author: WARNING !\Ref: WESTBROOK ESTIMATE !\Comment: WARNING
HO2+CH3COCH2O2=C3KET21+O2    1.0E12 0.0 0.0E0
!-----
!\ENDSUBMECH: CH3COCH3
!-----
!-----
!\SUBMECH: C2H3CHO
!-----
!_____
!\REACTIONCLASS: RH(=)PRODUCTS
!_____
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
C2H3+HCO=C2H3CHO    1.81E13 0.0 0.0E0
!_____
!\REACTIONCLASS: RH+R_ABSTRACTION
!_____
!\Author: WARNING !\Ref: BASED ON CH3CHO+H !\Comment: WARNING
C2H3CHO+H=C2H3CO+H2    6.9E5 2.4 1.905E3
!\Author: WARNING !\Ref: BASED ON CH3CHO+H !\Comment: WARNING
C2H3CHO+O=C2H3CO+OH    5.94E12 0.0 1.868E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
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C2H3CHO+OH=C2H3CO+H2O    3.73E4 2.6 -2.3E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H3CHO+O2=C2H3CO+HO2    9.0E12 0.5 4.22E4
!\Author: WARNING !\Ref: BASED ON CH3CHO+HO2 !\Comment: WARNING
C2H3CHO+HO2=C2H3CO+H2O2    3.01E12 0.0 1.192E4
!\Author: WARNING !\Ref: BASED ON CH3CHO+HO2 !\Comment: WARNING
C2H3CHO+CH3=C2H3CO+CH4    2.608E6 1.78 5.911E3
!\Author: WARNING !\Ref: ANALOGY WITH ACETALDEHYDE. !\Comment: WARNING
C2H3CHO+C2H3=C2H3CO+C2H4    1.74E12 0.0 8.44E3
!\Author: WARNING !\Ref: ANALOGY WITH CH3CHO+CH3O !\Comment: WARNING
C2H3CHO+CH3O=C2H3CO+CH3OH    1.0E12 0.0 3.3E3
!\Author: WARNING !\Ref: BASED ON CH3CHO+HO2 !\Comment: WARNING
C2H3CHO+CH3O2=C2H3CO+CH3O2H    3.01E12 0.0 1.192E4
!____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ALPHA_SCISSION
!____________________________________________________________________________________________________
!\Author: WARNING !\Ref: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15 !\Comment: WARNING
C2H3+CO=C2H3CO    1.51E11 0.0 4.81E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CHCHO+O2=CH3CH(OO)CHO    9.1E50 -12.2 1.563E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CH(OO)CHO=QCH2CH(OOH)CHO    1.0E0 2.934 2.5846957E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CH(OO)CHO=QCH3CH(OOH)CO    3.329E4 1.555 1.3271196E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CH(OO)CHO=C2H3CHO+HO2    6.4E25 -4.02 3.49139E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
QCH3CH(OOH)CO=>CO+CH3CHO+OH    1.494E13 0.153 1.0143214E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
QCH2CH(OOH)CHO=C2H3CHO+HO2    5.923E14 -0.714 9.134807E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
QCH2CH(OOH)CHO=CYC2H3OCHO+OH    1.573E14 -0.534 1.483154E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CH(OO)CHO=>CO+CH3CHO+OH    6.0E11 0.0 2.45E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CHCHO+HO2=>CO+CH3CHO+H2O    1.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CHCHO+HO2=>HCO+CH3CHO+OH    1.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING NO REFERENCE !\Comment: WARNING
CYC2H3OCHO+OH=>H2O+CH2CO+HCO    2.26E3 2.73 -4.6886E3
!\Author: WARNING !\Ref: WARNING NO REFERENCE !\Comment: WARNING
CYC2H3OCHO+HO2=>H2O2+CH2CO+HCO    1.72E1 3.46 9.7333E3
!-----------------------------------------------------------------------------------------------------------------------------
!\ENDSUBMECH: C3H6O3
!-----------------------------------------------------------------------------------------------------------------------------
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+++++++++++++++++++++++++++++++++++++
!\END_KINETICS_MODULE: C3
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+++++++++++++++++++++++++++++++++++++
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+++++++++++++++++++++++++++++++++++++
!\KINETICS_MODULE: C4
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+++++++++++++++++++++++++++++++++++++
!-----------------------------------------------------------------------------------------------------------------------------
!\SUBMECH: C4H10
!\MECHCOMMENTS: SOMEONE HAS UPDATED PC4H9 AND SC4H9 THERMAL DECOMPOSITIONS SINCE MECHANISM ASSEMBLY BEGAN. THIS ALTERATION MUST BE ADDRESSED BEFORE MECHANISM IS FINALISED. KPS 31 / 07 / 2015
!\MECHCOMMENTS: SOMEONE HAS REMOVED THE REACTIONS C4H8OOH1-2(=)C4H8-1+HO2 C4H8OOH2-1(=)C4H8-1+HO2 C4H8OOH2-3(=)C4H8-2+HO2 OUT OF BASEMECH2907 MUST BE ADDRESSED BEFORE FINALISATION
!\MECHCOMMENTS: COMMENTS ON RATE CONSTANTS IN USE IN C4 LTC ARE NOT VERY DETAILED. CAN WE IMPROVE UPON THIS?
!\MECHCOMMENTS: THESE REACTIONS HAVE BEEN STORED IN THE C4H8-1 / 2 CHEMISTRY
!-----------------------------------------------------------------------------------------------------------------------------
!____________________________________________________________________________________________________
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!\REACTIONCLASS: QOOH(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: VILLANO(FROM KUIWEN'S MECH) !\Comment: WARNING
C4H8OOH1-3=>OH+CH2O+C3H6    1.23E9 1.3 2.49E4
!\Author: WARNING !\Ref: VILLANO(FROM KUIWEN'S MECH) !\Comment: WARNING
C4H8OOH2-4=>OH+CH3CHO+C2H4    3.08E8 1.5 2.35E4
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RH(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: BASED ON OEHLSCHLAEGER ET AL. J. PHYS. CHEM. A 2004, 108 !\Comment: WARNING
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/
!\Author: WARNING !\Ref: BASED ON OEHLSCHLAEGER ET AL. J. PHYS. CHEM. A 2004, 108 !\Comment: WARNING
C4H10(+M)=NC3H7+CH3(+M)    6.6E52 -10.626 1.0033E5
   LOW/5.34E17 0.0E0 4.2959E4/
   TROE/9.502E-2 1.0E-20 5.348E3 4.326E3/
!\Author: WARNING !\Ref: ESTIMATE FROM RECOMBINATION(1E14 0 0) !\Comment: WARNING
C4H10=PC4H9+H    1.49E27 -3.15 1.07323E5
   PLOG/1.0E-2 4.45E90 -2.191E1 1.40564E5/
   PLOG/1.0E-1 4.63E76 -1.764E1 1.34669E5/
   PLOG/1.0E0 4.94E58 -1.232E1 1.25435E5/
   PLOG/1.0E1 4.8E40 -7.06E0 1.15302E5/
   PLOG/1.0E2 1.49E27 -3.15E0 1.07323E5/
!\Author: WARNING !\Ref: ESTIMATE FROM RECOMBINATION(1E14 0 0) !\Comment: WARNING
C4H10=SC4H9+H    5.4E26 -3.05 1.03313E5
   PLOG/1.0E-2 3.1E88 -2.124E1 1.36355E5/
   PLOG/1.0E-1 4.34E73 -1.676E1 1.2959E5/
   PLOG/1.0E0 7.39E55 -1.152E1 1.20199E5/
   PLOG/1.0E1 8.52E38 -6.58E0 1.10556E5/
   PLOG/1.0E2 5.4E26 -3.05E0 1.03313E5/
!\Author: WARNING !\Ref: MIYOSHI A / 2 COMPARED TO R+O2 080415A !\Comment: WARNING
C4H8OOH1-3+O2=C4H8OOH1-3O2    1.744E14 -0.816 -5.365E2
!\Author: WARNING !\Ref: MIYOSHI A / 2 COMPARED TO R+O2 080415A !\Comment: WARNING
C4H8OOH2-4+O2=C4H8OOH2-4O2    3.433E16 -1.627 1.987E2
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RH_H_ABSTRACTION
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887(1988) !\Comment: WARNING
C4H10+H=PC4H9+H2    3.49E5 2.69 6.45E3
!\Author: WARNING !\Ref: ANALOGY WITH C4H10+O2(=)PC4H9+HO2 !\Comment: WARNING
C4H10+O2=PC4H9+HO2    6.0E13 0.0 5.234E4
!\Author: WARNING !\Ref: MICHAEL, KEIL AND KLEM, INT. J. CHEM. KIN. 15, 705(1983) !\Comment: WARNING
C4H10+O=PC4H9+OH    1.13E14 0.0 7.85E3
!\Author: WARNING !\Ref: DROEGE, A. T. AND TULLY, F. P. !\Comment: WARNING
C4H10+OH=PC4H9+H2O    1.054E10 0.97 1.586E3
!\Author: SP !\Ref: 60% OF NEW FIT !\Comment: WARNING
C4H10+HO2=PC4H9+H2O2    2.08E1 3.59 1.56E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C4H10+CH3=PC4H9+CH4    3.45E1 3.44 1.04E4
!\Author: WARNING !\Ref: DRYER ESTIMATE !\Comment: WARNING
C4H10+CH3O=PC4H9+CH3OH    3.0E11 0.0 7.0E3
!\Author: WARNING !\Ref: ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523(1980) !\Comment: WARNING
C4H10+C2H5=PC4H9+C2H6    1.58E11 0.0 1.23E4
!\Author: WARNING !\Ref: SUNDARAM, K. M. AND FROMENT, G. F., I. AND E. C. FUNDAMENTALS 17, 174(1978) !\Comment: WARNING
C4H10+C2H3=PC4H9+C2H4    1.0E12 0.0 1.8E4
!\Author: WARNING !\Ref: ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523(1980) !\Comment: WARNING
C4H10+C3H5-A=PC4H9+C3H6    7.94E11 0.0 2.05E4
!\Author: WARNING !\Ref: ANALOGY TO C2H6+HO2 !\Comment: WARNING
C4H10+NC3H7O2=PC4H9+NC3H7O2H    1.7E13 0.0 2.046E4
!\Author: WARNING !\Ref: ANALOGY TO C2H6+HO2 !\Comment: WARNING
C4H10+IC3H7O2=PC4H9+IC3H7O2H    1.7E13 0.0 2.046E4
!\Author: WARNING !\Ref: WESTBROOK AND PITZ ESTIMATE(1983) !\Comment: WARNING
C4H10+PC4H9=SC4H9+C4H10    1.0E11 0.0 1.04E4
!\Author: WARNING !\Ref: ANALOGY TO C2H6+HO2 !\Comment: WARNING
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C4H10+SC4H9O2=PC4H9+SC4H9O2H 1.7E13 0.0 2.046E4
!\Author: WARNING !\Ref: ANALOGY TO C2H6+HO2 !\Comment: WARNING
C4H10+TC4H9O2=PC4H9+TC4H9O2H 1.7E13 0.0 2.046E4
!\Author: WARNING !\Ref: TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887(1988) !\Comment: WARNING
C4H10+H=SC4H9+H2 2.6E6 2.4 4.471E3
!\Author: WARNING !\Ref: INGHAM,T.; WALKER,R.W.; WOOLFORD,R.E., SYMP. INT. COMBUST. PROC. 25, 767-774(1994) !\Comment: WARNING
C4H10+O2=SC4H9+HO2 4.0E13 0.0 4.98E4
!\Author: WARNING !\Ref: MICHAEL, KEIL AND KLEM, INT. J. CHEM. KIN. 15, 705(1983) !\Comment: WARNING
C4H10+O=SC4H9+OH 5.62E13 0.0 5.2E3
!\Author: WARNING !\Ref: DROEGE, A. T. AND TULLY, F. P. !\Comment: WARNING
C4H10+OH=SC4H9+H2O 9.34E7 1.61 -3.5E1
!\Author: WARNING !\Ref: J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A(2008) 112(30) !\Comment: WARNING
C4H10+HO2=SC4H9+H2O2 1.264E2 3.37 1.372E4
!\Author: WARNING !\Ref: TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887(1988) !\Comment: WARNING
C4H10+CH3=SC4H9+CH4 3.02E0 3.46 5.481E3
!\Author: WARNING !\Ref: DRYER ESTIMATE !\Comment: WARNING
C4H10+CH3O=SC4H9+CH3OH 6.0E11 0.0 7.0E3
!\Author: WARNING !\Ref: ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523(1980) !\Comment: WARNING
C4H10+C2H5=SC4H9+C2H6 1.0E11 0.0 1.04E4
!\Author: WARNING !\Ref: SUNDARAM, K. M. AND FROMENT, G. F., I. AND E. C. FUNDAMENTALS 17, 174(1978) !\Comment: WARNING
C4H10+C2H3=SC4H9+C2H4 8.0E11 0.0 1.68E4
!\Author: WARNING !\Ref: ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523(1980) !\Comment: WARNING
C4H10+C3H5-A=SC4H9+C3H6 3.16E11 0.0 1.64E4
!\Author: WARNING !\Ref: ANALOGY TO C2H6+HO2 !\Comment: WARNING
C4H10+NC3H7O2=SC4H9+NC3H7O2H 1.12E13 0.0 1.77E4
!\Author: WARNING !\Ref: ANALOGY TO C2H6+HO2 !\Comment: WARNING
C4H10+IC3H7O2=SC4H9+IC3H7O2H 1.12E13 0.0 1.77E4
!\Author: WARNING !\Ref: ANALOGY TO C2H6+HO2 !\Comment: WARNING
C4H10+SC4H9O2=SC4H9+SC4H9O2H 1.12E13 0.0 1.77E4
!\Author: WARNING !\Ref: ANALOGY TO C2H6+HO2 !\Comment: WARNING
C4H10+TC4H9O2=SC4H9+TC4H9O2H 1.12E13 0.0 1.77E4
!\Author: SP !\Ref: 60% OF NEW FIT !\Comment: WARNING
C4H10+CH3O2=PC4H9+CH3O2H 2.08E1 3.59 1.76E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C4H10+CH3O2=SC4H9+CH3O2H 1.26E2 3.37 1.522E4
!\Author: SP !\Ref: 60% OF NEW FIT !\Comment: WARNING
C4H10+C2H5O2=PC4H9+C2H5O2H 2.08E1 3.59 1.76E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C4H10+C2H5O2=SC4H9+C2H5O2H 1.26E2 3.37 1.522E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C4H10+CH3CO3=CH3CO3H+PC4H9 2.08E1 3.59 1.11E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C4H10+CH3CO3=CH3CO3H+SC4H9 1.26E2 3.37 8.72E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C4H10+O2CHO=PC4H9+HO2CHO 2.08E1 3.59 1.11E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C4H10+O2CHO=SC4H9+HO2CHO 1.26E2 3.37 8.72E3
!\Author: WARNING !\Ref: MIYOSHI A / 2 COMPARED TO R+O2 080415A !\Comment: WARNING
C4H8OOH1-3O2=NC4KET13+OH 1.09E4 2.4 1.99E4
!\Author: WARNING !\Ref: MIYOSHI A / 2 COMPARED TO R+O2 080415A !\Comment: WARNING
C4H8OOH2-4O2=NC4KET24+OH 5.79E1 2.9 1.7E4
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
SC4H9+HO2=SC4H9O+OH 7.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
SC4H9+CH3O2=CH3O+SC4H9O 7.0E12 0.0 -1.0E3
!_____
!\REACTIONCLASS: RADICAL_BETA_SCISSION
!_____
!\Author: WARNING !\Ref: HENRY J. CURRAN INTERNATIONAL JOURNAL OF CHEMICAL KINETICS(2006) 38 !\Comment: WARNING
C2H5+CH3CHO=SC4H9O 3.33E10 0.0 6.397E3
!_____
!\REACTIONCLASS: R+O2(=)PRODUCTS
!_____
!\Author: WARNING !\Ref: IN ARAMCO(BASED ON KLIPPENSTEIN ET AL. N,IC3H7+O2) !\Comment: WARNING
PC4H9+O2=C4H8-1+HO2 8.37E-1 3.59 1.196E4

!\Author: WARNING !\Ref: IN ARAMCO(BASED ON KLIPPENSTEIN ET AL. N,IC3H7+O2) !\Comment: WARNING
