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N. Marinov
W. Pitz
C. Westbrook
M. Hori
N. Matsunaga

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AN EXPERIMENTAL AND KINETIC CALCULATION OF THE PROMOTION EFFECT OF HYDROCARBONS ON THE NO-NO2 CONVERSION IN A FLOW REACTOR

NICK MARINOV, WILLIAM PITZ and CHARLES WESTBROOK
Lawrence Livermore National Laboratory
P.O. Box 808, Livermore, California, USA

AND

MORIO HORI, NOAKI MATSUNAGA
Department of Mechanical System Engineering, Takushoku University
Hachioji, Tokyo, Japan

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ABSTRACT

Experimental and detailed chemical kinetic modeling work has been performed to investigate the role of hydrocarbon oxidation in NO-NO_2 conversion. An atmospheric pressure, quartz flow reactor was used to examine the dependence of NO oxidation to NO_2 by hydrocarbon type, reaction temperature and residence time. The five hydrocarbons examined in this study were methane, ethylene, ethane, propene and propane. In the experiment, probe measurement of the species concentrations was performed in the flow reactor using a mixture of NO (20ppm) /air/hydrocarbon (50ppm) at residence times of 0.16sec to 1.46sec, and temperatures from 600K to 1100K. In the chemical kinetic calculation, the temporal evolution of NO, NO_2, hydrocarbons and reaction intermediates was evaluated for a series of the hydrocarbons and the temperatures. The detailed chemical kinetic model consisted of 649 reversible reactions and 126 species.

Experimental results indicate that, in general, ethylene and propane effectively oxidize NO to NO_2 while methane is less effective. The calculation indicates the important chemical kinetic features which control NO-NO_2 conversion for each hydrocarbon type. The dependence of NO-NO_2 conversion with hydrocarbon type is qualitatively reproduced by the calculation. The calculation indicates that all five hydrocarbons oxidize NO to NO_2 predominantly through $NO+HO_2 \rightleftarrows NO_2+OH$, and that the contribution of oxidation by RO_2 and $HORO_2$ is minor. Highest effectiveness comes from hydrocarbons that produce reactive radicals (i.e., OH, O-atom) which promote hydrocarbon oxidation and lead to additional HO_2 production. On the other hand, if hydrocarbons produce radicals, such as methl and allyl, which resist oxidation by O_2, then these radicals will tend to reduce NO_2 to NO and limit NO oxidation to NO_2. Experimental results show that the effectiveness of hydrocarbons varies appreciably with temperature and only within the low temperature range. The dependence of the NO-NO_2 conversion with temperature is reasonably reproduced by the calculation. Propane shows the greatest NO-NO_2 conversion for the lowest temperatures. This ability is primarily due to the hydroperoxy-propyl plus O_2 reactions as indicated by the sensitivity analysis results.

INTRODUCTION

The main route to nitrogen dioxide (NO_2) formation in combustion systems is through the oxidation of nitric oxide (NO). This process was originally investigated in order to explain the high proportion of NO_2 found in NOx emissions from the exhaust of gas turbine engines [1]. Moreover, the understanding of the NO-NO_2 conversion mechanism is relevant to a number of issues including NO_2 emission from unflued space heaters, development of NOx control technologies, behavior of NO/NO_2 in the atmosphere, formation and reduction chemistry of NOx, and the probe sampling techniques for NOx concentration measurements. Originally, the NO-NO_2 conversion was thought to proceed through the rapid oxidation of NO by oxidative radicals without much attention to the effect of fuels on the conversion [2-4]. Although, in later studies, it was revealed that the conversion was greatly promoted by small quantities of fuels such as hydrocarbons, H_2, CO, and methanol [5-9]. In our former experiment and model calculation of the NO-NO_2 conversion in the mixing of hot combustion gas with cold air and nine different fuels [6], the results indicated that NO-NO_2 conversion appeared only in the low temperature range, and showed a strong dependence on fuel type. Thus, the interaction between the NO-NO_2 reactions and the oxidation reactions of the fuel in the low temperature range must be understood in order to explain the effect of fuel type on the NO-NO_2 conversion and consequently to predict the NO/NO_2 emission levels from combustion systems.

The objective of the present study is to compare the experimental results obtained by using a simple reacting flow reactor with the calculated results of a detailed chemical model in order to understand the effect of hydrocarbon oxidation kinetics on the NO to NO_2 conversion. The comparison is made in order to understand the NO-NO_2 conversion dependence on hydrocarbon type and reaction temperature. Detailed chemical kinetic modeling of the NO-NO_2 conversion in the presence of hydrocarbons has been previously reported for methane [10, 11], and ethylene [12]. The present study focuses on the NO-NO_2 conversion found in C_1 to C_3 hydrocarbons, i.e., methane, ethylene, ethane, propene, and propane. This problem is interesting not only in the area of NOx chemistry but also in low temperature hydrocarbon oxidation chemistry which has been investigated extensively in studies of engine knock, cool flames, and ignition phenomena [13-15]. In the experiment, a probe measurement of species concentrations was performed in an atmospheric flow reactor using a mixture of NO(20ppm)/air/hydrocarbon(50ppm). In the chemical kinetic calculations, the temporal evolution of NO, NO_2, hydrocarbons and reaction intermediates for a series of hydrocarbon types and reaction temperatures is shown. The important chemical kinetic features that control the NO-NO_2 conversion for each hydrocarbon type are discussed.

EXPERIMENTAL

Experimental Apparatus:

The experiment was performed using a constant temperature quartz flow reactor. Dry air was supplied to an electric heater at the bottom end of the flow reactor and the air was heated up to a desired reaction temperature. Just above the electric heater, an NO/hydrocarbon (balance N_2) mixture was doped as a counter-flow jet into the heated air stream. In the flow reactor, the initial NO(20ppm)/air/hydrocarbon(50ppm) mixture flowed up through the entrance section (8mm i.d.) and into the test section (16mm i.d., 590mm length) as a reacting flow at constant temperature. The types of hydrocarbons selected were methane, ethylene, ethane, propene, and propane, and the reaction temperatures were controlled from 600K to 1100K. The uniformity of the species concentrations and temperature across the test section was confirmed before measurements were taken. The sample was withdrawn by a quartz sampling probe at eleven axial positions (which corresponded to residence times from 0.16 to 1.46sec) in the test section. To attain iso-kinetic sampling, the sampling probe was designed to have a larger inlet diameter than the diameter of the downstream sampling tube. The samples were analyzed by a chemiluminescent NO/NOx analyzer continuously and by three gas chromatographs with thermal conductivity detectors and a flame ionization detector with batch method. The species detected by the gas chromatographs were oxygen, nitrogen, hydrogen, carbon monoxide, carbon dioxide and five hydrocarbons selected for the experiment.

Experimental Results and Discussion:

According to the experimental results, the NOx concentration remains essentially constant with residence time for all the experimental conditions investigated, and thus the decrease (increase) in the NO concentration corresponds to the increase (decrease) in the NO_2 concentration. When the hydrocarbons were not doped into the mixture, the NO_2 concentration was below 1ppm and did not vary against the residence time. From these results, it is clear that only the NO-NO_2 conversion occurs within the flow reactor, and that the formation of considerable levels of NO_2 is due to the role of hydrocarbon oxidation in the NO-NO_2 conversion.

Figure

Figure 2

The variations of the NO-NO_2 conversion with hydrocarbon type, that are shown as the NO_2/NO_x ratio against the residence time, are discussed at first. At the reaction temperature of 700K, only propane promotes the NO-NO_2 conversion as shown in Figure 1. In this case, it was found that only propane was consumed up to 30% which resulted in the NO_2/NO_x ratio above 0.9. At 800K, four hydrocarbons except methane promote the NO-NO_2 conversion, while, among them, ethylene and propane effectively oxidize NO to NO_2, and ethane is less effective (see Figures 3 and 4 in the later section). Although at 1000K, all five hydrocarbons promote the NO-NO_2 conversion and the NO_2/NO_x ratios decrease gradually in the later stage of the NO-NO_2 conversion due to the reduction of NO_2 to NO as shown in Figure 2. In this case, it was found that the concentrations of five hydrocarbons decreased monotonically against the residence time. It is suggested from these experimental results that methane promotes the NO-NO_2 conversion most weakly, and that the simple relationship is not found between the amount of hydrocarbon consumption and the level of the NO_2/NO_x ratio.