SC4H9+O2=C4H8-1+HO2 5.35E-1 3.71 9.322E3
!\Author: WARNING !\Ref: IN ARAMCO(BASED ON KLIPPENSTEIN ET AL. N,IC3H7+O2) !\Comment: WARNING
SC4H9+O2=C4H8-2+HO2 1.07E0 3.71 9.322E3
!_____
!\REACTIONCLASS: R+O2(=)RO2
!_____
!\Author: WARNING !\Ref: MIYOSHI !\Comment: WARNING
PC4H9+O2=PC4H9O2 6.865E16 -1.627 1.987E2
!\Author: WARNING !\Ref: MIYOSHI !\Comment: WARNING
SC4H9+O2=SC4H9O2 3.487E14 -0.816 -5.365E2
!\Author: WARNING !\Ref: WARNING !\Comment: EA+1.4K,20140430 KWZ
NC4KET13=>CH3CHO+CH2CHO+OH 1.05E16 0.0 4.3E4
!\Author: WARNING !\Ref: WARNING !\Comment: EA+1K,20140430 KWZ
NC4KET24=>CH2O+CH3COCH2+OH 1.5E16 0.0 4.3E4
!\Author: WARNING !\Ref: SHARMA !\Comment: A FACTOR REVALUED 20140425 KWZ 6.798E+006 1.300 18200.0
PC4H9O2=C4H8OOH1-3 1.36E7 1.3 1.82E4
!_____
!\REACTIONCLASS: RO2(=)ALKENE+HO2
!_____
!\Author: WARNING !\Ref: VILLANO !\Comment: WARNING
PC4H9O2=C4H8-1+HO2 1.258E8 1.38 2.89E4
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
SC4H9+IC3H7O2=SC4H9O+IC3H7O 7.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
SC4H9+NC3H7O2=SC4H9O+NC3H7O 7.0E12 0.0 -1.0E3
!_____
!\REACTIONCLASS: RH+RO2(=)PRODUCTS
!_____
!\Author: WARNING !\Ref: TSANG _ HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986 !\Comment: WARNING
SC4H9O2+H2=SC4H9O2H+H 3.01E13 0.0 2.603E4
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
SC4H9O2+HO2=SC4H9O2H+O2 1.75E10 0.0 -3.275E3
!\Author: WARNING !\Ref: ANALOGY TO CH2O+HO2 !\Comment: WARNING
SC4H9O2+CH2O=SC4H9O2H+HCO 5.6E12 0.0 1.36E4
!\Author: WARNING !\Ref: ANALOGY TO CH2O+HO2 !\Comment: WARNING
SC4H9O2+CH3CHO=SC4H9O2H+CH3CO 2.8E12 0.0 1.36E4
!\Author: WARNING !\Ref: WESTBROOK ESTIMATE !\Comment: WARNING
SC4H9O2+C2H6=SC4H9O2H+C2H5 1.7E13 0.0 2.046E4
!\Author: WARNING !\Ref: ANALOGY TO C3H6+HO2 !\Comment: WARNING
SC4H9O2+C3H6=SC4H9O2H+C3H5-A 5.35E-2 4.207 1.32881E4
!\Author: WARNING !\Ref: ANALOGY TO C2H4+HO2 !\Comment: WARNING
SC4H9O2+C2H4=SC4H9O2H+C2H3 1.13E13 0.0 3.043E4
!\Author: WARNING !\Ref: ANALOGY TO CH3OH+HO2 !\Comment: WARNING
SC4H9O2+CH3OH=SC4H9O2H+CH2OH 6.3E12 0.0 1.936E4
!\Author: WARNING !\Ref: HALF OF CH2O+HO2 !\Comment: WARNING
SC4H9O2+C2H3CHO=SC4H9O2H+C2H3CO 2.8E12 0.0 1.36E4
!\Author: WARNING !\Ref: ANALOGY TO CH4+HO2 !\Comment: WARNING
SC4H9O2+CH4=SC4H9O2H+CH3 1.12E13 0.0 2.464E4
!\Author: WARNING !\Ref: ANALOGY TO H2O2+CH3O2(=)HO2+CH3O2H !\Comment: WARNING
SC4H9O2+H2O2=SC4H9O2H+HO2 2.4E12 0.0 1.0E4
!\Author: WARNING !\Ref: ANALOGY TO C2H6+HO2 !\Comment: WARNING
SC4H9O2+C3H8=SC4H9O2H+NC3H7 1.7E13 0.0 2.046E4
!\Author: WARNING !\Ref: WALKER, R. W., REACTION KINETICS, VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975 !\Comment: WARNING
SC4H9O2+C3H8=SC4H9O2H+IC3H7 2.0E12 0.0 1.7E4
!_____
!\REACTIONCLASS: RO2+RO2(=)PRODUCTS
!_____
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
SC4H9O2+CH3O2=>SC4H9O+CH3O+O2 1.4E16 -1.61 1.86E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
SC4H9O2+CH3CO3=>SC4H9O+CH3CO2+O2 1.4E16 -1.61 1.86E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
SC4H9O2+NC3H7O2=>SC4H9O+NC3H7O+O2 1.4E16 -1.61 1.86E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING

SC4H9O2+IC3H7O2=>SC4H9O+IC3H7O+O2 1.4E16 -1.61 1.86E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
2SC4H9O2=>2SC4H9O+O2 1.4E16 -1.61 1.86E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
SC4H9O2+C2H5O2=>SC4H9O+C2H5O+O2 1.4E16 -1.61 1.86E3
!_____
!\REACTIONCLASS: R+RO2(=)PRODUCTS
!_____
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
SC4H9O2+CH3=SC4H9O+CH3O 7.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
SC4H9O2+C2H5=SC4H9O+C2H5O 7.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
SC4H9O2+IC3H7=SC4H9O+IC3H7O 7.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
SC4H9O2+NC3H7=SC4H9O+NC3H7O 7.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
SC4H9O2+SC4H9=2SC4H9O 7.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
SC4H9O2+C3H5-A=SC4H9O+C3H5O 7.0E12 0.0 -1.0E3
!_____
!\REACTIONCLASS: KHP_HOMOLYTIC_FISSION
!_____
!\Author: WARNING !\Ref: PITZ ESTIMATE !\Comment: WARNING
SC4H9O+OH=SC4H9O2H 1.0E15 -0.8 0.0E0
!\Author: WARNING !\Ref: SHARMA !\Comment: A FACTOR REVALUED 20140425 KWZ 4.795E+006 1.400 20800.0
SC4H9O2=C4H8OOH2-4 1.439E7 1.4 2.08E4
!_____
!\REACTIONCLASS: QOOH(=)ALKENE_HO2
!_____
!\Author: WARNING !\Ref: VILLANO !\Comment: WARNING
SC4H9O2=C4H8-1+HO2 5.13E9 1.0 3.04E4
!\Author: WARNING !\Ref: VILLANO(FROM KUIWEN'S MECH) !\Comment: WARNING
C4H8OOH1-3=C4H8O1-3+OH 2.59E9 0.69 1.6E4
!\Author: WARNING !\Ref: VILLANO(FROM KUIWEN'S MECH) !\Comment: WARNING
C4H8OOH2-4=C4H8O1-3+OH 2.44E9 0.78 1.8E4
!\Author: SP !\Ref: WARNING !\Comment: WARNING
C4H8O1-3+H=>C3H6+HCO+H2 2.5E12 0.0 0.0E0
!\Author: SP !\Ref: WARNING !\Comment: WARNING
C4H8O1-3+O=>C3H6+HCO+OH 2.5E12 0.0 0.0E0
!\Author: SP !\Ref: WARNING !\Comment: WARNING
C4H8O1-3+OH=>C3H6+HCO+H2O 2.5E12 0.0 0.0E0
!\Author: SP !\Ref: WARNING !\Comment: WARNING
C4H8O1-3+HO2=>C3H6+HCO+H2O2 5.0E12 0.0 1.5E4
!\Author: SP !\Ref: WARNING !\Comment: WARNING
C4H8O1-3+CH3=>C3H6+HCO+CH4 1.0E11 0.0 1.0E4
!\Author: SP !\Ref: WARNING !\Comment: WARNING
C4H8O1-3+CH3O2=>C3H6+HCO+CH3O2H 5.0E12 0.0 1.9E4
!\Author: SP !\Ref: WARNING !\Comment: WARNING
C4H8O1-3+H=>C2H4+CH3CO+H2 2.5E12 0.0 0.0E0
!\Author: SP !\Ref: WARNING !\Comment: WARNING
C4H8O1-3+O=>C2H4+CH3CO+OH 2.5E12 0.0 0.0E0
!\Author: SP !\Ref: WARNING !\Comment: WARNING
C4H8O1-3+OH=>C2H4+CH3CO+H2O 2.5E12 0.0 0.0E0
!\Author: SP !\Ref: WARNING !\Comment: WARNING
C4H8O1-3+HO2=>C2H4+CH3CO+H2O2 5.0E12 0.0 1.5E4
!\Author: SP !\Ref: WARNING !\Comment: WARNING
C4H8O1-3+CH3=>C2H4+CH3CO+CH4 1.0E11 0.0 1.0E4
!\Author: SP !\Ref: WARNING !\Comment: WARNING
C4H8O1-3+CH3O2=>C2H4+CH3CO+CH3O2H 5.0E12 0.0 1.9E4
!=====
!\ENDSUBSPECIES: C4_CYC_ETH
!=====
!---
!\ENDSUBMECH: C4H10

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!-----------------------------------------------------------------------------------------------------------------------
!-----------------------------------------------------------------------------------------------------------------------
!\SUBMECH: IC4H10
!\MECHCOMMENTS: NL: \KINETICS AND THERMO UPDATED AS PART OF IC4 09.09.19
!-----------------------------------------------------------------------------------------------------------------------
!_______________________________________________________________________________________________________________________
!\REACTIONCLASS: QOOH+O2(=)O2QOOH
!_______________________________________________________________________________________________________________________
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H8O2H-I+O2=IC4H8OOH-IO2    3.44E16 -1.627 1.99E2
!_______________________________________________________________________________________________________________________
!\REACTIONCLASS: R+O2(=)PRODUCTS
!_______________________________________________________________________________________________________________________
!\Author: NL !\Ref: IN ARAMCO(BASED ON KLIPPENSTEIN ET AL. N,IC3H7+O2) !\Comment: WARNING
IC4H9+O2=IC4H8+HO2    8.37E-1 3.59 1.196E4
!\Author: NL !\Ref: IN ARAMCO(BASED ON KLIPPENSTEIN ET AL. N,IC3H7+O2) !\Comment: WARNING
TC4H9+O2=IC4H8+HO2    5.35E-1 3.71 9.322E3
!_______________________________________________________________________________________________________________________
!\REACTIONCLASS: RH(=)PRODUCTS
!_______________________________________________________________________________________________________________________
!\Author: WARNING !\Ref: OEHLSCHLAEGER ET AL. J. PHYS. CHEM. A 2004, 108 !\Comment: WARNING
IC4H10(+M)=CH3+IC3H7(+M)    2.52E31 -4.102 9.1495E4
   LOW/2.41E19 0.0E0 5.2576E4/
   TROE/3.662E-1 8.153E2 6.079E1 1.0E20/
!\Author: WARNING !\Ref: OEHLSCHLAEGER ET AL. J. PHYS. CHEM. A 2004, 108 !\Comment: WARNING
IC4H10=TC4H9+H    2.51E98 -23.81 1.453E5
!\Author: WARNING !\Ref: OEHLSCHLAEGER ET AL. J. PHYS. CHEM. A 2004, 108 !\Comment: WARNING
IC4H10=IC4H9+H    9.85E95 -23.11 1.476E5
!_______________________________________________________________________________________________________________________
!\REACTIONCLASS: RH_R_ABSTRACTION
!_______________________________________________________________________________________________________________________
!\Author: WARNING !\Ref: WESTBROOK ESTIMATE !\Comment: WARNING
TC4H9O2+CH4=TC4H9O2H+CH3    1.13E13 0.0 2.046E4
!\Author: WARNING !\Ref: WESTBROOK ESTIMATE !\Comment: WARNING
TC4H9O2+C2H6=TC4H9O2H+C2H5    1.7E13 0.0 2.046E4
!\Author: WARNING !\Ref: WESTBROOK ESTIMATE !\Comment: WARNING
TC4H9O2+C3H8=TC4H9O2H+IC3H7    2.0E12 0.0 1.7E4
!\Author: WARNING !\Ref: WESTBROOK ESTIMATE !\Comment: WARNING
TC4H9O2+C3H8=TC4H9O2H+NC3H7    1.7E13 0.0 2.046E4
!\Author: WARNING !\Ref: WESTBROOK ESTIMATE !\Comment: WARNING
TC4H9O2+CH3OH=TC4H9O2H+CH2OH    6.3E12 0.0 1.936E4
!\Author: WARNING !\Ref: HALF OF CH2O+HO2 !\Comment: WARNING
TC4H9O2+CH3CHO=TC4H9O2H+CH3CO    2.8E12 0.0 1.36E4
!\Author: WARNING !\Ref: HALF OF CH2O+HO2 !\Comment: WARNING
TC4H9O2+C2H3CHO=TC4H9O2H+C2H3CO    2.8E12 0.0 1.36E4
!\Author: WARNING !\Ref: ESTIMATE? !\Comment: WARNING
TC4H9O2+HO2=TC4H9O2H+O2    1.75E10 0.0 -3.275E3
!\Author: WARNING !\Ref: WESTBROOK ESTIMATE !\Comment: WARNING
TC4H9O2+H2O2=TC4H9O2H+HO2    2.4E12 0.0 1.0E4
!\Author: WARNING !\Ref: WESTBROOK ESTIMATE !\Comment: WARNING
TC4H9O2+CH2O=TC4H9O2H+HCO    1.3E11 0.0 9.0E3
!\Author: WARNING !\Ref: PITZ ESTIMATE !\Comment: WARNING
TC4H9O2+C2H4=TC4H9O2H+C2H3    8.59E0 3.754 2.7132E4
!\Author: WARNING !\Ref: TSANG _ HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986 !\Comment: WARNING
TC4H9O2+H2=TC4H9O2H+H    3.01E13 0.0 2.603E4
!\Author: WARNING !\Ref: ANALOGY TO C3H6+HO2 !\Comment: WARNING
TC4H9O2+C3H6=TC4H9O2H+C3H5-A    5.35E-2 4.207 1.32881E4
!_______________________________________________________________________________________________________________________
!\REACTIONCLASS: O2QOOH(=)PRODUCTS
!_______________________________________________________________________________________________________________________
!\Author: WARNING !\Ref: GREEN 2003 WARNING !\Comment: WARNING
IC4H8OOH-IO2=IC4KETII+OH    5.2E4 1.9 1.88E4
!_______________________________________________________________________________________________________________________
!\REACTIONCLASS: R+O2(=)RO2
!_______________________________________________________________________________________________________________________
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!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H9+O2=IC4H9O2 6.86E16 -1.627 1.99E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
TC4H9+O2=TC4H9O2 9.752E11 0.325 -4.17E2
!_____
!\REACTIONCLASS: RH+R_ABSTRACTION
!_____
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H10+CH3=IC4H9+CH4 5.4E0 3.65 7.1463E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H10+H=IC4H9+H2 1.56E8 1.943 7.898325E3
!\Author: WARNING !\Ref: JOE MICHAELS SYMP. PAPER 2008. !\Comment: WARNING
IC4H10+OH=IC4H9+H2O 6.7E4 2.665 -1.69E2
!\Author: WARNING !\Ref: ALLARA AND SHAW ANALOG !\Comment: WARNING
IC4H10+C2H5=IC4H9+C2H6 1.51E12 0.0 1.04E4
!\Author: SP !\Ref: 60% OF NEW RATE !\Comment: WARNING
IC4H10+HO2=IC4H9+H2O2 3.12E1 3.59 1.56E4
!\Author: WARNING !\Ref: NIST STANDARD REFERENCE DATABASE 17 -2Q98 !\Comment: WARNING
IC4H10+O=IC4H9+OH 4.046E7 2.034 5.136E3
!\Author: WARNING !\Ref: ANALOGY TO C3H8+CH3O !\Comment: WARNING
IC4H10+CH3O=IC4H9+CH3OH 4.8E11 0.0 7.0E3
!\Author: WARNING !\Ref: ANALOGY WITH C4H10+O2(=)PC4H9+HO2 !\Comment: WARNING
IC4H10+O2=IC4H9+HO2 9.0E13 0.0 5.229E4
!\Author: WARNING !\Ref: J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A(2008) 112(30) !\Comment: WARNING
IC4H10+CH3O2=IC4H9+CH3O2H 2.77E0 3.97 1.828E4
!\Author: WARNING !\Ref: SCOTT AND WALKER C_F 129(4) 365--377 2002(*1.5) !\Comment: WARNING
IC4H10+C2H5O2=IC4H9+C2H5O2H 2.55E13 0.0 2.046E4
!\Author: WARNING !\Ref: ANALOGY TO C2H6+HO2 !\Comment: WARNING
IC4H10+CH3CO3=IC4H9+CH3CO3H 2.55E13 0.0 2.046E4
!\Author: WARNING !\Ref: ANALOGY TO C2H6+HO2 !\Comment: WARNING
IC4H10+NC3H7O2=IC4H9+NC3H7O2H 2.55E13 0.0 2.046E4
!\Author: WARNING !\Ref: ANALOGY TO C2H6+HO2 !\Comment: WARNING
IC4H10+IC3H7O2=IC4H9+IC3H7O2H 2.55E13 0.0 2.046E4
!\Author: WARNING !\Ref: ANALOGY TO C2H6+HO2 !\Comment: WARNING
IC4H10+TC4H9O2=IC4H9+TC4H9O2H 2.55E13 0.0 2.046E4
!\Author: WARNING !\Ref: ANALOGY TO C2H6+HO2 !\Comment: WARNING
IC4H10+O2CHO=IC4H9+HO2CHO 2.52E13 0.0 2.044E4
!\Author: WARNING !\Ref: ANALOGY TO C2H6+HO2 !\Comment: WARNING
IC4H10+SC4H9O2=IC4H9+SC4H9O2H 2.25E13 0.0 2.046E4
!\Author: WARNING !\Ref: WALKER, R. W., 22ND SYMPOSIUM(INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988 !\Comment: WARNING
IC4H10+SC4H9O2=TC4H9+SC4H9O2H 2.8E12 0.0 1.6E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H10+H=TC4H9+H2 5.7E7 1.849 4.07985E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H10+CH3=TC4H9+CH4 3.6E0 3.46 4.589E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H10+OH=TC4H9+H2O 4.85E6 1.84 -9.996E2
!\Author: WARNING !\Ref: FROM ISOBUTYL RATE !\Comment: WARNING
IC4H10+C2H5=TC4H9+C2H6 1.0E11 0.0 7.9E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H10+HO2=TC4H9+H2O2 9.75E2 3.01 1.209E4
!\Author: WARNING !\Ref: NIST STANDARD REFERENCE DATABASE 17 -2Q98 !\Comment: WARNING
IC4H10+O=TC4H9+OH 1.968E5 2.402 1.15E3
!\Author: WARNING !\Ref: TAMURA ESTIMATE !\Comment: WARNING
IC4H10+CH3O=TC4H9+CH3OH 1.9E10 0.0 2.8E3
!\Author: WARNING !\Ref: INGHAM,T.; WALKER,R.W.; WOOLFORD,R.E., SYMP. INT. COMBUST. PROC. 25, 767-774(1994) !\Comment: WARNING
IC4H10+O2=TC4H9+HO2 1.0E13 0.0 4.82E4
!\Author: WARNING !\Ref: ANALOGY WITH RH+RO2 --)R+RO2H !\Comment: WARNING
IC4H10+O2CHO=TC4H9+HO2CHO 2.8E12 0.0 1.601E4
!\Author: WARNING !\Ref: J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A(2008) 112(30) !\Comment: WARNING
IC4H10+CH3O2=TC4H9+CH3O2H 1.366E2 3.12 1.319E4
!\Author: WARNING !\Ref: WALKER, R. W., 22ND SYMPOSIUM(INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988 !\Comment: WARNING
IC4H10+C2H5O2=TC4H9+C2H5O2H 2.8E12 0.0 1.6E4
!\Author: WARNING !\Ref: WALKER, R. W., 22ND SYMPOSIUM(INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988 !\Comment: WARNING
IC4H10+CH3CO3=TC4H9+CH3CO3H 2.8E12 0.0 1.6E4

!\Author: WARNING !\Ref: WALKER, R. W., 22ND SYMPOSIUM(INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988 !\Comment: WARNING
IC4H10+NC3H7O2=TC4H9+NC3H7O2H 2.8E12 0.0 1.6E4
!\Author: WARNING !\Ref: WALKER, R. W., 22ND SYMPOSIUM(INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988 !\Comment: WARNING
IC4H10+IC3H7O2=TC4H9+IC3H7O2H 2.8E12 0.0 1.6E4
!\Author: WARNING !\Ref: WALKER, R. W., 22ND SYMPOSIUM(INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988 !\Comment: WARNING
IC4H10+TC4H9O2=TC4H9+TC4H9O2H 2.8E12 0.0 1.6E4
!\Author: WARNING !\Ref: WESTBROOK AND PITZ ESTIMATE(1983) !\Comment: WARNING
IC4H10+IC4H9=TC4H9+IC4H10 2.5E10 0.0 7.9E3
!_____
!\REACTIONCLASS: O2QOOH(=)ALKENEKHP+HO2
!_____
!\Author: NL !\Ref: WARNING NO REFERENCE !\Comment: WARNING
IC4H8OOH-IO2=IC4H7OOH+HO2 1.26E8 1.32 2.89E4
!_____
!\REACTIONCLASS: RO2(=)ALKENE+HO2
!_____
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H9O2=IC4H8+HO2 2.0E8 1.27 2.96E4
!_____
!\REACTIONCLASS: R+RO2(=)PRODUCTS
!_____
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
TC4H9+HO2=TC4H9O+OH 9.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
TC4H9+CH3O2=TC4H9O+CH3O 9.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
TC4H9+NC3H7O2=TC4H9O+NC3H7O 9.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
TC4H9+SC4H9O2=TC4H9O+SC4H9O 9.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
TC4H9+IC3H7O2=TC4H9O+IC3H7O 9.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
IC4H9+HO2=IC4H9O+OH 9.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
IC4H9+CH3O2=IC4H9O+CH3O 9.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
IC4H9+NC3H7O2=IC4H9O+NC3H7O 9.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
IC4H9+SC4H9O2=IC4H9O+SC4H9O 9.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
IC4H9+IC3H7O2=IC4H9O+IC3H7O 9.0E12 0.0 -1.0E3
!_____
!\REACTIONCLASS: RO2+RO2(=)PRODUCTS
!_____
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H9O2+CH3O2=>IC4H9O+CH3O+O2 1.4E16 -1.61 1.86E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H9O2+C2H5O2=>IC4H9O+C2H5O+O2 1.4E16 -1.61 1.86E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H9O2+CH3CO3=>IC4H9O+CH3CO2+O2 1.4E16 -1.61 1.86E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
2IC4H9O2=>O2+2IC4H9O 1.4E16 -1.61 1.86E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H9O2+TC4H9O2=>IC4H9O+TC4H9O+O2 1.4E16 -1.61 1.86E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H9O2+SC4H9O2=>IC4H9O+SC4H9O+O2 1.4E16 -1.61 1.86E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H9O2+NC3H7O2=>IC4H9O+NC3H7O+O2 1.4E16 -1.61 1.86E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H9O2+IC3H7O2=>IC4H9O+IC3H7O+O2 1.4E16 -1.61 1.86E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H9O2+HO2=>IC4H9O+OH+O2 1.4E16 -1.61 1.86E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
TC4H9O2+CH3O2=>TC4H9O+CH3O+O2 1.4E16 -1.61 1.86E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING

TC4H9O2+C2H5O2=>TC4H9O+C2H5O+O2 1.4E16 -1.61 1.86E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
TC4H9O2+CH3CO3=>TC4H9O+CH3CO2+O2 1.4E16 -1.61 1.86E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
2TC4H9O2=>2TC4H9O+O2 1.4E16 -1.61 1.86E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
TC4H9O2+SC4H9O2=>TC4H9O+SC4H9O+O2 1.4E16 -1.61 1.86E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
TC4H9O2+NC3H7O2=>TC4H9O+NC3H7O+O2 1.4E16 -1.61 1.86E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
TC4H9O2+IC3H7O2=>TC4H9O+IC3H7O+O2 1.4E16 -1.61 1.86E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
TC4H9O2+HO2=>TC4H9O+OH+O2 1.4E16 -1.61 1.86E3
!_____
!\REACTIONCLASS: KHP_HOMOLYTIC_FISSION
!_____
!\Author: NL_ALKANE RATE RULES !\Ref: WARNING !\Comment: WARNING
IC4KETII=>CH2O+CH3CHCHO+OH 1.5E16 0.0 4.3E4
!_____
!\REACTIONCLASS: R+RO2(=)PRODUCTS
!_____
!\Author: NL_16.9.19 !\Ref: WARNING !\Comment: WARNING
IC4H9O2+CH3=IC4H9O+CH3O 9.0E12 0.0 -1.0E3
!\Author: NL_16.9.19 !\Ref: WARNING !\Comment: WARNING
IC4H9O2+C2H5=IC4H9O+C2H5O 9.0E12 0.0 -1.0E3
!\Author: NL_16.9.19 !\Ref: WARNING !\Comment: WARNING
IC4H9O2+IC3H7=IC4H9O+IC3H7O 9.0E12 0.0 -1.0E3
!\Author: NL_16.9.19 !\Ref: WARNING !\Comment: WARNING
IC4H9O2+NC3H7=IC4H9O+NC3H7O 9.0E12 0.0 -1.0E3
!\Author: NL_16.9.19 !\Ref: WARNING !\Comment: WARNING
IC4H9O2+SC4H9=IC4H9O+SC4H9O 9.0E12 0.0 -1.0E3
!\Author: NL_16.9.19 !\Ref: WARNING !\Comment: WARNING
IC4H9O2+IC4H9=2IC4H9O 9.0E12 0.0 -1.0E3
!\Author: NL_16.9.19 !\Ref: WARNING !\Comment: WARNING
IC4H9O2+TC4H9=IC4H9O+TC4H9O 9.0E12 0.0 -1.0E3
!\Author: NL_16.9.19 !\Ref: WARNING !\Comment: WARNING
IC4H9O2+C3H5-A=IC4H9O+C3H5O 9.0E12 0.0 -1.0E3
!\Author: NL_16.9.19 !\Ref: WARNING !\Comment: WARNING
IC4H9O2+IC4H7=IC4H9O+IC4H7O 9.0E12 0.0 -1.0E3
!\Author: NL_16.9.19 !\Ref: WARNING !\Comment: WARNING
TC4H9O2+CH3=TC4H9O+CH3O 9.0E12 0.0 -1.0E3
!\Author: NL_16.9.19 !\Ref: WARNING !\Comment: WARNING
TC4H9O2+C2H5=TC4H9O+C2H5O 9.0E12 0.0 -1.0E3
!\Author: NL_16.9.19 !\Ref: WARNING !\Comment: WARNING
TC4H9O2+IC3H7=TC4H9O+IC3H7O 9.0E12 0.0 -1.0E3
!\Author: NL_16.9.19 !\Ref: WARNING !\Comment: WARNING
TC4H9O2+NC3H7=TC4H9O+NC3H7O 9.0E12 0.0 -1.0E3
!\Author: NL_16.9.19 !\Ref: WARNING !\Comment: WARNING
TC4H9O2+SC4H9=TC4H9O+SC4H9O 9.0E12 0.0 -1.0E3
!\Author: NL_16.9.19 !\Ref: WARNING !\Comment: WARNING
TC4H9O2+IC4H9=TC4H9O+IC4H9O 9.0E12 0.0 -1.0E3
!\Author: NL_16.9.19 !\Ref: WARNING !\Comment: WARNING
TC4H9O2+TC4H9=2TC4H9O 9.0E12 0.0 -1.0E3
!\Author: NL_16.9.19 !\Ref: WARNING !\Comment: WARNING
TC4H9O2+C3H5-A=TC4H9O+C3H5O 9.0E12 0.0 -1.0E3
!_____
!\REACTIONCLASS: RO2(=)QOOH
!_____
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H9O2=IC4H8O2H-I 7.14E6 1.6 2.1E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H9O2=IC4H8O2H-T 2.32E9 0.8 2.71E4
!\Author: WARNING !\Ref: GREEN 2003 !\Comment: WARNING
IC4H8O2H-I=>OH+CH2O+C3H6 3.08E13 0.0 2.67688E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING

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IC4H8O2H-I=AC3H5OOH+CH3    5.0E10 0.83 2.8E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H8O2H-T=IC4H7OOH+H    1.8E9 1.52 2.95E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H8O2H-I=IC4H8O2H-T    5.26E-7 5.64 2.4541E4
!=============================================================================================================
!\SUBSPECIES: TC4H9O
!=============================================================================================================
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_BETA_SCISSION
!_____________________________________________________________________________________________________________
!\Author: WARNING !\Ref: CURRAN INC. INT J CHEM KINET 38 !\Comment: WARNING
CH3COCH3+CH3=TC4H9O    1.5E11 0.0 1.19E4
!\Author: WARNING !\Ref: CURRAN INC. INT J CHEM KINET 38 !\Comment: WARNING
CH2O+IC3H7=IC4H9O    5.0E10 0.0 2.33E3
!\Author: NL !\Ref: WARNING NO REFERENCE !\Comment: WARNING
TC4H9O2H=TC4H9O+OH    8.618E20 -1.641 4.51556E4
!=============================================================================================================
!\ENDSUBSPECIES: IC4H9O2H
!=============================================================================================================
!-------------------------------------------------------------------------------------------------------------
!\ENDSUBMECH: IC4H10
!-------------------------------------------------------------------------------------------------------------
!-------------------------------------------------------------------------------------------------------------
!\SUBMECH: IC4H8
!-------------------------------------------------------------------------------------------------------------
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: RH(=)PRODUCTS
!_____________________________________________________________________________________________________________
!\Author: NL WARNING !\Ref: WARNING !\Comment: WARNING
CH2(S)+C3H6=IC4H8    6.07E47 -9.85 2.21E4
   PLOG/1.0E-2 4.82E57 -1.43E1 1.71E4/
   PLOG/1.0E-2 1.15E45 -1.11E1 6.1452E3/
   PLOG/1.0E-1 3.84E59 -1.44E1 1.84E4/
   PLOG/1.0E-1 1.83E45 -1.07E1 6.6385E3/
   PLOG/1.0E0 2.13E58 -1.35E1 2.04E4/
   PLOG/1.0E0 1.3E40 -8.77E0 5.8638E3/
   PLOG/1.0E1 8.48E52 -1.16E1 2.07E4/
   PLOG/1.0E1 2.27E32 -6.14E0 4.3179E3/
   PLOG/1.0E2 6.07E47 -9.85E0 2.21E4/
   PLOG/1.0E2 1.28E24 -3.49E0 2.5299E3/
!\Author: NL WARNING !\Ref: WARNING !\Comment: WARNING
CH2(S)+C3H6=IC4H7+H    6.51E26 -3.58 1.89E4
   PLOG/1.0E-2 8.2E19 -2.06E0 1.15E3/
   PLOG/1.0E-2 1.08E7 1.62E0 -3.1746E3/
   PLOG/1.0E-1 2.27E21 -2.44E0 2.65E3/
   PLOG/1.0E-1 1.37E5 2.15E0 -3.7992E3/
   PLOG/1.0E0 4.44E35 -6.55E0 1.39E4/
   PLOG/1.0E0 3.89E14 -4.2E-1 1.2376E3/
   PLOG/1.0E1 1.18E28 -4.09E0 1.4E4/
   PLOG/1.0E1 2.45E10 6.7E-1 7.5093E2/
   PLOG/1.0E2 6.51E26 -3.58E0 1.89E4/
   PLOG/1.0E2 1.81E2 2.97E0 -7.4603E2/
!\Author: NL WARNING !\Ref: WARNING !\Comment: WARNING
CH2(S)+C3H6=C3H5-T+CH3    7.36E29 -4.28 2.38E4
   PLOG/1.0E-2 1.77E19 -1.94E0 6.79E3/
   PLOG/1.0E-2 4.3E12 1.9E-1 -1.1041E2/
   PLOG/1.0E-1 1.68E19 -1.8E0 4.31E3/
   PLOG/1.0E-1 2.26E11 5.4E-1 4.781E1/
   PLOG/1.0E0 4.16E24 -3.19E0 9.76E3/
   PLOG/1.0E0 4.92E9 1.02E0 5.9977E2/
   PLOG/1.0E1 7.89E24 -3.07E0 1.39E4/
   PLOG/1.0E1 1.47E8 1.33E0 1.2284E3/
   PLOG/1.0E2 7.36E29 -4.28E0 2.38E4/
   PLOG/1.0E2 8.11E10 5.5E-1 5.5065E3/
```

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!\Author: NL WARNING !\Ref: WARNING !\Comment: WARNING
C3H5-T+CH3=IC4H7+H    5.16E28 -4.03 2.38E4
   PLOG/1.0E-2 4.12E29 -4.95E0 8.0E3/
   PLOG/1.0E-2 5.73E15 -7.7E-1 1.1959E3/
   PLOG/1.0E-1 4.86E30 -5.03E0 1.13E4/