The effectiveness of hydrocarbons varies appreciably with reaction temperature and only within a low temperature range (see Figure 5 in the later section). Propane shows the greatest NO-NO_2 conversion for the lowest temperatures and even methane and ethane show fairly large NO-NO_2 conversion for the higher temperatures. The variations of the hydrocarbon consumption with the reaction temperature obtained in the experiment showed that the consumption was accelerated with increasing the reaction temperature.

CHEMICAL KINETIC CALCULATIONS

Numerical Model:

The numerical calculations were performed using the CHEMKIN-II/SENKIN computer programs [16, 17]. The SENKIN code was used to calculate the temporal evolution of a homogeneous reacting gas mixture in an adiabatic system at constant pressure. The detailed chemical model used in the numerical calculations was based on a hierarchical structure of hydrocarbon oxidation kinetics starting from hydrogen and building up to propane. The main portion of the detailed kinetics mechanism was taken from our previous modeling works of hydrogen [18], methane[19], ethylene [20], ethane[19], propane[21], and ethanol [22] flame chemistry. The chemical model was extended to include NO_X chemistry and was primarily taken from GRI-MECH2.11 [23], Dean and Bozzelli [24], and Atkinson [25]. The chemical kinetic calculations performed for propane at temperatures less than ca. 800K by the above mechanism showed no fuel conversion. A low temperature chemistry submechanism was added to the above mechanism to achieve the amount of reactivity observed in the experiments. These reactions were taken from Bozzelli and coworkers [26,27] and involve the addition of molecular oxygen to hydroperoxy-propyl radicals which eventually lead to OH radical formation and chain branching. Thermodynamic properties of the chemical compounds were obtained from the CHEMKIN Thermodynamic database [28] or calculated by group additivity techniques as described by Benson [29] and fitted to a polynomial form using THERM [30]. The complete listing of the chemical kinetic mechanism used in the modeling portion of the study can be found in Table 1 and may be obtained from the authors [31]. The detailed chemical kinetic model consisted of 639 reversible reactions and 126 species.

Detailed Chemical Kinetic Calculations - Results

Fig. 3

In this section, the calculated results are compared to the experimental results. The NO2/NOx ratio against the residence time at 800K is shown in Figure 3. The experiments indicate a small amount of NO is oxidized for methane and ethane, while the model suggests relatively little to no conversion for these fuels. The ethylene experimental data shows a fairly rapid rise in NO conversion at early residence times and slowly levels out with time. The calculation shows similar behavior although the NO2/NOx ratio increases a little more rapidly at longer residence times. The propene experimental data shows a fairly linear increase in NO2 formation with time which is reproduced by the model calculation. Propane exhibits nearly the same measured NO2/NOx profile as ethylene, although the calculation shows an over oxidation of NO at the early residence times than indicated by the experiment. There are a number of possibilitities that could account for this problem. The over oxidation of NO could be due to the inadequate understanding of the propyl-O_2 isomerization to the hydroperoxy-propyl radical versus chemical activation of the propyl-O_2 adduct to propene and HO_2, thermochemical assignments in the propyl-O_2 and hydroperoxy-propyl adducts etc. Figure 4

Figure 4 shows the hydrocarbon consumption with residence time at 800K. The hydrocarbon concentration has been nondimensionalized to the initial hydrocarbon concentration of 50ppm. Experimental results for methane and ethane are reproduced by the calculation and show very little hydrocarbon consumption with residence time. The experimental ethylene consumption profile is also well reproduced by the calculation. The propene experimental data shows a longer induction time prior to the start of its oxidation than indicated by the calculation. At longer residence times, the propene experimental consumption profile exhibits a linear change in concentration with residence time which is a similiar characteristic exhibited by the calculation. The modeling results for propane show an over oxidation of the fuel in comparison with the experimental data, and the causes for this disagreement have been previosuly discussed in connection to the over oxidation of NO with residence time. Figure 5

The calculated change in the NO_2/NOx ratio with temperature is compared to measurement in Figure 5. The NO_2/NOx ratios for five hydrocarbons are reasonably reproduced by the model, although the amount of NO oxidized to NO_2 tends to be underpredicted at the highest temperatures of this study. The model was able to reproduce the low temperature NO-NO_2 conversion behavior for propane, and the mechanism for this behavior will be discussed in the next section.

Detailed Chemical Kinetic Calculations - Analysis:

Reaction flux calculations indicate that all five hydrocarbons oxidize NO to NO_2 predominantly through the $NO+HO_2 \rightleftarrows NO_2+OH$ mechanism for the operating conditions examined in this study. Alkyl, alkenyl or hydroxyalkyl plus molecular oxygen addition and subsequent stabilization of the adduct does not produce any appreciable concentration of these peroxy species which would otherwise convert the NO to NO_2 via (RO_2 or $HORO_2$)+NO $\rightleftarrows$ (RO+HORO)+NO_2. This particular NO-NO_2 conversion step was found to contribute less than 15% to NO-NO_2 conversion at the lowest temperature examined. Our numerical calculations strongly suggest that the effectiveness of hydrocarbon type toward NO-NO_2 conversion will depend on the hydrocarbon's propensity to produce reactive radicals like OH to sustain fuel oxidation while simultaneously producing HO_2 radicals for subsequent NO to NO_2 conversion. The production source of HO_2 was determined to occur primarily through the reaction steps of Alkyl+$O_2 \rightleftarrows$ Olefin+HO_2 (e.g., alkyl = iC_3H_7, nC_3H_7, C_2H_5), Alkyl-O_2 $\rightleftarrows$ Olefin+HO, $HCO+O_2 \rightleftarrows CO_2+HO_2$, and $H+O_2+M \rightleftarrows HO_2+M$ for the fuels studied at one atmosphere.

Methane does not readily promote NO-NO_2 conversion in comparison to other alkane fuels as suggested in Figures 3 and 5. This is primarily due to the slow nature of methane oxidation which produces a limited amount of HO_2 radicals and the role of methyl radicals plays in reducing NO_2 via $CH_3+NO_2 \rightleftarrows CH_3O+NO$. The CH_3 radical, produced predominantly from CH_4+OH, has a ca. 110kcal/mol C-H bond strength which makes direct abstraction of H-atom by O_2 very difficult. Such an elementary step would require overcoming a ca. 62kcal/mol endothermic enthalpy difference in the overall reaction. Instead, methyl radical is initially oxidized by $CH_3+O_2 \rightleftarrows CH_2O+OH$. A rate constant of $3.51\times10^{11}\exp(-7368K/T)$ $cm^3/mol/sec$ was used in the mechanism and is in agreement with Grela and Teitelboim [32]. This reaction initially sustains the early stages of methane oxidation and allows the HO_2 concentration to become established through the reaction steps of $CH_2O+OH \rightleftarrows HCO+H_2O$, $HCO+O_2 \rightleftarrows CO+HO_2$, $CO+OH \rightleftarrows CO_2+H$, and $H+O_2+M \rightleftarrows HO_2+M$. The HO_2 reacts with NO to make NO_2 and OH, whereupon the OH is recycled back to oxidize additional methane, formaldehyde, and CO. The NO_2 can further oxidize methyl through $CH_3+NO_2 \rightleftarrows CH_3O+NO$. This reaction allows the net production of OH radical to increase via $CH_3O(+M) \rightleftarrows CH_2O+H(+M)$, $H+O_2+N_2 \rightleftarrows HO_2+N_2$, $H+O_2 \rightleftarrows OH+O$ and $NO+HO_2 \rightleftarrows NO_2+OH$. As the temperature is raised, the amount of NO_2 formed increases as methane becomes further oxidized but is limited in the conversion due to the slow HO_2 production rate and fast NO_2 reduction to NO by CH_3. The NO to NO_2 oxidation process then declines at the highest temperatures as $H+O_2 \rightleftarrows OH+O$ dominates over $H+O_2+M \rightleftarrows HO_2+M$ thereby limiting HO_2 formation, and the additional O-atom formed aids in NO_2 reduction via $NO_2+O \rightleftarrows NO+O_2$.