   PLOG/1.0E-1 2.06E13 -7.4E-2 1.4287E3/
   PLOG/1.0E0 5.3E29 -4.57E0 1.44E4/
   PLOG/1.0E0 4.48E10 6.0E-1 1.4216E3/
   PLOG/1.0E1 1.32E30 -4.54E0 1.93E4/
   PLOG/1.0E1 4.1E6 1.71E0 1.0569E3/
   PLOG/1.0E2 5.16E28 -4.03E0 2.38E4/
   PLOG/1.0E2 1.37E-1 3.91E0 -3.5355E2/
!\Author: NL WARNING !\Ref: WARNING !\Comment: WARNING
IC4H8=C3H5-T+CH3    2.15E64 -13.4 1.35E5
   PLOG/1.0E-2 3.76E78 -1.87E1 1.3E5/
   PLOG/1.0E-2 3.38E59 -1.36E1 1.13E5/
   PLOG/1.0E-1 1.75E77 -1.79E1 1.32E5/
   PLOG/1.0E-1 4.0E60 -1.37E1 1.15E5/
   PLOG/1.0E0 1.16E76 -1.72E1 1.34E5/
   PLOG/1.0E0 1.34E55 -1.18E1 1.14E5/
   PLOG/1.0E1 1.62E72 -1.58E1 1.36E5/
   PLOG/1.0E1 2.12E47 -9.27E0 1.12E5/
   PLOG/1.0E2 4.3E64 -1.34E1 1.35E5/
   PLOG/1.0E2 1.46E39 -6.7E0 1.09E5/
!\Author: NL WARNING !\Ref: YE, GEORGIEVSKII, KLIPPENSTEIN, PROC. COMBUST. 35(2015) 223-230 !\Comment: WARNING
IC4H8=IC4H7+H    8.05E56 -11.5 1.22E5
   PLOG/1.0E-2 1.83E75 -1.76E1 1.2E5/
   PLOG/1.0E-2 5.96E54 -1.23E1 1.01E5/
   PLOG/1.0E-1 3.46E70 -1.6E1 1.2E5/
   PLOG/1.0E-1 2.74E43 -8.87E0 9.64E4/
   PLOG/1.0E0 2.16E71 -1.59E1 1.25E5/
   PLOG/1.0E0 1.26E43 -8.51E0 9.8E4/
   PLOG/1.0E1 1.28E66 -1.42E1 1.25E5/
   PLOG/1.0E1 9.46E35 -6.26E0 9.56E4/
   PLOG/1.0E2 1.61E57 -1.15E1 1.22E5/
   PLOG/1.0E2 8.68E28 -4.06E0 9.31E4/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RH+R_ABSTRACTION
!_____________________________________________________________________________________________________
!\Author: NL_PROPENE ANALOGY IN THE SAME BASE !\Ref: WARNING !\Comment: WARNING
IC4H8+H=IC4H7+H2    7.3E5 2.455 4.3612E3
!\Author: NL !\Ref: ZHOU, SIMMIE, SOMERS, GOLDSMITH, CURRAN, J. PHYS. CHEM. A 2017, 121, 1890-1899 !\Comment: WARNING
IC4H8+O2=IC4H7+HO2    1.323E18 -1.156 4.5131673E4
!\Author: NL PROPENE ANALOGY !\Ref: BEDJANIAN, MORIN, J. PHYS. CHEM. A 2017, 121, 1553-1562 !\Comment: WARNING
IC4H8+O=IC4H7+OH    1.936E-2 4.54 -2.4684E3
!\Author: NL !\Ref: KHALED ET AL. 2017 PROCI !\Comment: WARNING
IC4H8+OH=IC4H7+H2O    4.2E7 1.77 2.714E2
!\Author: NL !\Ref: ZADOR, KLIPPENSTEIN, AND MILLER - J. PHYS. CHEM. A, 2011, 115(36), PP 10218-10225 !\Comment: WARNING
IC4H8+HO2=IC4H7+H2O2    2.92E-1 4.12 1.2802E4
!\Author: NL_KUN WANG'S MECHANISM(2019) !\Ref: WARNING !\Comment: WARNING
IC4H8+CH3=IC4H7+CH4    1.104E2 3.27 7.15E3
!\Author: NL_PROPENE ANALOGY IN THE SAME BASE !\Ref: WARNING !\Comment: WARNING
IC4H8+CH3O=IC4H7+CH3OH    1.68E11 0.0 2.6E3
!\Author: NL_PROPENE ANALOGY IN THE SAME BASE !\Ref: WARNING !\Comment: WARNING
IC4H8+CH3O2=IC4H7+CH3O2H    1.54E-1 4.403 1.35472E4
!\Author: NL_PROPENE ANALOGY IN THE SAME BASE !\Ref: WARNING !\Comment: WARNING
IC4H8+C2H5=IC4H7+C2H6    2.0E11 0.0 9.8E3
!\Author: NL_PROPENE ANALOGY IN THE SAME BASE !\Ref: WARNING !\Comment: WARNING
IC4H8+C2H5O2=IC4H7+C2H5O2H    1.152E-1 4.403 1.35472E4
!\Author: !REF !\Ref: WARNING !\Comment: WARNING
IC4H8+CH3CO3=IC4H7+CH3CO3H    1.54E-1 4.403 1.35472E4
!\Author: !REF !\Ref: WARNING !\Comment: WARNING
IC4H8+O2CHO=IC4H7+HO2CHO    1.928E4 2.6 1.391E4
!\Author: !REF !\Ref: WARNING !\Comment: WARNING
IC4H8+TC4H9O2=IC4H7+TC4H9O2H    1.4E12 0.0 1.49E4
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!\Author: !REF !\Ref: WARNING !\Comment: WARNING
IC4H8+SC4H9O2=IC4H7+SC4H9O2H 1.4E12 0.0 1.49E4
!\Author: !REF !\Ref: WARNING !\Comment: WARNING
IC4H8+IC3H7O2=IC4H7+IC3H7O2H 1.4E12 0.0 1.49E4
!\Author: !REF !\Ref: WARNING !\Comment: WARNING
IC4H8+NC3H7O2=IC4H7+NC3H7O2H 1.4E12 0.0 1.49E4
!\Author: NL_ANALOGY !\Ref: RAMAN, CARSTENSEN, INT J CHEM KINET 44.5(2012) !\Comment: WARNING
IC4H8+C2H3=IC4H7+C2H4 1.08E2 3.34 3.0E3
!\Author: !REF !\Ref: WARNING !\Comment: WARNING
IC4H8+C3H5-A=IC4H7+C3H6 7.94E11 0.0 2.05E4
!\Author: !REF !\Ref: WARNING !\Comment: WARNING
IC4H8+C3H5-S=IC4H7+C3H6 7.94E11 0.0 2.05E4
!\Author: !REF !\Ref: WARNING !\Comment: WARNING
IC4H8+C3H5-T=IC4H7+C3H6 7.94E11 0.0 2.05E4
!\Author: NL_PROPENE ANALOGY !\Ref: BEDJANIAN, MORIN, J. PHYS. CHEM. A 2017, 121, 1553-1562 !\Comment: WARNING
IC4H8+O=CH3COCH2+CH3 1.17E-3 4.94 -2.4228E3
  DUP
!\Author: NL_PROPENE ANALOGY !\Ref: BEDJANIAN, MORIN, J. PHYS. CHEM. A 2017, 121, 1553-1562 !\Comment: WARNING
IC4H8+O=CH3COCH2+CH3 9.24E8 1.2 -2.383E2
  DUP
!\Author: NL_PROPENE ANALOGY !\Ref: BEDJANIAN, MORIN, J. PHYS. CHEM. A 2017, 121, 1553-1562 !\Comment: WARNING
IC4H8+O=IC3H7+HCO 6.23E9 0.79 -1.47E2
!\Author: NL_PROPENE ANALOGY !\Ref: BEDJANIAN, MORIN, J. PHYS. CHEM. A 2017, 121, 1553-1562 !\Comment: WARNING
IC4H8+O=C3H6+CH2O 1.46E5 2.365 -8.321E2
!_____
!\REACTIONCLASS: RADICAL_ADDITIONH
!_____
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H8+H=IC4H9 1.22111337E21 -2.30044118 8.97295916E3
  PLOG/1.0E-2 5.08177554E60 -1.53291958E1 1.82033909E4/
  PLOG/1.0E-1 1.32987545E57 -1.38481426E1 1.95398908E4/
  PLOG/1.0E0 1.49024916E47 -1.05045446E1 1.78342512E4/
  PLOG/1.0E1 1.50969538E33 -6.06218608E0 1.34115071E4/
  PLOG/1.0E2 1.22111337E21 -2.30044118E0 8.97295916E3/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H8+H=TC4H9 4.46407033E23 -2.83965302 6.67801904E3
  PLOG/1.0E-2 5.73956633E61 -1.53227045E1 1.70532182E4/
  PLOG/1.0E-1 1.35152506E57 -1.35640258E1 1.71159581E4/
  PLOG/1.0E0 1.18344142E47 -1.02255249E1 1.46880129E4/
  PLOG/1.0E1 1.17235992E36 -6.69847535E0 1.13111983E4/
  PLOG/1.0E2 4.46407033E23 -2.83965302E0 6.67801904E3/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H8+H=C3H6+CH3 1.93202678E11 1.3035533 1.50855325E4
  PLOG/1.0E-2 5.84575102E19 -1.71979462E0 7.30358052E3/
  PLOG/1.0E-1 2.53518239E27 -3.85920702E0 1.30947947E4/
  PLOG/1.0E0 8.32015681E31 -5.03135957E0 1.83405586E4/
  PLOG/1.0E1 8.60341274E26 -3.39703976E0 1.94913021E4/
  PLOG/1.0E2 1.93202678E11 1.3035533E0 1.50855325E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H9=C3H6+CH3 2.68765606E28 -4.31510745 3.80665531E4
  PLOG/1.0E-2 3.06678836E59 -1.48679929E1 4.45949176E4/
  PLOG/1.0E-1 2.73169026E56 -1.3556788E1 4.52360935E4/
  PLOG/1.0E0 5.23049393E49 -1.11739312E1 4.44248061E4/
  PLOG/1.0E1 3.31238228E39 -7.82434163E0 4.17721259E4/
  PLOG/1.0E2 2.68765606E28 -4.31510745E0 3.80665531E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
TC4H9=C3H6+CH3 2.99954026E26 -3.47712836 5.3263557E4
  PLOG/1.0E-2 2.31802144E57 -1.40132722E1 5.22216763E4/
  PLOG/1.0E-1 2.11533307E57 -1.36178037E1 5.5375839E4/
  PLOG/1.0E0 2.0231547E53 -1.20256567E1 5.7484892E4/
  PLOG/1.0E1 4.77650923E43 -8.81277619E0 5.73612501E4/
  PLOG/1.0E2 2.99954026E26 -3.47712836E0 5.3263557E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H9=TC4H9 1.58476133E25 -3.85678223 3.47611859E4
  PLOG/1.0E-2 8.77258715E59 -1.55127981E1 4.24465458E4/

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   PLOG/1.0E-1 1.46467336E56 -1.39946385E1 4.29907024E4/
   PLOG/1.0E0 2.23785573E48 -1.12863917E1 4.18028818E4/
   PLOG/1.0E1 1.45144498E37 -7.63709644E0 3.87752972E4/
   PLOG/1.0E2 1.58476133E25 -3.85678223E0 3.47611859E4/
!_____________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_BETA_SCISSION
!_____________________________________________________________________________________________
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H7=C3H4-A+CH3    2.246E54 -11.14216 8.50228251E4
   PLOG/1.0E-2 3.682E54 -1.247531E1 7.15978436E4/
   PLOG/1.0E-1 1.396E55 -1.231844E1 7.43852009E4/
   PLOG/1.0E0 2.519E55 -1.207106E1 7.75106364E4/
   PLOG/1.0E1 1.368E55 -1.167732E1 8.10161398E4/
   PLOG/1.0E2 2.246E54 -1.114216E1 8.50228251E4/
!_____________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONHO2
!_____________________________________________________________________________________________
!\Author: WARNING !\Ref: ZADOR(J. PHYS. CHEM. A., 2011,115,10218) !\Comment: WARNING
IC4H8+HO2=TC4H9O2    1.04E-1 3.45 4.338E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H8+HO2=IC4H8O2H-T    3.25E26 -4.89 1.9948E4
   PLOG/1.33E-2 6.62E6 -1.4E-1 1.1076E4/
   PLOG/1.0E0 7.2E4 8.8E-1 7.816E3/
   PLOG/1.0E1 1.69E16 -2.21E0 1.3289E4/
   PLOG/1.0E2 3.25E26 -4.89E0 1.9948E4/
!_____________________________________________________________________________________________
!\REACTIONCLASS: R+R(=)RH+RH
!_____________________________________________________________________________________________
!\Author: WARNING !\Ref: KLIPPENSTEIN _ HARDING 2007 !\Comment: WARNING
IC4H7+H=C3H4-A+CH4    1.232E3 3.035 2.582E3
!\Author: WARNING !\Ref: TSANG, W. J.PHYS.CHEM.REF.DATA 1991, 20, 221. !\Comment: WARNING
IC4H7+OH=C3H4-A+CH3OH    6.0E12 0.0 0.0E0
!\Author: WARNING !\Ref: LASKIN ET AL. IJCK 32 589-614 2000 !\Comment: WARNING
IC4H7+CH3=C3H4-A+C2H6    3.0E12 -0.32 -1.31E2
!\Author: WARNING !\Ref: DAGAUT, P. ET AL., CST 71, 111(1990). !\Comment: WARNING
IC4H7+C2H5=C3H4-A+C3H8    4.0E11 0.0 0.0E0
!\Author: WARNING !\Ref: DAGAUT, P. ET AL., CST 71, 111(1990). !\Comment: WARNING
IC4H7+C2H3=C3H4-A+C3H6    1.0E12 0.0 0.0E0
!_____________________________________________________________________________________________
!\REACTIONCLASS: R+R(=)PRODUCTS
!_____________________________________________________________________________________________
!\Author: WARNING !\Ref: DAGAUT, P. ET AL., CST 71, 111(1990). !\Comment: WARNING
IC4H7+C2H5=C2H4+IC4H8    4.0E11 0.0 0.0E0
!\Author: WARNING !\Ref: LASKIN ET AL. IJCK 32 589-614 2000 !\Comment: WARNING
IC4H7+HCO=IC4H8+CO    6.0E13 0.0 0.0E0
!_____________________________________________________________________________________________
!\REACTIONCLASS: R+O(=)PRODUCTS
!_____________________________________________________________________________________________
!\Author: WARNING !\Ref: TSANG, W. J.PHYS.CHEM.REF.DATA 1991, 20, 221. !\Comment: WARNING
IC4H7+O=IC3H5CHO+H    6.0E13 0.0 0.0E0
!_____________________________________________________________________________________________
!\REACTIONCLASS: R+OH(=)PRODUCTS
!_____________________________________________________________________________________________
!\Author: WARNING !\Ref: TSANG, W. J.PHYS.CHEM.REF.DATA 1991, 20, 221. !\Comment: WARNING
IC4H7+OH=>IC3H5CHO+2H    1.6E20 -1.56 2.633E4
   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/
!_____________________________________________________________________________________________
!\REACTIONCLASS: R+O2(=)PRODUCTS
!_____________________________________________________________________________________________
!\Author: WARNING !\Ref: LASKIN ET AL. IJCK 32 589-614 2000 !\Comment: WARNING
IC4H7+O2=>C3H4-A+CH2O+OH    2.18E21 -2.85 3.0755E4
   PLOG/1.0E0 4.99E15 -1.4E0 2.2428E4/
   PLOG/1.0E1 2.18E21 -2.85E0 3.0755E4/
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!\Author: WARNING !\Ref: LASKIN ET AL. IJCK 32 589-614 2000 !\Comment: WARNING
IC4H7+O2=IC3H5CHO+OH    2.47E13 -0.45 2.3017E4
   PLOG/1.0E0 1.82E13 -4.1E-1 2.2859E4/
   PLOG/1.0E1 2.47E13 -4.5E-1 2.3017E4/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+HO2(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H7+HO2=IC4H7OOH    3.9E34 -6.795 7.654E3
   PLOG/1.0E-1 6.1E17 -3.062E0 -6.394E3/
   PLOG/1.0E0 3.3E35 -7.872E0 3.123E3/
   PLOG/1.0E1 3.64E40 -8.906E0 8.118E3/
   PLOG/1.0E2 3.9E34 -6.795E0 7.654E3/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H7+HO2=IC4H7O+OH    4.81E17 -1.228 7.798E3
   PLOG/1.0E-1 7.88E9 7.83E-1 -2.33E3/
   PLOG/1.0E0 1.0E13 -8.7E-2 -1.1E1/
   PLOG/1.0E1 1.6E18 -1.503E0 4.824E3/
   PLOG/1.0E2 4.81E17 -1.228E0 7.798E3/
!\Author: WARNING !\Ref: FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325?346 \COMMENT !\Comment: WARNING
IC4H7+HO2=IC3H5CHO+H2O    5.07E-5 4.59 9.275E2
   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/
!\Author: WARNING !\Ref: FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325?346 \COMMENT !\Comment: WARNING
IC4H7OOH=IC3H5CHO+H2O    1.48E16 -1.12 4.59493E4
   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/
!\Author: WARNING !\Ref: FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325?346 \COMMENT !\Comment: DECOMP BELONGS TO THE
ALLYL+HO2 MECHANISM.
IC4H7OOH=IC4H7O+OH    1.28E27 -3.61 4.63331E4
   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/
!\Author: WARNING !\Ref: FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325?346 \COMMENT !\Comment: WARNING
IC4H7O=C3H5-T+CH2O    8.52E25 -3.61 2.78634E4
   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/
!\Author: WARNING !\Ref: FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325?346 \COMMENT !\Comment: WARNING
IC4H7O=IC3H5CHO+H    2.57E20 -2.06 2.20401E4
   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/
!\Author: WARNING !\Ref: FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325?346 \COMMENT !\Comment: WARNING
IC4H7O=C3H6+HCO    4.75E8 1.14 2.09225E4
   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/
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   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/
!\Author: WARNING !\Ref: FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325?346 \COMMENT !\Comment: WARNING
C3H5-T+CH2O=IC3H5CHO+H    6.01E5 2.09 7.8956E3
   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/
!\Author: WARNING !\Ref: FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325?346 \COMMENT !\Comment: WARNING
C3H5-T+CH2O=C3H6+HCO    1.65E1 3.17 9.3998E3
   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/
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: R+CH3O2(=)PRODUCTS
!_____________________________________________________________________________________________________________
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H7+CH3O2=IC4H7O+CH3O    9.62E17 -1.228 7.798E3
   PLOG/1.0E-1 1.576E10 7.83E-1 -2.33E3/
   PLOG/1.0E0 2.0E13 -8.7E-2 -1.1E1/
   PLOG/1.0E1 3.2E18 -1.503E0 4.824E3/
   PLOG/1.0E2 9.62E17 -1.228E0 7.798E3/
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: R+RO2(=)PRODUCTS
!_____________________________________________________________________________________________________________
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
IC4H7+NC3H7O2=IC4H7O+NC3H7O    7.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
IC4H7+SC4H9O2=IC4H7O+SC4H9O    7.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
IC4H7+IC3H7O2=IC4H7O+IC3H7O    7.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ESTIMATE !\Comment: WARNING
IC4H7+TC4H9O2=IC4H7O+TC4H9O    7.0E12 0.0 -1.0E3
!\Author: WARNING !\Ref: ZADOR PHYS. CHEM. CHEM. PHYS., 2009, 11, 11040?1053 !\Comment: WARNING
IC4H8+OH=CH3COCH3+CH3    5.45E-5 4.22 1.141E3
   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/
!-------------------------------------------------------------------------------------------------------------
!\ENDSUBMECH: IC4H8
!-------------------------------------------------------------------------------------------------------------
!-------------------------------------------------------------------------------------------------------------
!\SUBMECH: C4H8-1
!\MECHCOMMENTS: PC4H9O AND SC4H9O MOVED TO N-BUTANE MECHANISM
!\MECHCOMMENTS: IF SIMULATING BUTENE, OR ANY MECHANISM THAT IS DEPENDENT ON BUTENE, DON'T REMOVE BUTANOL
!\MECHCOMMENTS: PC4H8OH-1: THIS SPECIES HAS NO FORMATION PATHWAYS IN THE MODEL, IT SHOULD BE REMOVED, MAYBE THIS IS A PART
OF THE BUTANOL CHEMISTRY
!-------------------------------------------------------------------------------------------------------------
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: RH(=)PRODUCTS
!_____________________________________________________________________________________________________________
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!\Author: WARNING !\Ref: YIJUN ZHANG ET AL. COMBUSTION AND FLAME 159(2012) 905 C917 !\Comment: WARNING
C3H5-A+CH3(+M)=C4H8-1(+M)    1.0E14 -0.32 -2.623E2
   AR/0.7/
   CO/1.5/
   CH4/2.0/
   H2/2.0/
   CO2/2.0/
   C2H6/3.0/
   H2O/6.0/
   LOW/3.91E60 -1.281E1 6.25E3/
   TROE/1.04E-1 1.606E3 6.0E4 6.1184E3/
!\Author: WARNING !\Ref: YIJUN ZHANG ET AL. COMBUSTION AND FLAME 159(2012) 905 C917 !\Comment: WARNING
C2H5+C2H3(+M)=C4H8-1(+M)    1.5E13 0.0 0.0E0
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   H2/2.0/
   CH4/2.0/
   C2H6/3.0/
   H2O/6.0/
   LOW/1.55E56 -1.179E1 8.9845E3/
   TROE/1.98E-1 2.2779E3 6.0E4 5.7232E3/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C4H8-1=C4H71-3+H    5.83E26 -3.586 9.0516E4
   PLOG/1.0E-3 1.59E62 -1.5388E1 9.839E4/
   PLOG/1.0E-2 2.86E63 -1.5341E1 1.01589E5/
   PLOG/1.0E-1 3.25E64 -1.5255E1 1.05036E5/
   PLOG/1.0E0 1.35E57 -1.2776E1 1.03861E5/
   PLOG/1.0E1 1.63E42 -8.199E0 9.7893E4/
   PLOG/1.0E2 5.83E26 -3.586E0 9.0516E4/
!\Author: WARNING !\Ref: KPS, TST /RRHO+HRS !\Comment: WARNING
C4H8-1+H=C4H71-3+H2    2.42E3 3.05 1.995E3
!\Author: WARNING !\Ref: IN ARAMCO !\Comment: WARNING
C4H8-1+O=C4H71-3+OH    1.75E11 0.7 5.884E3
!\Author: WARNING !\Ref: IN ARAMCO(TSANG '91) !\Comment: WARNING
C4H8-1+CH3O2=C4H71-3+CH3O2H    2.7E4 0.7 5.884E3
!\Author: WARNING !\Ref: IN ARAMCO(TSANG '91) !\Comment: WARNING
C4H8-1+CH3O=C4H71-3+CH3OH    4.0E1 2.9 8.609E3
!\Author: WARNING !\Ref: IN ARAMCO(DECHAUX, J.C., OXID. COMM. 2, 95(1981)) !\Comment: WARNING
C4H8-1+CH3CO3=C4H71-3+CH3CO3H    1.0E11 0.0 8.0E3
!\Author: WARNING !\Ref: IN ARAMCO(DECHAUX, J.C., OXID. COMM. 2, 95(1981)) !\Comment: WARNING
C4H8-1+C3H5-A=C4H71-3+C3H6    7.9E10 0.0 1.24E4
!\Author: WARNING !\Ref: IN ARAMCO(ALLARA, D. L. AND EDELSON, D., INT. J. CHEM. KINET. 7, 479(1975).) !\Comment: WARNING
C4H8-1+C2H5O2=C4H71-3+C2H5O2H    1.4E12 0.0 1.49E4
!\Author: WARNING !\Ref: IN ARAMCO(ALLARA, D. L. AND EDELSON, D., INT. J. CHEM. KINET. 7, 479(1975).) !\Comment: WARNING
C4H8-1+NC3H7O2=C4H71-3+NC3H7O2H    1.4E12 0.0 1.49E4
!\Author: WARNING !\Ref: IN ARAMCO(ALLARA, D. L. AND EDELSON, D., INT. J. CHEM. KINET. 7, 479(1975).) !\Comment: WARNING
C4H8-1+IC3H7O2=C4H71-3+IC3H7O2H    1.4E12 0.0 1.49E4
!\Author: WARNING !\Ref: IN ARAMCO(ALLARA, D. L. AND EDELSON, D., INT. J. CHEM. KINET. 7, 479(1975).) !\Comment: WARNING
C4H8-1+SC4H9O2=C4H71-3+SC4H9O2H    1.4E12 0.0 1.49E4
!\Author: WARNING !\Ref: IN ARAMCO(WESTBROOK ESTIMATE) !\Comment: WARNING
C4H8-1+TC4H9O2=C4H71-3+TC4H9O2H    1.4E12 0.0 1.49E4
!\Author: SD !\Ref: WANG, KUN, ET AL. PHYSICAL CHEMISTRY CHEMICAL PHYSICS 17.9(2015) !\Comment: WARNING
C4H8-1+CH3=C4H71-3+CH4    1.694E2 3.12 5.78E3
!\Author: WARNING !\Ref: JUDIT ZADOR,STEPHEN J. KLIPPENSTEIN,AND JAMES A. MILLER J. PHYS. CHEM. A 2011, 115, 10218 C10225 !\Comment: *2
C4H8-1+HO2=C4H71-3+H2O2    7.82E-1 3.97 1.1702E4
!\Author: SD !\Ref: ZHOU, CHONG-WEN, ET AL. THE JOURNAL OF PHYSICAL CHEMISTRY A 121.9(2017) !\Comment: WARNING
C4H8-1+O2=C4H71-3+HO2    4.88E1 3.48 3.48E4
!\Author: WARNING !\Ref: VASU, SUBITH S., ET AL. THE JOURNAL OF PHYSICAL CHEMISTRY A 115.12(2011) !\Comment: WARNING
C4H8-1+OH=C4H71-3+H2O    1.616E6 2.2 -4.372E2
!_____
!\REACTIONCLASS: RADICAL_ADDITIONH
!_____
!\Author: WARNING !\Ref: WARNING !\Comment: QRRK /MSC ANALYSIS WITH CHEMDIS
C4H8-1+H=C2H4+C2H5    7.02E32 -5.22 3.1754E4
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PLOG/1.0E-3 2.55E6 1.93E0 5.564E3/
PLOG/1.0E-3 3.45E7 1.81E0 2.263E3/
PLOG/1.0E-2 5.56E6 1.83E0 5.802E3/
PLOG/1.0E-2 8.06E7 1.71E0 2.522E3/
PLOG/1.0E-1 1.21E9 1.18E0 7.472E3/
PLOG/1.0E-1 1.18E10 1.1E0 4.077E3/
PLOG/1.0E0 9.47E16 -1.03E0 1.3413E4/
PLOG/1.0E0 6.02E15 -4.9E-1 8.452E3/
PLOG/1.0E1 4.5E28 -4.24E0 2.3618E4/
PLOG/1.0E1 7.58E21 -2.14E0 1.4245E4/
PLOG/1.0E2 7.02E32 -5.22E0 3.1754E4/
PLOG/1.0E2 2.29E21 -1.87E0 1.7243E4/
!\Author: WARNING !\Ref: WARNING !\Comment: QRRK /MSC ANALYSIS WITH CHEMDIS
C4H8-1+H=C3H6+CH3 1.32E20 -1.46 1.5383E4
PLOG/1.0E-3 7.83E9 1.17E0 1.442E3/
PLOG/1.0E-3 1.8E6 1.76E0 5.9E3/
PLOG/1.0E-2 3.39E10 1.0E0 1.895E3/
PLOG/1.0E-2 3.46E6 1.68E0 6.1E3/
PLOG/1.0E-1 4.02E8 1.1E0 7.574E3/
PLOG/1.0E-1 3.7E13 1.4E-1 4.127E3/
PLOG/1.0E0 4.57E19 -1.54E0 9.061E3/
PLOG/1.0E0 1.21E16 -9.9E-1 1.3175E4/
PLOG/1.0E1 8.57E23 -2.66E0 1.414E4/
PLOG/1.0E1 7.14E27 -4.23E0 2.3319E4/
PLOG/1.0E2 1.32E20 -1.46E0 1.5383E4/
PLOG/1.0E2 1.0E33 -5.49E0 3.1922E4/
!\Author: WARNING !\Ref: WARNING !\Comment: QRRK /MSC ANALYSIS WITH CHEMDIS
C4H8-1+H=PC4H9 1.44E37 -7.21 2.4896E4
PLOG/1.0E-3 1.35E15 -2.81E0 1.57E3/
PLOG/1.0E-3 4.33E20 -4.16E0 -2.63E2/
PLOG/1.0E-2 5.2E16 -2.97E0 1.992E3/
PLOG/1.0E-2 1.78E22 -4.33E0 1.86E2/
PLOG/1.0E-1 1.91E21 -3.97E0 4.636E3/
PLOG/1.0E-1 1.98E26 -5.18E0 2.518E3/
PLOG/1.0E0 1.9E31 -6.46E0 1.1968E4/
PLOG/1.0E0 3.78E32 -6.63E0 7.265E3/
PLOG/1.0E1 2.1E40 -8.6E0 2.1058E4/
PLOG/1.0E1 8.79E34 -6.91E0 1.0952E4/
PLOG/1.0E2 1.44E37 -7.21E0 2.4896E4/
PLOG/1.0E2 7.8E28 -4.79E0 1.0355E4/
!\Author: WARNING !\Ref: WARNING !\Comment: QRRK /MSC ANALYSIS WITH CHEMDIS
C4H8-1+H=SC4H9 1.37E26 -3.79 8.012E3
PLOG/1.0E-3 4.07E22 -4.51E0 -7.71E2/
PLOG/1.0E-3 3.52E12 -2.15E0 1.466E3/
PLOG/1.0E-2 3.9E24 -4.78E0 -3.4E1/
PLOG/1.0E-2 1.02E14 -2.28E0 1.799E3/
PLOG/1.0E-1 2.03E29 -5.81E0 2.97E3/
PLOG/1.0E-1 1.16E18 -3.13E0 4.049E3/
PLOG/1.0E0 3.53E34 -6.95E0 7.525E3/
PLOG/1.0E0 5.22E27 -5.53E0 1.0963E4/
PLOG/1.0E1 1.19E34 -6.42E0 9.81E3/
PLOG/1.0E1 4.33E37 -7.92E0 2.0354E4/
PLOG/1.0E2 1.37E26 -3.79E0 8.012E3/
PLOG/1.0E2 2.22E36 -7.06E0 2.5203E4/
!\Author: WARNING !\Ref: WARNING !\Comment: QRRK /MSC ANALYSIS WITH CHEMDIS
C4H8-2+H=C2H4+C2H5 5.15E33 -5.39 3.2601E4
PLOG/1.0E-3 8.96E6 1.86E0 6.209E3/
PLOG/1.0E-2 1.92E7 1.77E0 6.443E3/
PLOG/1.0E-1 3.97E9 1.11E0 8.097E3/
PLOG/1.0E0 3.01E17 -1.09E0 1.4023E4/
PLOG/1.0E1 1.88E29 -4.33E0 2.4297E4/
PLOG/1.0E2 5.15E33 -5.39E0 3.2601E4/
!\Author: WARNING !\Ref: WARNING !\Comment: QRRK /MSC ANALYSIS WITH CHEMDIS
C4H8-2+H=C3H6+CH3 1.23E20 -1.35 1.5762E4
PLOG/1.0E-3 6.39E9 1.29E0 1.834E3/

PLOG/1.0E-2 2.6E10 1.12E0 2.267E3/
PLOG/1.0E-1 2.48E13 2.9E-1 4.456E3/
PLOG/1.0E0 2.91E19 -1.39E0 9.365E3/
PLOG/1.0E1 6.13E23 -2.53E0 1.4463E4/
PLOG/1.0E2 1.23E20 -1.35E0 1.5762E4/
!\Author: WARNING !\Ref: WARNING !\Comment: QRRK /MSC ANALYSIS WITH CHEMDIS
C4H8-2+H=PC4H9 5.17E36 -6.98 2.5063E4
PLOG/1.0E-3 3.9E14 -2.55E0 1.729E3/
PLOG/1.0E-2 1.41E16 -2.71E0 2.133E3/
PLOG/1.0E-1 4.31E20 -3.69E0 4.719E3/
PLOG/1.0E0 4.03E30 -6.17E0 1.202E4/
PLOG/1.0E1 5.19E39 -8.33E0 2.1137E4/
PLOG/1.0E2 5.17E36 -6.98E0 2.5063E4/
!\Author: WARNING !\Ref: WARNING !\Comment: QRRK /MSC ANALYSIS WITH CHEMDIS
C4H8-2+H=SC4H9 3.27E25 -3.51 8.145E3
PLOG/1.0E-3 8.34E21 -4.21E0 -6.02E2/
PLOG/1.0E-2 6.79E23 -4.46E0 8.2E1/
PLOG/1.0E-1 2.85E28 -5.47E0 3.003E3/
PLOG/1.0E0 5.45E33 -6.61E0 7.559E3/
PLOG/1.0E1 2.33E33 -6.11E0 9.893E3/
PLOG/1.0E2 3.27E25 -3.51E0 8.145E3/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C4H8-1+H=C4H8-2+H 1.21970567E-14 8.42230129 6.17748467E3
PLOG/1.0E-2 1.13970471E6 2.19098257E0 4.47777098E3/
PLOG/1.0E-1 5.35017843E11 5.65128682E-1 8.0862242E3/
PLOG/1.0E0 2.01661348E19 -1.55491233E0 1.38675893E4/
PLOG/1.0E1 5.76162919E17 -9.35851505E-1 1.63693033E4/
PLOG/1.0E2 6.37751035E2 3.5689757E0 1.22710156E4/
PLOG/1.0E3 1.21970567E-14 8.42230129E0 6.17748467E3/