Ethylene readily promotes the conversion of NO to NO_2, as shown in Figures 3 and 5, due to the main oxidation pathways producing HO_2 and reactive radicals like OH and O-atom for further ethylene conversion to products. Ethylene is primarily consumed by OH radical to make C_2H_3 and H_2O. The C_2H_3 is oxidized by two competing pathways [33] and the net reaction schemes can be expressed as:

(1)

$$\begin{array}{c} C_2H_3+O_2 \rightleftarrows CH_2O+HCO \\ CH_2O+OH \rightleftarrows HCO+H_2O \\ \underline{(2\times)\ HCO+O_2 \rightleftarrows CO+HO_2} \\ C_2H_3+3O_2+OH \rightleftarrows 2CO+H_2O+2HO_2 \end{array}$$

(2)

$$\begin{array}{c} C_2H_3+O_2 \rightleftarrows CH_2HCO+O \\ \underline{CH_2HCO+O_2 \rightleftarrows CH_2O+CO+OH} \\ C_2H_3+O_2 \rightleftarrows CH_2O+CO+OH+O \end{array}$$

In reaction sequence (1), two HO_2 molecules may form per ethylene consumed thus making this pathway effective in promoting NO to NO_2. Reaction sequence (2) is an important chain branching pathway which sustains ethylene oxidation and allows ethylene to convert NO to NO_2 at lower temperatures than ethane. Complete NO to NO_2 conversion for ethylene oxidation is limited by NO_2 recycle back to NO via $NO_2+O \rightleftarrows NO+O_2$ and $NO_2+HO_2 \rightleftarrows HONO+O_2$ followed by $HONO+M \rightleftarrows NO+OH+M$. The rate constant for NO_2+HO_2 direct H-atom abstraction has been measured over the temperature range considered in this study. Glanzer and Troe [34] report a rate constant of 1.1×10^{12} $cm^3/mol/sec$ for the 1350-1700K temperature range. Tyndall et al. [35] report an upper limit to this reaction of 5.0×10^{8} $cm^3/mol/sec$ at 300K. We have used a rate expression of $6.31\times10^{8}T^{1.25}$ $\exp(-2516K/T)$ $cm^3/mol/sec$ which is in agreement with the aforementioned studies and has a comparable activation energy found for typical direct abstraction (metathesis) type reactions [29]. The highest temperatures examined in the ethylene case showed the conversion of NO to NO_2 declining for the same reasons as discussed previously for the methane case.

Ethane shows a greater NO-NO_2 conversion relative to methane as indicated in Figures 3 and 5. This is primarily due to the ease of producing HO_2 from $C_2H_5+O_2 \rightleftarrows C_2H_4+HO_2$ and the subsequent radical production that occurs once C_2H_4 is consumed. Ethane is oxidized by OH to make C_2H_5 and H_2O. The ethyl radical reacts with O_2 and either collisionally stabilizes to the peroxy compound, $C_2H_5O_2$, and/or forms $C_2H_4+HO_2$ through the chemically activated reactions of $C_2H_5+O_2 \rightleftarrows C_2H_4+HO_2$ or $C_2H_5+O_2 \rightleftarrows C_2H_5O_2$ followed by $C_2H_5O_2 \rightleftarrows C_2H_4+HO_2$. The $C_2H_5+O_2 \rightleftarrows$

C_2H_4+HO_2 reaction exhibits an overall exothermicity of ca. 12kcal/mol and has no energy barriers greater than the entrance channel's incoming energy. The favorable thermodynamics portrayed in $C_2H_5+O_2 \rightleftarrows C_2H_4+HO_2$ opposed to $CH_3+O_2 \rightleftarrows CH_2+HO_2$ allows for rapid HO_2 production in ethane oxidation while simultaneously consuming C_2H_5 thus limiting its participation in NO_2 reduction kinetics via $C_2H_5+NO_2 \rightleftarrows CH_3CH_2O+NO$. These are important differences when considering the NO-NO_2 promotion effect between ethane and methane fuels.

The NO-NO_2 conversion in propene oxidation lies in between ethylene and ethane as shown in Figures 3 and 5. The conversion is not as great as ethylene primarily due to NO_2 reduction via aC_3H_5 (allyl)+$NO_2 \rightleftarrows CH_2CHCH_2O+NO$, yet the conversion temperature range is wider than ethane due to the greater carbon content of propene introduced into the reactive flow. Propene is initially consumed by O_2 to produce aC_3H_5 and HO_2. The $NO+HO_2 \rightleftarrows NO_2+OH$ reaction provides the initial source of OH radicals for propene consumption. Propene is primarily removed by OH to make aC_3H_5 and H_2O. Allyl is a resonantly stabilized radical that is difficult to oxidize by O_2. This may be explained by noting the rate determining energy barriers for allyl-O_2 isomerization to products typically exceed the allyl+O_2 incoming energy by at least 12kcal/mol [36], and given the ca. 20kcal/mol bond strength of allyl-O_2 suggests allyl-O_2 dissociation will tend to dominate over any product formation processes. Allyl's ability to resist O_2 oxidative attack allows aC_3H_5 to react with NO_2 via $aC_3H_5+NO_2 \rightleftarrows CH_2CHCH_2O+NO$ analogous to $CH_3+NO_2 \rightleftarrows CH_3O+NO$. The CH_2CHCH_2O radical produced by this NO_2 reduction step then decomposes to acrolein and H-atom and makes this a reactive chain sequence. The acrolein is consumed by OH to form CH_2CHCO and CHCHCHO. The CH_2CHCO decomposes to C_2H_3+CO, and CHCHCHO reacts with O_2 to make C_2H_2+CO+HO_2. Acrolein is also removed by O-atom to produce CH_2HCO (vinoxy) and HCO radicals. Interestingly, the acrolein oxidation sequence yields radicals typically found in ethylene oxidation [33]. The consumption of C_2H_3 and CH_2HCO by O_2 yields CH_2O, HCO, and radicals like OH, O-atom and HO_2. The reaction of $C_3H_6+OH \rightleftarrows C_3H_6OH$ followed by $HOC_3H_6+O_2 \rightleftarrows HOC_3H_6O_2$ and $HOC_3H_6O_2 \rightleftarrows CH_3HCO$ +CH_2O+OH is of secondary importance to HO_2 formation. Propene reactions with O-atom to form C_2H_5+HCO or CH_3CO+CH_3 products are of minor importance in the overall propene oxidation chemistry, although these reactions provide additional sources of HO_2 and CH_3 radicals.