!\Author: WARNING !\Ref: WARNING !\Comment: QRRK /MSC ANALYSIS WITH CHEMDIS
SC4H9=PC4H9 6.02E45 -10.07 5.3399E4
PLOG/1.0E-3 9.6E37 -1.104E1 3.884E4/
PLOG/1.0E-2 6.05E40 -1.126E1 3.9461E4/
PLOG/1.0E-1 1.64E47 -1.249E1 4.3112E4/
PLOG/1.0E0 6.53E55 -1.427E1 5.0351E4/
PLOG/1.0E1 2.13E56 -1.371E1 5.4866E4/
PLOG/1.0E2 6.02E45 -1.007E1 5.3399E4/
!\Author: WARNING !\Ref: WARNING !\Comment: QRRK /MSC ANALYSIS WITH CHEMDIS
PC4H9=C2H4+C2H5 1.48E29 -4.71 3.595E4
PLOG/1.0E-3 3.44E34 -8.1E0 2.8397E4/
PLOG/1.0E-2 1.11E39 -9.05E0 3.1891E4/
PLOG/1.0E-1 7.74E42 -9.78E0 3.5771E4/
PLOG/1.0E0 7.47E43 -9.67E0 3.8722E4/
PLOG/1.0E1 2.06E39 -7.97E0 3.8955E4/
PLOG/1.0E2 1.48E29 -4.71E0 3.595E4/
!\Author: WARNING !\Ref: WARNING !\Comment: QRRK /MSC ANALYSIS WITH CHEMDIS
PC4H9=C3H6+CH3 2.23E42 -8.68 5.6601E4
PLOG/1.0E-3 3.71E25 -5.81E0 3.4965E4/
PLOG/1.0E-2 1.85E27 -6.01E0 3.5481E4/
PLOG/1.0E-1 2.46E32 -7.16E0 3.8637E4/
PLOG/1.0E0 2.05E42 -9.61E0 4.6415E4/
PLOG/1.0E1 4.98E48 -1.097E1 5.4456E4/
PLOG/1.0E2 2.23E42 -8.68E0 5.6601E4/
!\Author: WARNING !\Ref: WARNING !\Comment: QRRK /MSC ANALYSIS WITH CHEMDIS
SC4H9=C2H4+C2H5 9.94E42 -8.7 6.1203E4
PLOG/1.0E-3 8.3E25 -5.75E0 3.9343E4/
PLOG/1.0E-2 4.12E27 -5.94E0 3.9859E4/
PLOG/1.0E-1 5.57E32 -7.1E0 4.3029E4/
PLOG/1.0E0 4.54E42 -9.54E0 5.0839E4/
PLOG/1.0E1 1.06E49 -1.09E1 5.8899E4/
PLOG/1.0E2 9.94E42 -8.7E0 6.1203E4/
!\Author: WARNING !\Ref: WARNING !\Comment: QRRK /MSC ANALYSIS WITH CHEMDIS
SC4H9=C3H6+CH3 4.79E26 -4.01 3.6898E4
PLOG/1.0E-3 2.89E40 -9.76E0 3.3601E4/
PLOG/1.0E-2 1.8E44 -1.05E1 3.7007E4/

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   PLOG/1.0E-1 2.51E46 -1.073E1 4.0237E4/
   PLOG/1.0E0 4.74E44 -9.85E0 4.1841E4/
   PLOG/1.0E1 3.79E37 -7.44E0 4.0604E4/
   PLOG/1.0E2 4.79E26 -4.01E0 3.6898E4/
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONO
!_____________________________________________________________________________________________________________
!\Author: WARNING !\Ref: ANALOGY WITH C3H6+O !\Comment: WARNING
C4H8-1+O=NC3H7+HCO    7.45E6 1.88 1.83E2
!\Author: WARNING !\Ref: ANALOGY WITH C3H6+O !\Comment: WARNING
C4H8-1+O=>CH2CO+C2H5+H    3.05E6 1.88 1.83E2
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: R+O(=)PRODUCTS
!_____________________________________________________________________________________________________________
!\Author: WARNING !\Ref: IN ARAMCO(ESTIMATE) !\Comment: WARNING
C4H71-3+O=C2H3CHO+CH3    6.03E13 0.0 0.0E0
!\Author: WARNING !\Ref: GOLDSMITH, C. FRANKLIN, ET AL. PROCEEDINGS OF THE COMBUSTION INSTITUTE 33.1(2011) !\Comment: WARNING
C4H71-3+HO2=C4H7O2-1+OH    8.2E3 2.74 1.1444E3
   PLOG/1.0E-2 5.1E12 -1.58E-1 -1.417E3/
   PLOG/1.0E-1 2.49E14 -6.42E-1 -3.491E2/
   PLOG/1.0E0 3.885E17 -1.52E0 2.3792E3/
   PLOG/1.0E1 1.465E15 -6.84E-1 3.6153E3/
   PLOG/1.0E2 8.2E3 2.74E0 1.1444E3/
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_BETA_SCISSION
!_____________________________________________________________________________________________________________
!\Author: WARNING !\Ref: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116(13), PP 3325? 3346 !\Comment: WARNING
C4H7O2-1=C3H6+HCO    4.75E8 1.14 2.09225E4
!\Author: WARNING !\Ref: IN ARAMCO(ESTIMATE) !\Comment: WARNING
C4H71-3+C2H5=C4H8-1+C2H4    2.59E12 0.0 -1.31E2
!\Author: WARNING !\Ref: IN ARAMCO(ESTIMATE) !\Comment: WARNING
C4H71-3+CH3O=C4H8-1+CH2O    2.41E13 0.0 0.0E0
!-------------------------------------------------------------------------------------------------------------
!\ENDSUBMECH: C4H6-1
!-------------------------------------------------------------------------------------------------------------
!-------------------------------------------------------------------------------------------------------------
!\SUBMECH: C4H8-2
!-------------------------------------------------------------------------------------------------------------
!_____________________________________________________________________________________________________________
!\REACTIONCLASS: RH(=)PRODUCTS
!_____________________________________________________________________________________________________________
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H5-S+CH3(+M)=C4H8-2(+M)    5.0E13 0.0 0.0E0
   AR/0.7/
   CO/1.5/
   CO2/2.0/
   H2/2.0/
   CH4/2.0/
   C2H4/3.0/
   C2H6/3.0/
   C2H2/3.0/
   H2O/6.0/
   LOW/8.54E58 -1.194E1 9.7698E3/
   TROE/1.75E-1 1.3406E3 6.0E4 1.01398E4/
!\Author: WARNING !\Ref: ASSUME BY THIS WORK !\Comment: WARNING
C4H8-2=C3H5-A+CH3    7.5E65 -15.6 9.73E4
!\Author: SN !WAGNON1@LLNL.GOV !A*2(DEG) AS C3H6=C3H5-A+H YE PROCI 35(2015) 223-230 !\Ref: WARNING !\Comment: WARNING
C4H8-2=C4H71-3+H    1.61E57 -11.52 1.2182E5
   PLOG/1.0E-2 1.83E75 -1.761E1 1.2037E5/
   PLOG/1.0E-2 5.96E54 -1.232E1 1.012E5/
   PLOG/1.0E-1 3.46E70 -1.601E1 1.1951E5/
   PLOG/1.0E-1 2.76E43 -8.87E0 9.6365E4/
   PLOG/1.0E0 2.16E71 -1.591E1 1.2486E5/
   PLOG/1.0E0 1.26E43 -8.51E0 9.8004E4/
   PLOG/1.0E1 1.28E66 -1.4219E1 1.2498E5/
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   PLOG/1.0E1 9.46E35 -6.26E0 9.5644E4/
   PLOG/1.0E2 1.61E57 -1.152E1 1.2182E5/
   PLOG/1.0E2 8.7E28 -4.06E0 9.3114E4/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RH+R_ABSTRACTION
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: ANALOGY WITH C3H6+OH(=)C3H5-A+H2O *2 / 2 !\Comment: WARNING
C4H8-2+OH=C4H71-3+H2O    4.46E6 2.072 1.0508E3
!\Author: WARNING !\Ref: JUDIT ZADOR,STEPHEN J. KLIPPENSTEIN,AND JAMES A. MILLER J. PHYS. CHEM. A 2011, 115, 10218 C10225 !\Comment: *2
C4H8-2+HO2=C4H71-3+H2O2    6.9E-1 4.0 1.2103E4
!\Author: WARNING !\Ref: KPS, TST /RRHO+HRS !*2 EA-1 !\Comment: WARNING
C4H8-2+H=C4H71-3+H2    5.62E2 3.5 1.627E3
!\Author: WARNING !\Ref: BEDJANIAN, YURI, AND JULIEN MORIN. THE JOURNAL OF PHYSICAL CHEMISTRY A 121.8(2017) !\Comment: WARNING
C4H8-2+O=C4H71-3+OH    1.936E-2 4.54 -2.4698E3
!\Author: CWZ !\Ref: DIRECT CALCULATION BY STATED AUTHOR !\Comment: WARNING
C4H8-2+O2=C4H71-3+HO2    7.74E1 3.52 3.62E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C4H8-2+CH3=C4H71-3+CH4    1.11E2 3.27 7.15E3
!\Author: WARNING !\Ref: IN ARAMCO(ESTIMATE) !\Comment: WARNING
C4H8-2+CH3O=C4H71-3+CH3OH    1.8E1 2.95 1.199E4
!\Author: WARNING !\Ref: IN ARAMCO( !TWICE RATE OF C3H6+HO2) !\Comment: WARNING
C4H8-2+NC3H7O2=C4H71-3+NC3H7O2H    3.2E12 0.0 1.49E4
!\Author: WARNING !\Ref: IN ARAMCO( !TWICE RATE OF C3H6+HO2) !\Comment: WARNING
C4H8-2+IC3H7O2=C4H71-3+IC3H7O2H    3.2E12 0.0 1.49E4
!\Author: WARNING !\Ref: IN ARAMCO( !TWICE RATE OF C3H6+HO2) !\Comment: WARNING
C4H8-2+SC4H9O2=C4H71-3+SC4H9O2H    3.2E12 0.0 1.49E4
!\Author: WARNING !\Ref: IN ARAMCO(WESTBROOK ESTIMATE) !\Comment: WARNING
TC4H9O2+C4H8-2=TC4H9O2H+C4H71-3    1.4E12 0.0 1.49E4
!\Author: WARNING !\Ref: ANALOGY WITH C3H6+O !\Comment: WARNING
C4H8-2+O=>CH2CO+C2H5+H    3.05E6 1.88 1.83E2
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RADICAL_ADDITIONHO2
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: VILLANO(FROM KUIWEN'S MECH) !\Comment: WARNING
SC4H9O2=C4H8-2+HO2    7.25E9 0.8 2.99E4
   DUP
!\Author: WARNING !\Ref: VILLANO(FROM KUIWEN'S MECH) !\Comment: WARNING
SC4H9O2=C4H8-2+HO2    1.7E10 0.67 3.07E4
   DUP
!=====================================================================================================
!\ENDSUBSPECIES: C2CY(COC)OHCCY(CCO)COH\CCY(CCO)COH\CCY(CCOC)OH
!=====================================================================================================
!-----------------------------------------------------------------------------------------------------
!\ENDSUBMECH: IC4H9OH
!-----------------------------------------------------------------------------------------------------
!-----------------------------------------------------------------------------------------------------
!\SUBMECH: H15DE2M
!\MECHCOMMENTS: OTHER IC4H7O DECOMPOSITIONS ARE IN THE IC4H8 MECAHNISM
!\MECHCOMMENTS: IC4H8OH HAS NOT CONSUMPTION PATHWAYS, KPS, 12 / 05 / 2016
!-----------------------------------------------------------------------------------------------------
!_____________________________________________________________________________________________________
!\REACTIONCLASS: RH(=)PRODUCTS
!_____________________________________________________________________________________________________
!\Author: NL \REF !\Ref: WARNING !\Comment: WARNING
2IC4H7=C3H4-A+AC5H10    1.31E54 -12.995 1.6742E4
   PLOG/3.9E-2 3.76E65 -1.5935E1 2.0251E4/
   PLOG/7.8E-2 8.65E58 -1.449E1 1.8566E4/
   PLOG/1.56E-1 1.31E54 -1.2995E1 1.6742E4/
!_____________________________________________________________________________________________________
!\REACTIONCLASS: R+R(=)RH+RH
!_____________________________________________________________________________________________________
!\Author: WARNING !\Ref: FROM BAULCH ET AL. J. PHYS. CHEM. REF. DATA, 21, 411--429, 1992 !\Comment: WARNING
IC4H7O+O2=IC3H5CHO+HO2    3.0E10 0.0 1.649E3
!\Author: WARNING !\Ref: ANALOGY CH3O+X --)CH2O+HX !\Comment: WARNING
IC4H7O+HO2=IC3H5CHO+H2O2    3.0E11 0.0 0.0E0
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!\Author: WARNING !\Ref: ANALOGY CH3O+X --)CH2O+HX !\Comment: WARNING
IC4H7O+CH3=IC3H5CHO+CH4 2.4E13 0.0 0.0E0
!\Author: WARNING !\Ref: ANALOGY CH3O+X --)CH2O+HX !\Comment: WARNING
IC4H7O+O=IC3H5CHO+OH 6.0E12 0.0 0.0E0
!\Author: WARNING !\Ref: ANALOGY CH3O+X --)CH2O+HX !\Comment: WARNING
IC4H7O+OH=IC3H5CHO+H2O 1.81E13 0.0 0.0E0
!\Author: WARNING !\Ref: ANALOGY CH3O+X --)CH2O+HX !\Comment: WARNING
IC4H7O+H=IC3H5CHO+H2 1.99E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C4H71-3=C2H4+C2H3 3.7E6 2.13 5.901E4
  PLOG/1.0E-2 5.65E72 -1.832E1 7.782E4/
  PLOG/1.0E-2 1.83E49 -1.165E1 6.541E4/
  PLOG/1.0E-1 2.53E70 -1.714E1 8.055E4/
  PLOG/1.0E-1 3.08E42 -9.35E0 6.516E4/
  PLOG/1.0E0 5.29E69 -1.652E1 8.49E4/
  PLOG/1.0E0 3.5E29 -5.14E0 6.306E4/
  PLOG/1.0E1 4.15E25 -3.37E0 6.5602E4/
  PLOG/1.0E2 3.7E6 2.13E0 5.901E4/
  PLOG/1.0E2 3.75E73 -1.682E1 1.009E5/
!\Author: P. ZHANG ET AL., JPCA, 2013, 117, 1890-1906. !ANALOGY TO BUTANOL !\Ref: WARNING !\Comment: WARNING
C4H7O2-1=CH2O+C3H5-S 1.03E23 -3.11 1.7691E4
  PLOG/1.3E-1 5.09E23 -3.85E0 1.5721E4/
  PLOG/1.0E0 6.73E34 -7.46E0 1.9332E4/
  PLOG/1.0E1 1.48E30 -5.62E0 1.9026E4/
  PLOG/1.0E2 1.03E23 -3.11E0 1.7691E4/
!---
!\ENDSUBMECH: C4H2
!---
!---
!\SUBMECH: NC3H7CHO
!\MECHCOMMENTS: THIS SUBMECH IS COMPLETELY STAND-ALONE WITHIN THE C4 MODULE, THIS SPECIES IS NOT FORMED FROM ANY C4 /C5 INTERMEDIATES. MATTEO PELUCCHI ALDEHYDES MECHANISMS NEED TO BE INCORPORATED.
!\MECHCOMMENTS: NAMING SCHEMES FOR PELUCCHI ALDEHYDE CHEMISTRY MAY BE DIFFERENT IN HIS MECHANISM
!---
!_____
!\REACTIONCLASS: RH(=)PRODUCTS/UNIMOLECULARDECOMPOSITION
!_____
!\Author: SD !\Ref: M. PELUCCHI,COMBUST. FLAME 162(2015) 265-286. !\Comment: WARNING
NC3H7CHO=CH3+CH2CH2CHO 1.63E24 -2.246 9.03693E4