Propane shows the greatest NO-NO_2 conversion for the lowest temperatures and widest temperature range of all five fuels studied both experimentally and computationally. The ability of propane to convert NO to NO_2 at the lower temperatures is primarily due to the hydroperoxy-propyl plus O_2 reactions which lead to the production of oxygenates and two OH radicals. The OH radicals further consume propane through $C_3H_8+OH \rightleftarrows iC_3H_7+H_2O$ and $C_3H_8+OH \rightleftarrows nC_3H_7+H_2O$. The generated propyl radicals react with O_2 and leads to two possible general outcomes. The reaction could produce HO_2 via chemically activated routes of $iC_3H_7+O_2 \rightleftarrows C_3H_6+HO_2$ and $nC_3H_7+O_2 \rightleftarrows C_3H_6+HO_2$, $iC_3H_7+O_2 \rightleftarrows iC_3H_7O_2$ followed by $iC_3H_7O_2 \rightleftarrows C_3H_6+HO_2$, and $nC_3H_7+O_2 \rightleftarrows nC_3H_7O$ followed by $nC_3H_7O2 \rightleftarrows C_3H_6+HO_2$ or the reaction could form the stabilized hydroperoxy-propyl (or C_3H_6OOH) adduct. The degree of reactivity exhibited in propane is essentially controlled by the competition of chemically activated reactions producing HO_2 and olefin (i.e., C_3H_6) versus the partial equilibrium established in the $C_3H_7+O_2 \rightleftarrows C_3H_7O_2 \rightleftarrows C_3H_6OOH$ reaction sequence as determined from reaction flux analysis and suggested by the sensitivity analysis results for NO in Figure 6. The stabilized hydroperoxy-propyl adduct readily reacts with O_2 and establishes a partial equilibrium with $O_2C_3H_6OOH$. The $O_2C_3H_6OOH$ species undergoes internal H-atom abstraction to make $HOOC_3H_5OOH$ (e.g., C(OO.)CCOOH $\rightleftarrows$ C(OOH)CC.OOH) followed by beta-scission of the O-O bond leading to a ketohydroperoxide (e.g., C(OOH)CC*O) and OH radical. The ketohydroperoxides primarily undergo O-O bond scission which leads to further OH radical production, chain branching, and propane consumption. The decomposition of the ketohydroperoxides tends to increase NO-NO_2 conversion as indicated by the negative sensitivity coefficients shown for the C(OOH)CC*O $\rightleftarrows$ $CH_2HCO+CH_2O+OH$, CC(OOH)C*O $\rightleftarrows$ $CH_3HCO+HCO+OH$, and CC*OCOOH $\rightleftarrows$ CH_3CO+CH_2O+OH reactions. Sensitivity analysis shows hydroperoxy-propyl plus O_2 reactions and the ketohydroperoxide decomposition reactions play an important promoting role in the NO-NO_2 conversion for propane.

Figure 6

The sensitivity analysis results for $NO+HO_2 \rightleftarrows NO_2+OH$ showed a relatively small sensitivity coefficient in spite of its importance in promoting NO-NO_2 conversion. Reaction flux analysis indicates that this reaction dominates HO_2 consumption, and therefore a small perturbation in the rate constant A-factor leads to a minor effect on the NO conversion. The reactions of CCCOO. or

C_2COO. with NO exhibit larger in magnitude sensitivity coefficients than $NO+HO_2 \rightleftarrows NO_2+OH$ since these reactions reduce the net production of alkyl-peroxy species and, in effect, indirectly limit OH radical production thereby showing HO_2 production as well.

CONCLUSIONS

The flow reactor experiment indicated the following results:

1. In general, ethylene and propane effectively oxidize NO to NO_2 while methane and ethane are less effective.
2. High NO_2/NOx ratios are obtained only within a relatively low reaction temperature range, though the hydrocarbon consumption is accerelated with increasing the reaction temperature. At higher reaction temperatures, the reduction of NO_2 to NO is observed at longer residence times.

The chemical kinetics modeling indicated the following results:

1. The kinetic calculation reproduces the experimental results qualitatively for the dependence of NO-NO_2 conversion with hydrocarbon type and reasonably for that with reaction temperature.
2. Highest level of NO-NO_2 promotion comes from hydrocarbons that produce reactive radicals (i.e., OH, O-atom) which further consume the parent hydrocarbon while at the same time producing HO_2 radicals for NO-NO_2 conversion via $NO+HO_2 \rightleftarrows NO_2+OH$ (propane and ethylene).
3. If parent hydrocarbons (i.e. CH_4, C_3H_6) produce a daughter radicals (i.e., CH_3, aC_3H_5) that are resistant to oxidation by O_2 then the daughter radicals will reduce NO_2 to NO via the reaction $R+NO_2 \rightleftarrows RO+NO$ ($R=CH_3$, aC_3H_5). This reaction limits NO to NO_2 conversion. The $R+NO_2 \rightleftarrows RO+NO$ reaction type was found to be important in the methane and propene studies.
4. If the parent fuel can be oxidized to C_2H_4 or C_2H_3, then NO will be readily promoted to NO_2 as reactive radicals (i.e., OH, O-atom) and HO_2 are produced when C_2H_3 is oxidized by O_2 (propene and ethane).

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FIGURE CAPTIONS

Figure 1 NO_2/NO_x ratios against residence time obtained by the flow reactor experiment for five hydrocarbons at 700K.

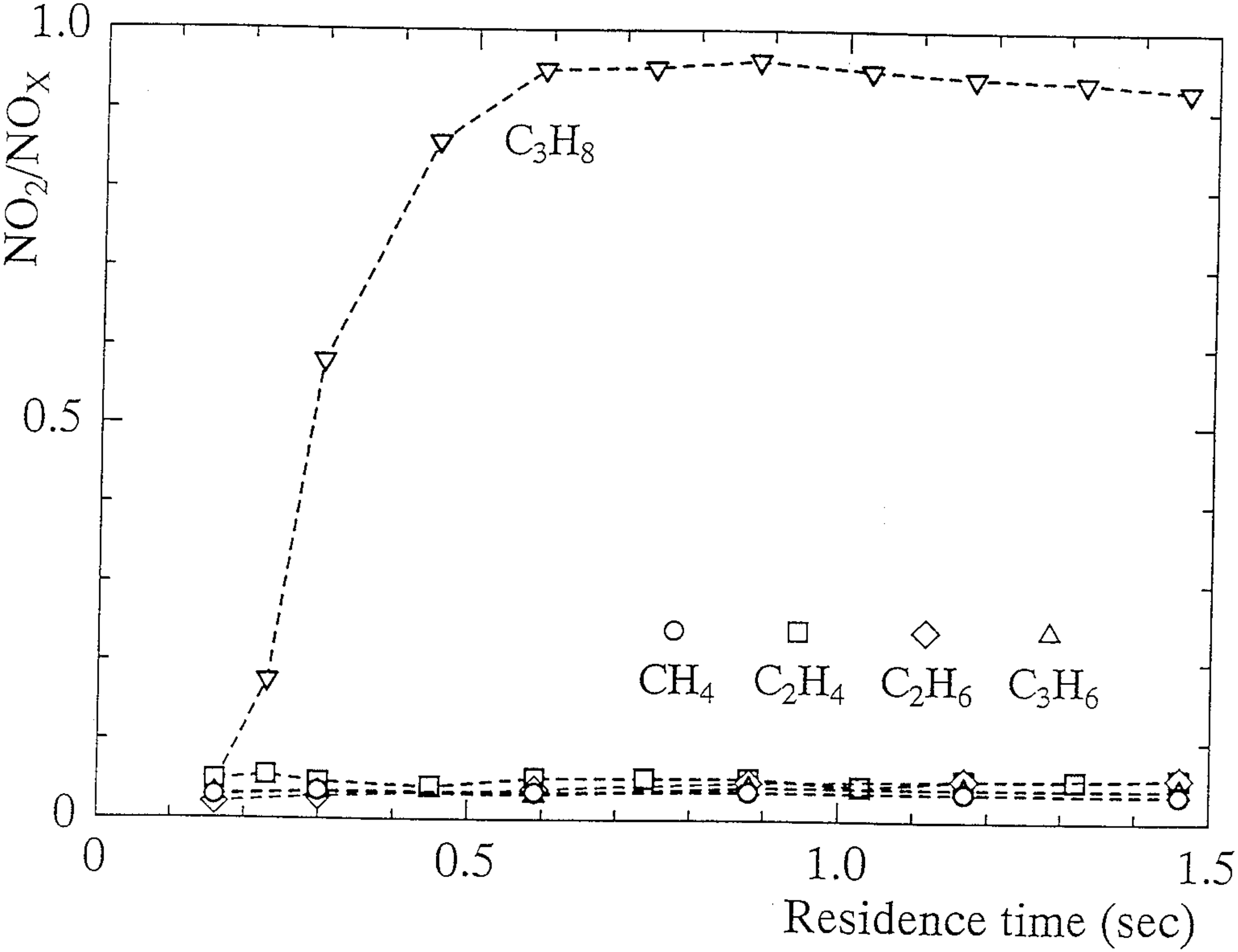
Figure 2 NO_2/NO_x ratios against residence time obtained by the flow reactor experiment for five hydrocarbons at 1000K.

Figure 3 Comparison between the flow reactor experiment and the chemical kinetic calculation. NO_2/NO_x ratios against residence time for five hydrocarbons at 800K.

Figure 4 Comparison between the flow reactor experiment and the chemical kinetic calculation. Nondimensional hydrocarbon concentrations against residence time for five hydrocarbons at 800K. (Hydrocarbon concentrations are nondimensionalized to the initial hydrocarbon concentrations)

Figure 5 Comparison between the flow reactor experiment and the chemical kinetic calculation. NO_2/NO_x ratios at the residence time of 1.46 sec against the reaction temperature for five hydrocarbons.

Figure 6 Propane sensitivity analysis at 650K. The logarithmic sensitivity coefficient determined by perturbing reaction's pre-exponential term by a factor of 1.3 and calculating the new NO value relative to the baseline, unperturbed case. A negative (positive) coefficient indicates the reaction promotes (reduces) NO-NO_2 conversion.



1.0
0.5
0
NO_2/NO_X
C_3H_8
○ CH_4
□ C_2H_4
◇ C_2H_6
△ C_3H_6
0
0.5
1.0
1.5
Residence time (sec)

Figure 1

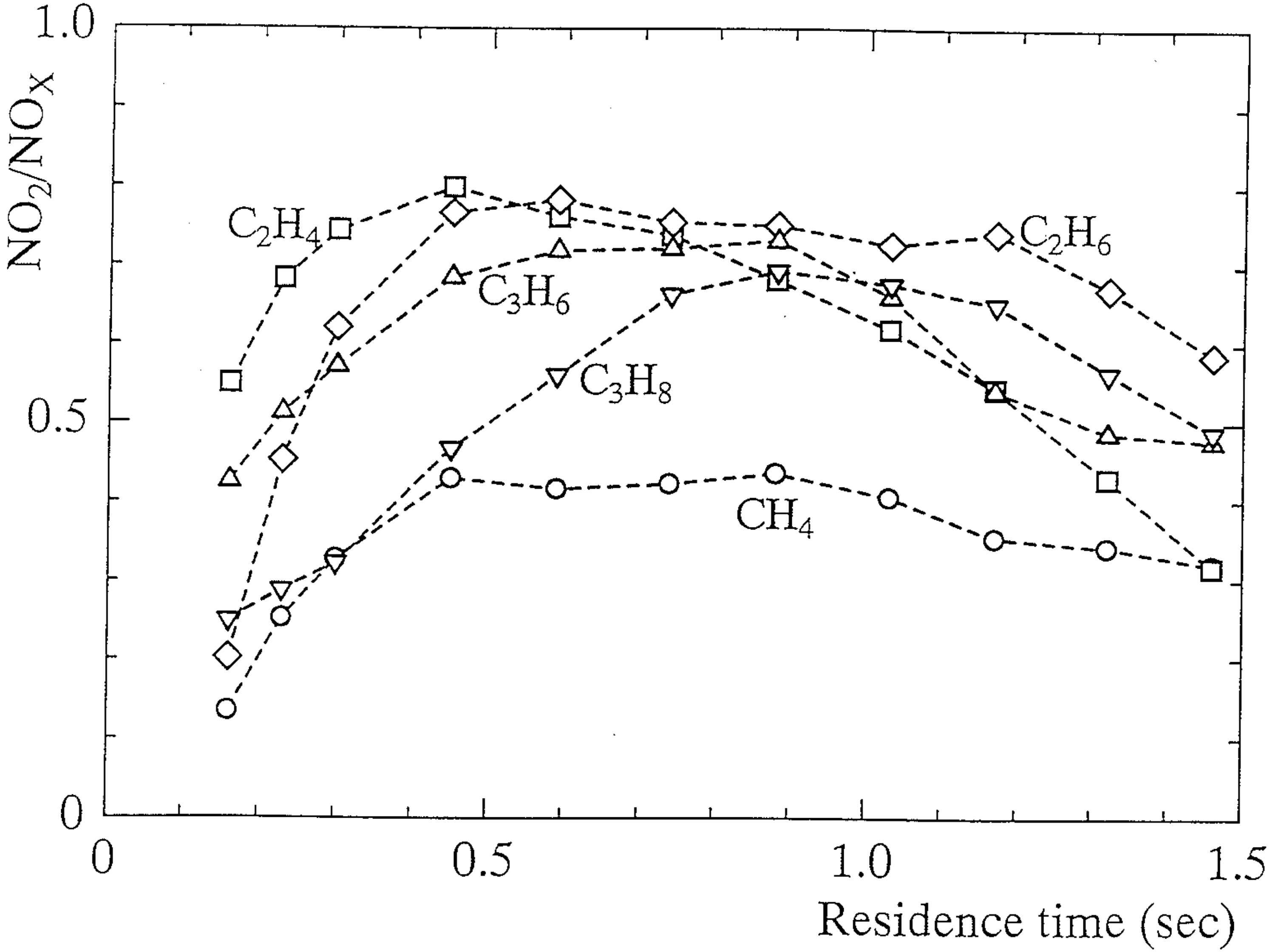

1.0
0.5
0
NO_2/NO_X
0
0.5
1.0
1.5
Residence time (sec)
C_2H_4
C_2H_6
C_3H_6
C_3H_8
CH_4