!\Author: WARNING !\Ref: M. PELUCCHI,COMBUST. FLAME 162(2015) 265-286. !\Comment: WARNING
NC3H7CHO=C2H5+CH2CHO 7.56E27 -3.5 8.14791E4
!\Author: WARNING !\Ref: M. PELUCCHI,COMBUST. FLAME 162(2015) 265-286. !\Comment: WARNING
NC3H7CHO=NC3H7+HCO 1.12E28 -3.51 8.37575E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NC3H7CHO=CO+C3H8 1.0E14 0.0 7.5E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NC3H7CHO=CH2CO+C2H6 1.0E14 0.0 7.5E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H4+IC3H7=C4H8-2+CH3 4.21E-26 11.32 2.055E4
  PLOG/1.0E-2 1.39E5 1.87E0 1.728E4/
  PLOG/1.0E-1 1.3E11 2.1E-1 2.183E4/
  PLOG/1.0E0 1.36E14 -5.5E-1 2.6E4/
  PLOG/1.0E1 2.09E9 1.02E0 2.76E4/
  PLOG/1.0E2 2.12E-6 5.55E0 2.527E4/
  PLOG/1.0E3 4.21E-26 1.132E1 2.055E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H4+IC3H7=IC4H8+CH3 2.19E-27 11.42 1.864E4
  PLOG/1.0E-2 1.67E7 9.6E-1 1.606E4/
  PLOG/1.0E-1 1.17E13 -6.5E-1 2.091E4/
  PLOG/1.0E0 8.54E14 -1.06E0 2.484E4/
  PLOG/1.0E1 6.12E8 9.0E-1 2.598E4/
  PLOG/1.0E2 1.16E-7 5.65E0 2.338E4/
  PLOG/1.0E3 2.19E-27 1.142E1 1.864E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H4+IC3H7=C4H8-1+CH3 1.55E-23 10.35 1.693E4

PLOG/1.0E-2 2.37E19 -2.53E0 1.757E4/
PLOG/1.0E-1 4.69E23 -3.69E0 2.187E4/
PLOG/1.0E0 2.81E23 -3.48E0 2.505E4/
PLOG/1.0E1 9.37E14 -8.3E-1 2.53E4/
PLOG/1.0E2 4.18E-2 4.06E0 2.23E4/
PLOG/1.0E3 1.55E-23 1.035E1 1.693E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H4+IC3H7=AC5H10+H 1.69E-29 12.0 1.771E4
PLOG/1.0E-2 5.5E6 1.05E0 1.602E4/
PLOG/1.0E-1 1.18E12 -4.2E-1 2.041E4/
PLOG/1.0E0 8.28E13 -8.3E-1 2.424E4/
PLOG/1.0E1 6.27E7 1.13E0 2.539E4/
PLOG/1.0E2 1.59E-8 5.84E0 2.284E4/
PLOG/1.0E3 1.69E-29 1.2E1 1.771E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H4+IC3H7=BC5H10+H 5.2E-30 12.22 2.046E4
PLOG/1.0E-2 4.7E-2 3.5E0 1.605E4/
PLOG/1.0E-1 1.53E5 1.67E0 2.084E4/
PLOG/1.0E0 8.31E8 7.0E-1 2.529E4/
PLOG/1.0E1 1.1E5 2.0E0 2.726E4/
PLOG/1.0E2 6.29E-10 6.32E0 2.525E4/
PLOG/1.0E3 5.2E-30 1.222E1 2.046E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C4H8-2+CH3=IC4H8+CH3 1.48E-25 11.16 2.034E4
PLOG/1.0E-2 6.58E13 -6.7E-1 1.971E4/
PLOG/1.0E-1 3.0E19 -2.23E0 2.448E4/
PLOG/1.0E0 3.17E20 -2.38E0 2.812E4/
PLOG/1.0E1 4.55E12 8.0E-2 2.862E4/
PLOG/1.0E2 2.42E-5 5.27E0 2.537E4/
PLOG/1.0E3 1.48E-25 1.116E1 2.034E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C4H8-2+CH3=C3H6+C2H5 3.87E-26 11.25 2.161E4
PLOG/1.0E-2 1.34E10 3.2E-1 1.966E4/
PLOG/1.0E-1 2.06E16 -1.39E0 2.465E4/
PLOG/1.0E0 1.34E18 -1.78E0 2.86E4/
PLOG/1.0E1 1.56E11 4.1E-1 2.947E4/
PLOG/1.0E2 3.68E-6 5.42E0 2.65E4/
PLOG/1.0E3 3.87E-26 1.125E1 2.161E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C4H8-2+CH3=C4H8-1+CH3 4.39E-27 11.55 2.23E4
PLOG/1.0E-2 1.07E7 1.25E0 1.965E4/
PLOG/1.0E-1 3.11E13 -5.6E-1 2.461E4/
PLOG/1.0E0 1.19E16 -1.18E0 2.881E4/
PLOG/1.0E1 1.05E10 7.6E-1 3.0E4/
PLOG/1.0E2 8.19E-7 5.62E0 2.726E4/
PLOG/1.0E3 4.39E-27 1.155E1 2.23E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C4H8-2+CH3=AC5H10+H 2.13E-28 12.01 2.217E4
PLOG/1.0E-2 1.33E5 1.88E0 1.96E4/
PLOG/1.0E-1 2.92E11 1.1E-1 2.432E4/
PLOG/1.0E0 2.92E14 -6.4E-1 2.857E4/
PLOG/1.0E1 9.14E8 1.14E0 2.994E4/
PLOG/1.0E2 1.3E-7 5.92E0 2.73E4/
PLOG/1.0E3 2.13E-28 1.201E1 2.217E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C4H8-2+CH3=BC5H10+H 2.5E-16 8.36 1.486E4
PLOG/1.0E-2 3.47E12 -1.3E-1 1.765E4/
PLOG/1.0E-1 2.92E14 -6.3E-1 1.998E4/
PLOG/1.0E0 3.62E12 2.0E-2 2.102E4/
PLOG/1.0E1 4.92E5 2.11E0 2.018E4/
PLOG/1.0E2 6.18E-6 5.36E0 1.762E4/
PLOG/1.0E3 2.5E-16 8.36E0 1.486E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H8+CH3=C3H6+C2H5 3.37E-21 10.04 2.305E4
PLOG/1.0E-2 7.79E12 -2.5E-1 2.053E4/

PLOG/1.0E-1 1.03E19 -1.95E0 2.532E4/
PLOG/1.0E0 1.73E21 -2.47E0 2.933E4/
PLOG/1.0E1 9.43E14 -4.7E-1 3.043E4/
PLOG/1.0E2 9.55E-2 4.35E0 2.771E4/
PLOG/1.0E3 3.37E-21 1.004E1 2.305E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H8+CH3=C4H8-1+CH3 3.41E-22 10.35 2.374E4
PLOG/1.0E-2 6.16E9 6.8E-1 2.056E4/
PLOG/1.0E-1 1.3E16 -1.09E0 2.529E4/
PLOG/1.0E0 1.24E19 -1.83E0 2.953E4/
PLOG/1.0E1 5.57E13 -1.0E-1 3.096E4/
PLOG/1.0E2 2.08E-2 4.56E0 2.848E4/
PLOG/1.0E3 3.41E-22 1.035E1 2.374E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H8+CH3=AC5H10+H 3.46E-14 8.12 1.555E4
PLOG/1.0E-2 4.54E11 5.0E-1 1.718E4/
PLOG/1.0E-1 2.19E14 -2.3E-1 1.969E4/
PLOG/1.0E0 3.6E13 8.0E-2 2.113E4/
PLOG/1.0E1 5.62E7 1.87E0 2.07E4/
PLOG/1.0E2 2.75E-3 4.95E0 1.841E4/
PLOG/1.0E3 3.46E-14 8.12E0 1.555E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC4H8+CH3=BC5H10+H 3.75E-14 7.84 1.474E4
PLOG/1.0E-2 2.0E13 -2.5E-1 1.697E4/
PLOG/1.0E-1 4.0E15 -8.5E-1 1.938E4/
PLOG/1.0E0 1.5E14 -3.7E-1 2.061E4/
PLOG/1.0E1 7.5E7 1.57E0 1.997E4/
PLOG/1.0E2 2.1E-3 4.73E0 1.757E4/
PLOG/1.0E3 3.75E-14 7.84E0 1.474E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H6+C2H5=AC5H10+H 2.23E-17 8.47 1.591E4
PLOG/1.0E-2 1.49E5 1.8E0 1.637E4/
PLOG/1.0E-1 2.26E8 9.2E-1 1.895E4/
PLOG/1.0E0 5.06E8 9.0E-1 2.077E4/
PLOG/1.0E1 1.27E4 2.33E0 2.081E4/
PLOG/1.0E2 3.04E-6 5.22E0 1.882E4/
PLOG/1.0E3 2.23E-17 8.47E0 1.591E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H6+C2H5=BC5H10+H 2.03E-27 11.36 2.148E4
PLOG/1.0E-2 1.49E3 2.08E0 1.786E4/
PLOG/1.0E-1 3.68E9 2.9E-1 2.253E4/
PLOG/1.0E0 1.12E13 -6.1E-1 2.691E4/
PLOG/1.0E1 2.51E8 9.2E-1 2.86E4/
PLOG/1.0E2 2.79E-7 5.44E0 2.632E4/
PLOG/1.0E3 2.03E-27 1.136E1 2.148E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C4H8-1+CH3=AC5H10+H 1.15E-16 8.35 1.528E4
PLOG/1.0E-2 2.28E4 2.12E0 1.521E4/
PLOG/1.0E-1 5.38E7 1.18E0 1.78E4/
PLOG/1.0E0 3.81E8 1.01E0 1.978E4/
PLOG/1.0E1 3.45E4 2.28E0 2.003E4/
PLOG/1.0E2 1.86E-5 5.07E0 1.82E4/
PLOG/1.0E3 1.15E-16 8.35E0 1.528E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C4H8-1+CH3=BC5H10+H 2.31E-26 11.12 2.079E4
PLOG/1.0E-2 2.75E2 2.37E0 1.664E4/
PLOG/1.0E-1 7.29E8 5.6E-1 2.119E4/
PLOG/1.0E0 8.12E12 -5.0E-1 2.572E4/
PLOG/1.0E1 1.15E9 7.9E-1 2.77E4/
PLOG/1.0E2 4.7E-6 5.15E0 2.565E4/
PLOG/1.0E3 2.31E-26 1.112E1 2.079E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
AC5H10+H=BC5H10+H 2.32E-11 7.43 5.31E3
PLOG/1.0E-2 2.02E11 7.2E-1 5.811E3/
PLOG/1.0E-1 3.64E14 -1.8E-1 8.414E3/

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   PLOG/1.0E0 8.18E14 -2.1E-1 1.024E4/
   PLOG/1.0E1 1.69E10 1.25E0 1.024E4/
   PLOG/1.0E2 3.5E0 4.16E0 8.228E3/
   PLOG/1.0E3 2.32E-11 7.43E0 5.31E3/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H6+C2H5=C4H8-1+CH3    5.91639257E-30 12.6856042 2.35242461E4
   PLOG/1.0E-2 1.28864537E8 9.94796567E-1 1.88907766E4/
   PLOG/1.0E-1 4.98106803E19 -2.3005532E0 2.67311744E4/
   PLOG/1.0E0 9.72617692E29 -5.10873378E0 3.59408045E4/
   PLOG/1.0E1 4.5409295E26 -3.84508066E0 4.02982725E4/
   PLOG/1.0E2 4.85834682E2 3.39809251E0 3.47733837E4/
   PLOG/1.0E3 5.91639257E-30 1.26856042E1 2.35242461E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H4+NC3H7=C4H8-1+CH3    1.46613849E-30 12.8140051 2.15111348E4
   PLOG/1.0E-2 4.65186422E6 1.33031135E0 1.6097355E4/
   PLOG/1.0E-1 3.21380736E18 -2.03965914E0 2.40568258E4/
   PLOG/1.0E0 3.18373724E29 -5.05106644E0 3.36902876E4/
   PLOG/1.0E1 3.69392927E26 -3.89519566E0 3.83361143E4/
   PLOG/1.0E2 7.45266743E2 3.27769524E0 3.30327766E4/
   PLOG/1.0E3 1.46613849E-30 1.28140051E1 2.15111348E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H4+NC3H7=C3H6+C2H5    1.34292319E-29 12.4863337 1.46743009E4
   PLOG/1.0E-2 6.87904356E27 -4.88579962E0 1.78162273E4/
   PLOG/1.0E-1 4.60176853E37 -7.60702496E0 2.58252199E4/
   PLOG/1.0E0 3.01242442E40 -8.17675315E0 3.23060244E4/
   PLOG/1.0E1 1.29369702E26 -3.64892665E0 3.17842345E4/
   PLOG/1.0E2 1.34306393E3 3.20579697E0 2.61776644E4/
   PLOG/1.0E3 1.34292319E-29 1.24863337E1 1.46743009E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
AC5H10+H=AC5H9-C+H2    1.26E5 2.62 2.61E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
BC5H10+H=AC5H9-C+H2    1.0E4 2.92 3.37E3
!\Author: WARNING !\Ref: S. WANG, D.F. DAVIDSON, R.K. HANSON, PROC. COMBUST. INST. 35(2015) 473-480. !\Comment: WARNING
CYC2H3OCHO+OH=>C2H3O1-2+CO+H2O    2.8E12 0.0 -7.09E2
!UPDATES FROM SN
!!C3H5-A+H=C3H6,RATE FROM YE, PROCI (2015), 223-230 KUKKADAPU1@LLNL.GOV
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!!
AC5H9-C+H=BC5H10    2.0E14 0.0 0.0E0
   PLOG/1.0E-2 1.0E64 -1.502E1 2.389E4/
   PLOG/1.0E-2 9.25E39 -8.59E0 6.466E3/
   PLOG/1.0E-1 7.0E60 -1.384E1 2.4846E4/
   PLOG/1.0E-1 1.69E34 -6.64E0 5.193E3/
   PLOG/1.0E0 5.0E57 -1.27E1 2.5947E4/
   PLOG/1.0E0 4.53E29 -5.1E0 4.172E3/
   PLOG/1.0E1 8.4E52 -1.113E1 2.591E4/
   PLOG/1.0E1 2.39E25 -3.68E0 3.143E3/
   PLOG/1.0E2 3.45E44 -8.62E0 2.2842E4/
   PLOG/1.0E2 5.5E20 -2.16E0 1.917E3/
   PLOG/1.0E3 7.7E14 -3.1E-1 4.35E2/
   PLOG/1.0E3 3.57E11 6.5E-1 -6.1E2/
!!
!!C3H5-A+H=C3H6,RATE FROM YE, PROCI (2015), 223-230 KUKKADAPU1@LLNL.GOV
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!!
AC5H9-C+H=AC5H10 2.0E14 0.0 0.0E0
  PLOG/1.0E-2 1.0E64 -1.502E1 2.389E4/
  PLOG/1.0E-2 9.25E39 -8.59E0 6.466E3/
  PLOG/1.0E-1 7.0E60 -1.384E1 2.4846E4/
  PLOG/1.0E-1 1.69E34 -6.64E0 5.193E3/
  PLOG/1.0E0 5.0E57 -1.27E1 2.5947E4/
  PLOG/1.0E0 4.53E29 -5.1E0 4.172E3/
  PLOG/1.0E1 8.4E52 -1.113E1 2.591E4/
  PLOG/1.0E1 2.39E25 -3.68E0 3.143E3/
  PLOG/1.0E2 3.45E44 -8.62E0 2.2842E4/
  PLOG/1.0E2 5.5E20 -2.16E0 1.917E3/
  PLOG/1.0E3 7.7E14 -3.1E-1 4.35E2/
  PLOG/1.0E3 3.57E11 6.5E-1 -6.1E2/
!\Author: WARNING !\Ref: WARNING NO REFERENCE !\Comment: WARNING !
BC5H10+OH=AC5H9-C+H2O 6.24E6 2.0 -2.98E2
!\Author: WARNING !\Ref: WARNING NO REFERENCE !\Comment: WARNING !
BC5H10+HO2=AC5H9-C+H2O2 1.928E4 2.6 1.391E4
!\Author: SN !\Ref: 2*RATE RULE PRIMARY !ALLYL WARNING NO REFERENCE !\Comment: WARNING !
BC5H10+CH3=AC5H9-C+CH4 1.11E2 3.27 7.15E3
!\Author: WARNING !\Ref: WARNING NO REFERENCE !\Comment: WARNING !
BC5H10+CH3O=AC5H9-C+CH3OH 1.8E2 2.95 1.199E4
!\Author: WARNING !\Ref: WARNING NO REFERENCE !\Comment: WARNING !
BC5H10+CH3O2=AC5H9-C+CH3O2H 1.928E4 2.6 1.391E4
!\Author: WARNING !\Ref: WARNING NO REFERENCE !\Comment: WARNING !
BC5H10+OH=IC3H7+CH3CHO 2.0E10 0.0 4.0E3
!---
!\ENDSUBMECH: CC5H10BC5H10
!---
!---
!\SUBMECH: AC5H10
!\MECHCOMMENTS: AC5H10 SUBMECH CONTAINS B13DE2M(BUTA-1,3-DIENE-2-METHYL OR 2-METHYL-1,3-BUTADIENE AS A SUBMECH BELOW
!\MECHCOMMENTS: IF SIMULATING IC4H10, AC5H10 SUBMECHANISM IN C5-MODULE IS NECESSARY ALONG WITH B13DE2M SUBMECH.
!\MECHCOMMENTS: KPS, 22 / 07 / 2015 WHEN COMBINING JBS PENTANE WITH CWS ISO-BUTENE KPS NOTICED THAT BOTH MECAHNISMS HAVE COMMON REACTIONS
!\MECHCOMMENTS: FOR AC5H10 AND BOTH AUTHORS ARE USING DIFFERENT KINETIC PARAMETERS. THIS WILL HAVE TO BE DISCUSSED
!\MECHCOMMENTS: I HAVE COMBINED JOHNS AC5H10 REACTIONS WITH CWS AND SEPERATED THEM INTO THEIR REACTION CLASSED. EACH RATE CONSTANT IS COMMENTED
!\MECHCOMMENTS: SEARCH FOR "!\\WARNING: DUPLICATED KINETICS" AT THE TOP OF THE AC5H10 SUBMECH. IT LOOKS LIKE CWS KINETICS ARE MUCH MORE DETAILED.