Figure 2

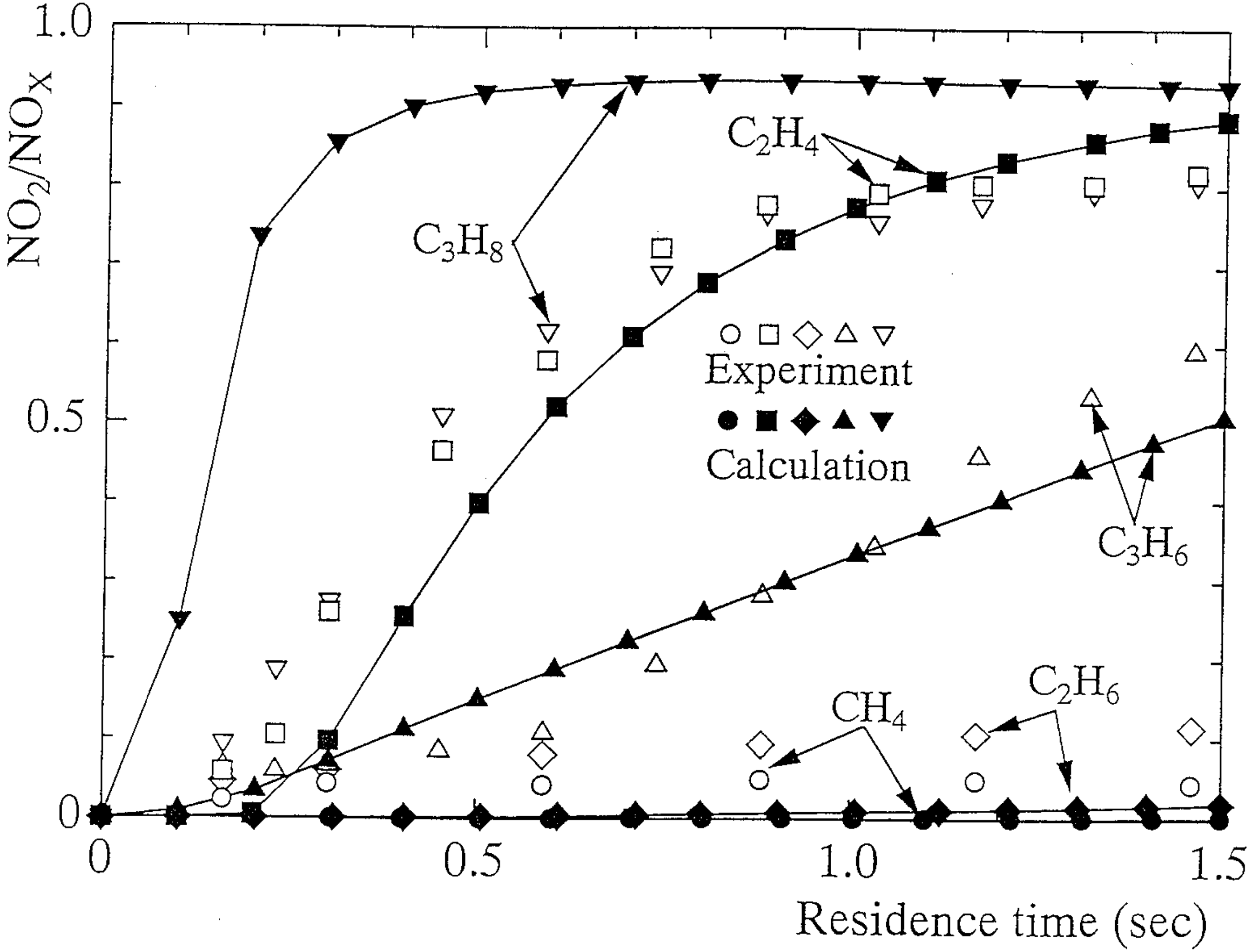
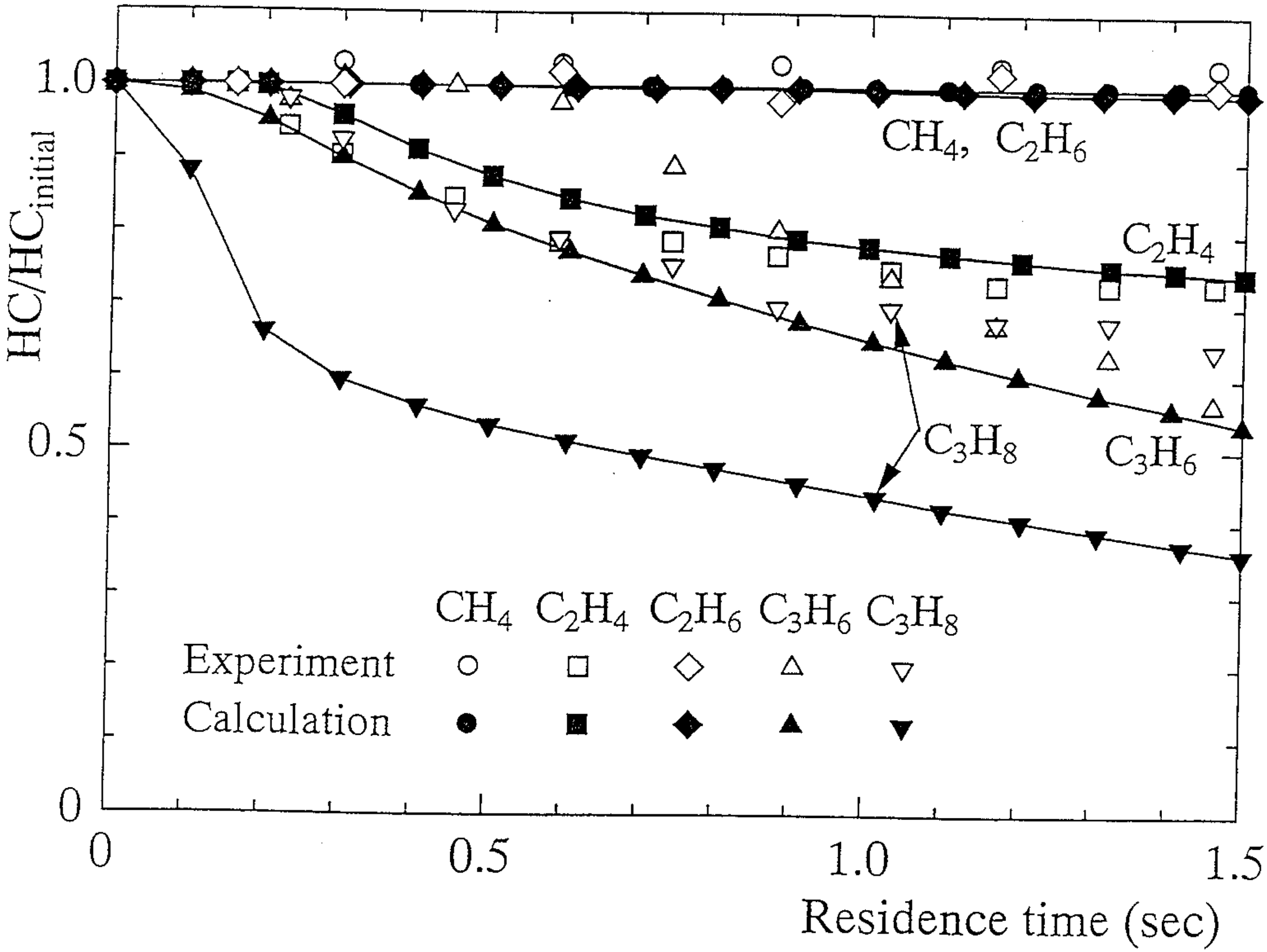

1.0
0.5
0
NO2/NOX
0
0.5
1.0
1.5
Residence time (sec)
C3H8
C2H4
C3H6
CH4
C2H6
○ □ ◇ △ ▽
Experiment
● ■ ◆ ▲ ▼
Calculation

Figure 3



1.0
0.5
0
HC/HC$_{initial}$
0
0.5
1.0
1.5
Residence time (sec)
CH$_4$, C$_2$H$_6$
C$_2$H$_4$
C$_3$H$_8$
C$_3$H$_6$
CH$_4$ C$_2$H$_4$ C$_2$H$_6$ C$_3$H$_6$ C$_3$H$_8$
Experiment ○ □ ◇ △ ▽
Calculation ● ■ ◆ ▲ ▼

Figure 4

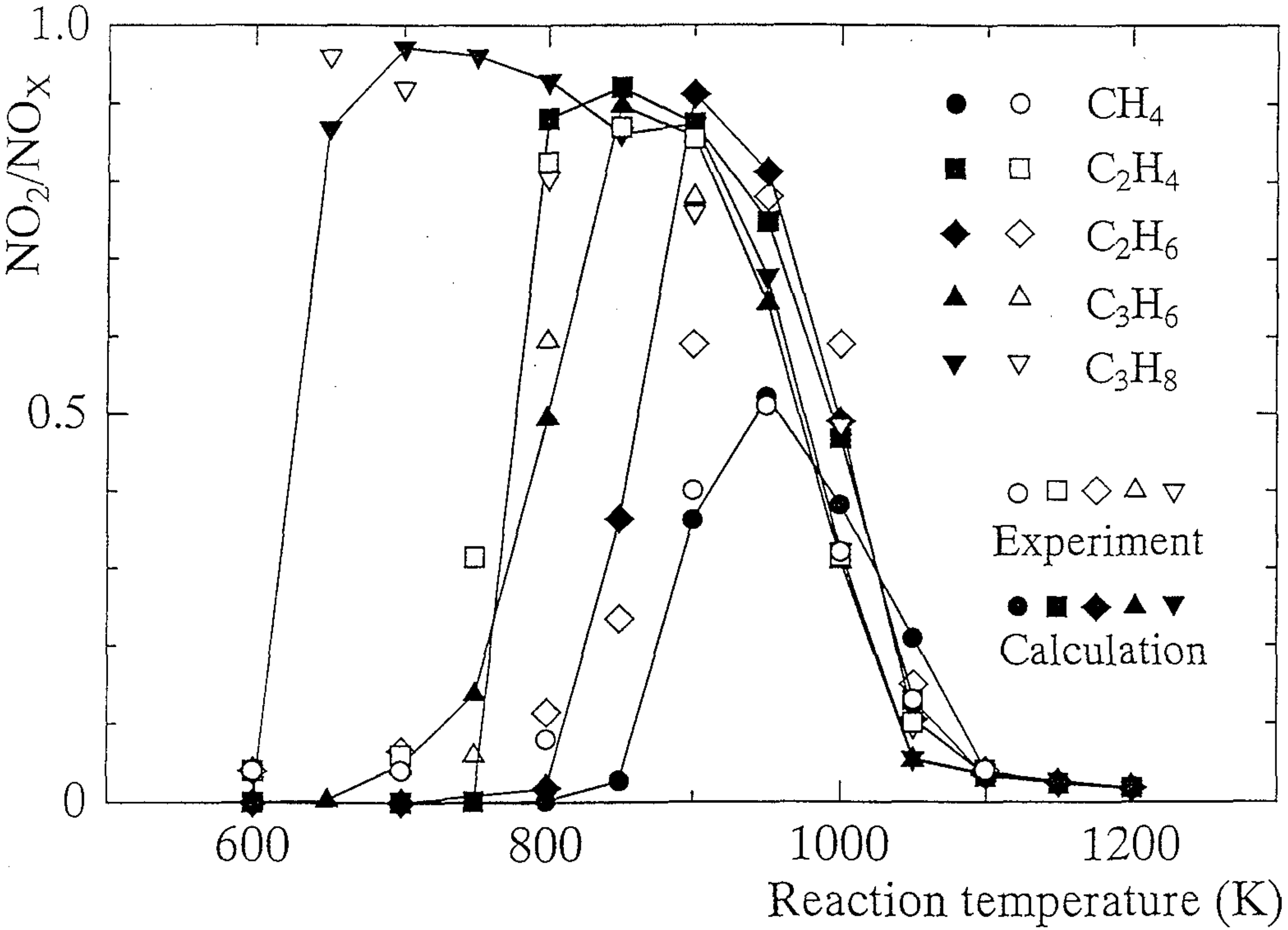

1.0
0.5
0
NO2/NOx
600
800
1000
1200
Reaction temperature (K)
● ○ CH4
■ □ C2H4
◆ ◇ C2H6
▲ △ C3H6
▼ ▽ C3H8
○ □ ◇ △ ▽ Experiment
● ■ ◆ ▲ ▼ Calculation

Figure 5

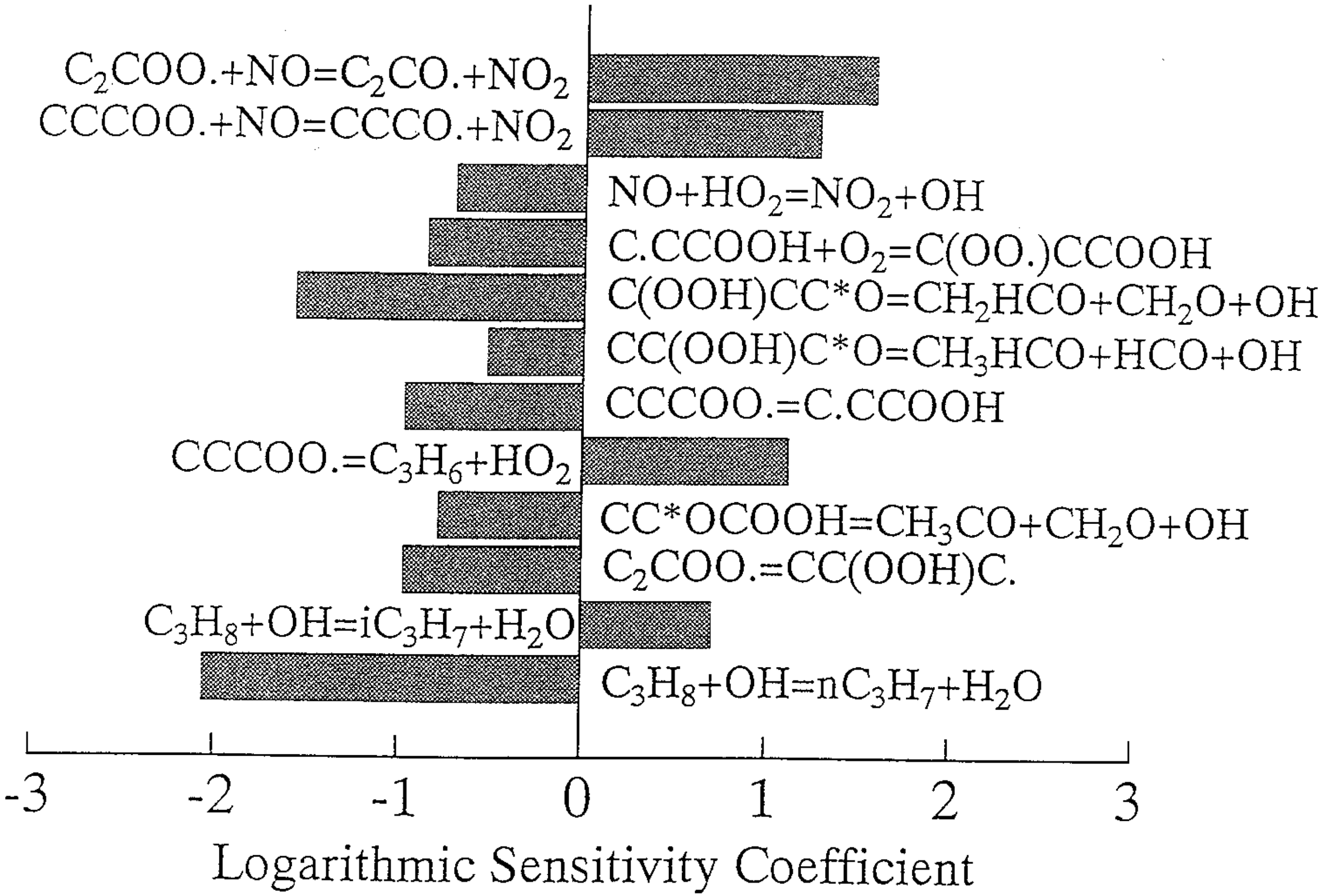

$C_2COO.+NO=C_2CO.+NO_2$
$CCCOO.+NO=CCCO.+NO_2$
$NO+HO_2=NO_2+OH$
$C.CCOOH+O_2=C(OO.)CCOOH$
$C(OOH)CC*O=CH_2HCO+CH_2O+OH$
$CC(OOH)C*O=CH_3HCO+HCO+OH$
$CCCOO.=C.CCOOH$
$CCCOO.=C_3H_6+HO_2$
$CC*OCOOH=CH_3CO+CH_2O+OH$
$C_2COO.=CC(OOH)C.$
$C_3H_8+OH=iC_3H_7+H_2O$
$C_3H_8+OH=nC_3H_7+H_2O$
-3
-2
-1
0
1
2
3
Logarithmic Sensitivity Coefficient