!\MECHCOMMENTS: DUPLICATED KINETICS
!\MECHCOMMENTS: POSSIBLE DUPLICATED REACTIONS, WE ALL NEED TO DISCUSS COMBINING THESE REACTIONS WITH OTHER PARTS OF MECHANISM
!---
!____
!\REACTIONCLASS: RH(=)PRODUCTS
!____
!\Author: KPS, THIS REACTION IS FROM CWS IC4H8 !\Ref: WARNING !\Comment: WARNING
AC5H10=C3H5-T+C2H5 8.922E24 -2.409 1.005E5
!\Author: KPS, THIS REACTION IS FROM CWS IC4H8 !\Ref: WARNING !\Comment: WARNING
IC4H7+CH3(+M)=AC5H10(+M) 1.5E14 -0.32 -2.623E2
  AR/0.7/
  CO/1.5/
  CO2/2.0/
  CH4/2.0/
  H2/2.0/

C2H6/3.0/
H2O/6.0/
LOW/5.865E60 -1.281E1 6.25E3/
TROE/1.04E-1 1.606E3 6.0E4 6.118E3/
!\Author: WARNING !\Ref: FROM LLNL C8-C16 N-ALKANES MECH !\Comment: WARNING
AC5H10+OH=AC5H9-C+H2O 2.764E4 2.64 -1.919E3
!\Author: WARNING !\Ref: FROM LLNL C8-C16 N-ALKANES MECH !\Comment: WARNING
AC5H10+HO2=AC5H9-C+H2O2 4.82E3 2.55 1.053E4
!\Author: SN !\Ref: WANG, !KUN, ET AL. ! !\Comment: WARNING
AC5H10+CH3=AC5H9-C+CH4 1.61E2 3.12 6.32E3
!\Author: WARNING !\Ref: FROM LLNL C8-C16 N-ALKANES MECH !\Comment: WARNING
AC5H10+CH3O2=AC5H9-C+CH3O2H 4.82E3 2.55 1.053E4
!\Author: WARNING !\Ref: FROM LLNL C8-C16 N-ALKANES MECH !\Comment: WARNING
AC5H10+CH3O=AC5H9-C+CH3OH 4.0E1 2.9 8.609E3
!_____
!\REACTIONCLASS: RADICAL_ADDITIONMISC
!_____
!\Author: KPS, THIS REACTION IS FROM CWS IC4H8 !\Ref: WARNING !\Comment: WARNING
AC5H10+OH=SC4H9+CH2O 2.0E10 0.0 4.0E3
!\Author: WARNING !\Ref: FROM LLNL C8-C16 N-ALKANES MECH !\Comment: WARNING
AC5H10+O=SC4H9+HCO 7.23E5 2.34 -1.05E3
!\Author: WARNING !\Ref: FROM LLNL C8-C16 N-ALKANES MECH !\Comment: WARNING
AC5H10+O=IC3H7+CH3CO 7.23E5 2.34 -1.05E3
!\Author: WARNING !\Ref: FROM LLNL C8-C16 N-ALKANES MECH !\Comment: WARNING
AC5H10+O=IC4H9+HCO 7.23E5 2.34 -1.05E3
!\Author: SD !\Ref: WARNING !\Comment: WARNING
C6H11OH1Q2-5=QC3H5OHP+C3H6 1.392E14 0.0 2.813709E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C6H11OH1Q2-5+O2=C6H11OH1Q2-5O2 8.715E13 -0.816 -5.365E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C6H11OH1Q2-3O2=C6H103OH1Q2+HO2 6.168E9 1.01 2.9362E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C6H11OH1Q2-4O2=C6H103OH1Q2+HO2 6.168E9 1.01 2.9362E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C6H11OH1Q2-4O2=C6H104OH1Q2+HO2 6.168E9 1.01 2.9362E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C6H11OH1Q2-5O2=C6H104OH1Q2+HO2 6.168E9 1.01 2.9362E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C6H11OH1Q2-5O2=C6H105OH1Q2+HO2 3.606E9 1.13 3.06E4
!_____
!\REACTIONCLASS: O2QOOHDECOMPOSITIONS
!_____
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C6H11OH1Q2-3O2=C6H10OH1KET2-3+OH 1.748E8 1.7 2.6E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C6H10OH1KET2-3=>NC3H7CHO+OH+CO+CH2OH 5.25E15 0.0 4.18E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NH+H=N+H2 3.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NH+O=NO+H 9.2E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NH+OH=HNO+H 3.2E14 -0.376 -4.6E1
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NH+OH=N+H2O 1.6E7 1.733 -5.76E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NH+O2=HNO+O 2.4E13 0.0 1.385E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NH+O2=NO+OH 9.9E10 0.0 1.53E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NH+N=N2+H 3.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NH+NO=N2O+H 2.7E15 -0.78 2.0E1
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NH+NO=N2+OH 6.8E14 -0.78 2.0E1
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING

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NH+NO2=N2O+OH    4.1E12 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NH+NO2=HNO+NO    5.9E12 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
N+OH=NO+H    3.8E13 0.0 0.0E0
!\Author: YJZ !\Ref: BAULCH ET AL., J. PHYS. CHEM. REF. DATE, 1994, 23 !\Comment: WARNING
N+O2=NO+O    9.03E9 1.0 6.498E3
!\Author: YJZ !\Ref: ABIAN, ALZUETA AND GLARBORG, IJCK, 2015, 47(8) !\Comment: 1.2A_9.4E12
N+NO=N2+O    1.128E13 0.14 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NNH=N2+H    1.0E9 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NNH+H=N2+H2    1.0E14 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NNH+O=N2O+H    1.9E14 -0.274 -2.2E1
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NNH+O=N2+OH    1.2E13 0.145 -2.17E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NNH+O=NH+NO    5.2E11 0.381 -4.09E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NNH+OH=N2+H2O    5.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NNH+O2=N2+HO2    5.6E14 -0.385 -1.3E1
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NNH+NO=N2+HNO    5.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
HNO+H=NO+H2    6.6E10 0.94 4.95E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
HNO+O=NO+OH    2.3E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
2HNO=N2O+H2O    9.0E8 0.0 3.1E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NO+HO2=NO2+OH    2.1E12 0.0 -4.97E2
!\Author: YJZ !\Ref: TSANG AND HERRON, JPCRD, 1991,20(4) !\Comment: WARNING
NO+O(+M)=NO2(+M)    1.3E15 -0.75 0.0E0
   AR/0.6/
   O2/0.8/
   NO/1.8/
   N2O/4.4/
   CO2/6.0/
   NO2/6.2/
   H2O/10.0/
   LOW/9.44E24 -2.87E0 1.551E3/
   TROE/9.62E-1 1.0E1 7.962E3/
!\Author: YJZ !\Ref: TSANG AND HERRON, JPCRD, 1991,20(4) !\Comment: BIG EFFECT ON CO 1.5A_3.91E12
NO2+O=NO+O2    5.86E12 0.0 -2.38E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NO2+HO2=HONO+O2    1.9E0 3.32 3.044E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
2NO2=2NO+O2    4.5E12 0.0 2.7599E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
HONO+O=NO2+OH    1.2E13 0.0 5.96E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
HONO+OH=NO2+H2O    1.7E12 0.0 -5.2E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
2HONO=NO+NO2+H2O    3.5E-1 3.64 1.214E4
!\Author: YJZ !\Ref: ZUEV AND STARIKOVSKII, KHIM. FIZ, 1991, 10 !\Comment: WARNING
N2O(+M)=N2+O(+M)    1.69E11 0.0 5.7653E4
   O2/1.4/
   N2/1.7/
   NO/3.0/
   N2O/3.5/
   H2O/12.0/
   LOW/7.2E14 0.0E0 5.741E4/
!\Author: YJZ !\Ref: KLIPPENSTEIN ET AL., CNF, 2011, 158 !\Comment: WARNING
```

```
N2O+H=N2+OH    6.4E7 1.835 1.3492E4
!\Author: YJZ !\Ref: HIDAKA J. PHY. CHEM.,1985, 89, 4903 !\Comment: WARNING
N2O+H=OHV+N2    1.6E14 0.0 5.03E4
!\Author: YJZ !\Ref: MEAGHER J ET AL., JPCA, 2000, 104(25) !\Comment: 0.8A_3.69E12
N2O+O=N2+O2    3.69E12 0.0 1.5936E4
!\Author: YJZ !\Ref: MEAGHER J ET AL., JPCA, 2000, 104(25) !\Comment: 1.2A_9.15E13
N2O+O=2NO    9.15E13 0.0 2.7679E4
!\Author: YJZ !\Ref: MEBEL ET AL., IJCK, 1996, 28(9) !\Comment: WARNING
N2O+OH=HO2+N2    1.3E-2 4.72 3.656E4
!\Author: YJZ !\Ref: MEBEL ET AL., IJCK, 1996, 28(9) !\Comment: WARNING
N2O+OH=HNO+NO    1.2E-4 4.33 2.508E4
!\Author: YJZ !\Ref: MEBEL ET AL., IJCK, 1996, 28(9) !\Comment: WARNING
N2O+NO=NO2+N2    5.3E5 2.23 4.6281E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
HCN+O=NCO+H    1.4E4 2.64 4.98E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
HCN+O=NH+CO    3.5E3 2.64 4.98E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
HCN+OH=HOCN+H    5.9E4 2.4 1.25E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
HOCN+H=H2+NCO    2.4E8 1.5 6.617E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
HOCN+O=OH+NCO    1.7E8 1.5 4.133E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
HOCN+OH=H2O+NCO    1.2E6 2.0 -2.48E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NCO+M=N+CO+M    2.2E14 0.0 5.405E4
   N2/1.5/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NCO+H=CO+NH    7.2E13 0.0 1.0E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NCO+O=NO+CO    2.0E15 -0.5 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NCO+OH=H+CO+NO    8.3E12 -0.05 1.8042E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NCO+O2=NO+CO2    2.0E12 0.0 2.0E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NCO+NO=N2O+CO    4.0E19 -2.19 1.743E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NCO+NO=N2+CO2    1.5E21 -2.74 1.824E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NCO+NO2=CO+2NO    2.5E11 0.0 -7.07E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NCO+NO2=CO2+N2O    3.0E12 0.0 -7.07E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NCO+N=N2+CO    2.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
2NCO=>2CO+N2    1.8E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CO+NO2=NO+CO2    9.0E13 0.0 3.38E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CO+N2O=N2+CO2    2.7E11 0.0 2.0237E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CO2+N=NO+CO    2.0E12 0.0 2.0E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2O+NO2=HONO+HCO    1.4E-7 5.64 9.22E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
HCO+NO=HNO+CO    6.9E12 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
HCO+HNO=NO+CH2O    5.8E-1 3.84 1.15E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
HCO+NO2=NO+CO2+H    2.3E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
HCO+NO2=HONO+CO    5.0E12 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
```

```
HCO+NO2=NO+CO+OH    5.0E12 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH4+NO2=CH3+HONO    1.1E-1 4.28 2.63E4
   DUP
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH4+NO2=CH3+HONO    7.4E1 3.42 3.31E4
   DUP
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3+NH=N+CH4    8.2E5 1.87 5.852E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3+HNO=NO+CH4    1.5E11 0.76 3.48E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3+NO=HCN+H2O    1.5E-1 3.52 3.95E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3+NO2=CH3O+NO    1.1E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2+N2=HCN+NH    1.0E13 0.0 7.4E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2+N=HCN+H    5.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2+NO=HCN+OH    3.9E11 0.0 -3.78E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2+NO2=CH2O+NO    5.9E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2(S)+NO=HCN+OH    2.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2(S)+NO=CH2+NO    1.0E14 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2(S)+N2O=CH2O+N2    3.8E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH+NO=CO+NH    9.1E12 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH+NO=NCO+H    1.8E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH+NO=HCN+O    7.9E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH+NO=HCO+N    6.8E12 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH+NO2=HCO+NO    1.0E14 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH+N2O=HCN+NO    1.9E13 0.0 -5.11E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3OH+NO2=HONO+CH2OH    1.5E2 3.32 2.0035E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3O+HNO=NO+CH3OH    3.2E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3O+NO=HNO+CH2O    7.5E12 0.0 2.017E3
   DUP
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3O+NO=HNO+CH2O    2.5E18 -2.56 0.0E0
   DUP
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3O+NO2=HONO+CH2O    6.0E12 0.0 2.285E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2OH+HNO=NO+CH3OH    3.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2OH+NO2=HONO+CH2O    5.0E12 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3O2+NO=CH3O+NO2    1.4E12 0.0 -7.15E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H6+NO2=C2H5+HONO    3.3E0 3.84 2.39E4
   DUP
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H6+NO2=C2H5+HONO    8.5E1 3.45 3.2E4
   DUP
```

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!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H5+N=C2H4+NH    4.3E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H5+NO2=C2H5O+NO    4.0E13 -0.2 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H3+NO=HCN+CH2O    7.0E21 -3.382 1.025E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H3+HONO=C2H4+NO2    8.1E5 1.87 5.504E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H3+NO2=CH2CHO+NO    7.7E14 -0.6 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H2+NCO=HCCO+HCN    1.4E12 0.0 1.815E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H+NO=HCN+CO    4.6E13 0.0 5.7E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H+NO2=HCCO+NO    4.6E13 0.0 -2.58E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H5O+NO=CH3CHO+HNO    6.6E12 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H5O+NO2=CH3CHO+HONO    1.7E12 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH2CHO+NO2=CH2CO+HONO    2.0E15 -0.68 1.43E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CO+NO2=>CH3+CO2+NO    1.5E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
HCCO+N=HCN+CO    5.0E13 0.0 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
HCCO+NO=HCN+CO2    2.1E12 0.0 -6.76E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3NO2=CH3+NO2    5.22E21 -1.56 6.1309E4
   PLOG/6.6E-3 2.68E50 -1.148E1 7.1011E4/
   PLOG/3.94E-2 1.04E48 -1.068E1 6.7928E4/
   PLOG/7.88E-2 1.19E48 -1.06E1 6.7175E4/
   PLOG/1.0E-1 3.78E50 -1.115E1 7.2239E4/
   PLOG/1.575E-1 9.51E47 -1.047E1 6.694E4/
   PLOG/1.0E0 2.93E49 -1.052E1 7.3097E4/
   PLOG/1.0E1 1.39E46 -9.27E0 7.3087E4/
   PLOG/1.0E2 5.22E21 -1.56E0 6.1309E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3NO2=CH3O+NO    9.078E39 -7.875 6.6229E4
   PLOG/1.0E-1 2.851E48 -1.102E1 6.6953E4/
   PLOG/2.0E-1 1.644E48 -1.088E1 6.7057E4/
   PLOG/5.0E-1 4.932E47 -1.0635E1 6.7138E4/
   PLOG/1.0E0 4.932E47 -1.0635E1 6.7138E4/
   PLOG/2.0E0 2.333E46 -1.011E1 6.7089E4/
   PLOG/5.0E0 1.349E45 -9.66E0 6.6924E4/
   PLOG/1.0E1 1.002E44 -9.265E0 6.6722E4/
   PLOG/2.0E1 6.266E42 -8.85E0 6.6507E4/
   PLOG/5.0E1 6.266E42 -7.85E0 6.6507E4/
   PLOG/1.0E2 9.078E39 -7.875E0 6.6229E4/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
H+NO2=OH+NO    1.01E11 0.84 -1.058E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
OH+NO=HONO    7.29E22 -3.41 2.66E3
   PLOG/1.0E-2 5.02E21 -4.24E0 8.989E2/
   PLOG/1.0E-1 5.31E22 -4.24E0 1.184E3/
   PLOG/3.16E-1 1.38E23 -4.22E0 1.376E3/
   PLOG/1.0E0 3.09E23 -4.17E0 1.621E3/
   PLOG/3.16E0 5.45E23 -4.09E0 1.911E3/
   PLOG/1.0E1 6.35E23 -3.97E0 2.222E3/
   PLOG/3.16E1 3.68E23 -3.75E0 2.501E3/
   PLOG/1.0E2 7.29E22 -3.41E0 2.66E3/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
H+HONO=H2+NO2    1.89E3 2.83 1.4227E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
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H+HONO=NO+H2O    2.79E10 0.8 6.146E3
   PLOG/1.0E-2 3.91E9 9.9E-1 4.049E3/
   PLOG/1.0E-1 3.93E9 9.9E-1 4.049E3/
   PLOG/3.16E-1 3.97E9 9.9E-1 4.051E3/
   PLOG/1.0E0 4.3E9 9.8E-1 4.07E3/
   PLOG/3.16E0 7.04E9 9.2E-1 4.225E3/
   PLOG/1.0E1 2.6E10 7.6E-1 4.736E3/
   PLOG/3.16E1 7.91E10 6.4E-1 5.519E3/
   PLOG/1.0E2 2.79E10 8.0E-1 6.146E3/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
HNO+OH=H+HONO    1.03E5 2.24 6.951E3
   PLOG/1.0E-2 1.06E3 2.76E0 4.439E3/
   PLOG/1.0E-1 1.09E3 2.75E0 4.45E3/
   PLOG/3.16E-1 1.18E3 2.74E0 4.476E3/
   PLOG/1.0E0 1.48E3 2.72E0 4.554E3/
   PLOG/3.16E0 2.71E3 2.64E0 4.768E3/
   PLOG/1.0E1 9.67E3 2.49E0 5.253E3/
   PLOG/3.16E1 5.31E4 2.29E0 6.063E3/
   PLOG/1.0E2 1.03E5 2.24E0 6.951E3/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
HNO+OH=NO+H2O    4.18E10 0.51 5.532E3
   PLOG/1.0E-2 5.82E10 4.0E-1 3.762E3/
   PLOG/1.0E-1 5.85E10 4.0E-1 3.763E3/
   PLOG/3.16E-1 5.92E10 4.0E-1 3.764E3/
   PLOG/1.0E0 6.3E10 3.9E-1 3.782E3/
   PLOG/3.16E0 9.53E10 3.4E-1 3.931E3/
   PLOG/1.0E1 2.6E11 2.3E-1 4.413E3/
   PLOG/3.16E1 3.83E11 2.0E-1 5.099E3/
   PLOG/1.0E2 4.18E10 5.1E-1 5.532E3/
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
N2O+H2=N2+H2O    7.0E12 0.0 3.25E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NO+H(+M)=HNO(+M)    1.52E15 -0.41 0.0E0
   AR/0.75/
   O2/1.5/
   N2/1.6/
   H2/2.0/
   CO2/3.0/
   H2O/10.0/
   LOW/2.4E14 2.06E-1 -1.55E3/
   TROE/8.2E-1 1.0E-30 1.0E30 1.0E30/
!\Author: QW !FUEL 243(2019) 288 297, G4 / / B3LYP / 6 311+G(D,P) !\Ref: WARNING !\Comment: WARNING
HNO+NO2=NO+HONO    7.847E2 3.059 3.8824E3
!\Author: QW !CCSDT/CBS CALCULATION !\Ref: WARNING !\Comment: WARNING
HNO+O2=NO+HO2    3.98956E5 2.3026 1.46054E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C2H5O2+NO=C2H5O+NO2    1.4E12 0.0 -7.15E2
!-----------------------------------------------------------------------------------------------------------------------
!-----------------------------------------------------------------------------------------------------------------------
!\SUBMECH: C3H8+NOX
!-----------------------------------------------------------------------------------------------------------------------
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H8+NO2=NC3H7+HONO    1.32E14 0.0 3.11E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C3H8+NO2=IC3H7+HONO    1.16E13 0.0 2.819E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NC3H7O2+NO=NC3H7O+NO2    1.4E12 0.0 -7.15E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC3H7O2+NO=IC3H7O+NO2    1.4E12 0.0 -7.15E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
CH3CHO+NO2=CH3+CO+HONO    1.4E-7 5.64 9.22E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NC3H7+NO2=NC3H7O+NO    4.0E13 -0.2 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC3H7+NO2=IC3H7O+NO    4.0E13 -0.2 0.0E0
```

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!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NC3H7+HNO=C3H8+NO    1.5E11 0.76 3.48E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
IC3H7+HNO=C3H8+NO    1.5E11 0.76 3.48E2
!-----------------------------------------------------------------------------------------------------------------------
!\ENDSUBMECH: C3H8+NOX
!-----------------------------------------------------------------------------------------------------------------------
!+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
++++++++++++++++++++++++++++++++++++
!-----------------------------------------------------------------------------------------------------------------------
!\SUBMECH: C4H10+NOX
!-----------------------------------------------------------------------------------------------------------------------
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C4H10+NO2=PC4H9+HONO    1.32E14 0.0 3.11E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
C4H10+NO2=SC4H9+HONO    2.32E13 0.0 2.81E4
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
SC4H9O2+NO=SC4H9O+NO2    1.4E12 0.0 -7.15E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
NC3H7CHO+NO2=NC3H7+CO+HONO    1.4E-7 5.64 9.22E3
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
SC4H9+NO2=SC4H9O+NO    4.0E13 -0.2 0.0E0
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
PC4H9+HNO=C4H10+NO    1.5E11 0.76 3.48E2
!\Author: WARNING !\Ref: WARNING !\Comment: WARNING
SC4H9+HNO=C4H10+NO    1.5E11 0.76 3.48E2
END
```