Figure 6

Table 1

Reaction Mechanism Rate Coefficients

(Kf = A T**b exp(-Ea/RT); cm3, mol, sec, and cal/mol)

```
REACTION                         A         b        Ea      Reference

oh+h2=h+h2o                  2.14E+08  1.52   3449.0 !Marinov 1995a
o+oh=o2+h                    2.02E+14  -0.4      0.0 !Marinov 1995a
o+h2=oh+h                    5.06E+04  2.67   6290.0 !Marinov 1995a
h+o2(+m)=ho2(+m)             4.52E+13  0.0       0.0 !Marinov 1995a
low /  1.05E+19  -1.257  0.0 /                       !Marinov 1995a
h2o/0.0/ h2/0.0/ n2/0.0/ ch4/10.0/ co2/3.8/ co/1.9/
h+o2(+n2)=ho2(+n2)           4.52E+13  0.0       0.0 !Marinov 1995a
low / 2.03E+20  -1.59    0.0  /                      !Marinov 1995a
h+o2(+h2)=ho2(+h2)           4.52E+13  0.0       0.0 !Marinov 1995a
low / 1.52E+19  -1.133   0.0 /                       !Marinov 1995a
h+o2(+h2o)=ho2(+h2o)         4.52E+13  0.0       0.0 !Marinov 1995a
low / 2.10E+23  -2.437   0.0 /                       !Marinov 1995a
oh+ho2=h2o+o2                2.13E+28 -4.827 3500.0 !Hippler 1995
 dup
oh+ho2=h2o+o2                9.10E+14  0.0  10964.0 !Hippler 1995
 dup
h+ho2=oh+oh                  1.50E+14  0.0  1000.0  !Marinov 1995a
h+ho2=h2+o2                  6.63E+13  0.0  2126.0  !Tsang   1986x
h+ho2=o+h2o                  3.01E+13  0.0  1721.0  !Marinov 1995a
o+ho2=o2+oh                  3.25E+13  0.0     0.0  !Marinov 1995a
oh+oh=o+h2o                  3.57E+04  2.4 -2112.0  !Marinov 1995a
h+h+m=h2+m                   1.00E+18 -1.0     0.0  !Marinov 1995a
h2o/0.0/ h2/0.0/
h+h+h2=h2+h2                 9.20E+16 -0.6     0.0  !Marinov 1995a
h+h+h2o=h2+h2o               6.00E+19 -1.25    0.0  !Marinov 1995a
h+oh+m=h2o+m                 2.21E+22 -2.0     0.0  !Marinov 1995a
 h2o/6.4/
h+o+m=oh+m                   4.71E+18 -1.0     0.0  !Marinov 1995a
 h2o/6.4/
o+o+m=o2+m                   1.89E+13  0.0 -1788.0  !Marinov 1995a
ho2+ho2=h2o2+o2              4.20E+14  0.0 11982.0  !Marinov 1995a
dup
ho2+ho2=h2o2+o2              1.30E+11  0.0 -1629.0  !Marinov 1995a
dup
oh+oh(+m)=h2o2(+m)           1.24E+14 -0.37    0.0  !Marinov 1995a
low /  3.04E+30   -4.63   2049.0 /                  !Marinov 1995a
 troe / 0.470   100.0   2000.0  1.0E+15/
h2o2+h=ho2+h2                1.98E+06  2.0  2435.0  !Marinov 1995a
h2o2+h=oh+h2o                3.07E+13  0.0  4217.0  !Marinov 1995a
h2o2+o=oh+ho2                9.55E+06  2.0  3970.0  !Marinov 1995a
h2o2+oh=h2o+ho2              2.40E+00 4.042 -2162.0 !Marinov 1995a
ch3+ch3(+m)=c2h6(+m)         9.22E+16 -1.174 636.0  !Walter  1990
low / 1.14E+36 -5.246 1705.0/                       !Walter  1990
troe/ 0.405  1120.0   69.6    1.0E+15/
 h2o/5.0/ h2/2.0/ co2/3.0/ co/2.0/
ch3+h(+m)=ch4(+m)            2.14E+15 -0.4     0.0   !Tsang 1986
low/  3.31E+30   -4.0  2108.0 /                      !Marinov 1996
troe / 0.0   1.0E-15   1.0E-15   40.0/
h2o/5.0/ h2/2.0/ co2/3.0/ co/2.0/
ch4+h=ch3+h2                 2.20E+04 3.0    8750.0  !Miller 1992
ch4+oh=ch3+h2o               4.19E+06 2.0    2547.0  !Marinov 1995
ch4+o=ch3+oh                 6.92E+08 1.56   8485.0  !Marinov 1995
ch4+ho2=ch3+h2o2             1.12E+13 0.0    24640.0 !Marinov 1995
ch3+ho2=ch3o+oh              7.00E+12 0.0       0.0  !Troe  1993
ch3+ho2=ch4+o2               3.00E+12 0.0       0.0  !Marinov 1995
ch3+o=ch2o+h                 8.00E+13 0.0       0.0  !Marinov 1995
ch3+o2=ch3o+o                1.45E+13 0.0    29209.0 !Klatt 1991
ch3+o2=ch2o+oh               3.51E+11 0.0    14640.0 !Marinov 1995
ch3+o2=ch3o2                 9.03E+58 -15.0 17023.0 !Tsang 1986
```

```
ch3o2+o=ch3o+o2           2.60E+13 0.0       0.0  !Zellner 1988
ch3o2+h=ch3o+oh           9.64E+13 0.0       0.0  !Tsang 1986
ch3o2+ch3=ch3o+ch3o       2.40E+13 0.0       0.0  !Tsang 1986
ch3o2+ho2=ch3ooh+o2       2.29E+11 0.0   -1550.0  !Atkinson 1992
ch3ooh=ch3o+oh            6.00E+14 0.0   42300.0  !Lightfoot 1991
ch3ooh+oh=ch3o2+h2o       3.12E+6  2.0    -298.0  !This Study
ch3o+h=ch3+oh             1.00E+13 0.0       0.0  !Marinov 1998
ch2oh+h=ch3+oh            1.00E+13 0.0       0.0  !Marinov 1998
ch3+oh=ch2(s)+h2o         2.65E+13 0.0    2186.0  !Humpfer 1994
ch3+oh=ch2+h2o            3.00E+06 2.0    2500.0  !Marinov 1996
ch3+oh=hcoh+h2            5.48E+13 0.0    2981.0  !Humpfer 1994
ch3+oh=ch2o+h2            2.25E+13 0.0    4300.0  !Marinov 1996
ch3+h=ch2+h2              9.00E+13 0.0    15100.0 !Miller 1992
ch3+m=ch+h2+m             6.90E+14 0.0    82469.0 !Markus 1992
ch3+m=ch2+h+m             1.90E+16 0.0    91411.0 !Markus 1992
ch3+oh(+m)=ch3oh(+m)      8.70E+13 0.1        0.0 !Fagerstrom 1993
low/ 8.84E+41   -7.4   626.0 /                    !Marinov 1996
troe /  0.025   1.0E-15   8000.0   3000.0/
h2o /10.0/ h2/2.0/ co2/3.0/ co/2.0/
ch3oh(+m)=ch2(s)+h2o  2.837e10 1.0 89871.         !Marinov 1998
low / 1.78e49 -8.81 99369./
troe /0.9 740. 980. 5100./
h2o/10.0/ h2/2.0/ co2/3.0/ co/2.0/
ch3oh(+m)=hcoh+h2(+m) 4.2e9 1.12 85604.           !Marinov 1998
low / 5.02e47 -8.402 94823./
troe/ 0.9 615. 915. 4615./
h2o /10.0/ h2/2.0/ co2/3.0/ co/2.0/
ch3oh(+m)=ch2o+h2(+m) 2.03e9 1.0 91443.           !Marinov 1998
low /9.784e47 -8.4 101761./
troe/ 0.9 825. 1125. 5700./
h2o/10./ h2/2.0/ co2/3.0/ co/2.0/
ch3oh+oh=ch2oh+h2o        2.61E+05  2.182 -1344.0   !Tsang  1987
ch3oh+oh=ch3o+h2o         2.62E+06  2.056   916.0   !Tsang  1987
ch3oh+o=ch2oh+oh          3.88E+05  2.5    3080.0   !Tsang  1987
ch3oh+h=ch2oh+h2          1.70E+07  2.1    4868.0   !Tsang  1987
ch3oh+h=ch3o+h2           4.24E+06  2.1    4868.0   !Tsang  1987
ch3oh+ho2=ch2oh+h2o2      9.64E+10  0.0   12578.0   !Tsang  1987
ch2o+h(+m)=ch3o(+m)       5.40E+11  0.454  2600.0   !GRI-Mech2.11
low/ 1.50E+30 -4.80 5560./
troe/ 0.758 94. 1555. 4200./
h2o/5.0/
ch2o+h(+m)=ch2oh(+m)      5.40E+11  0.454  3600.0   !GRI-Mech2.11
low / 9.10E+31 -4.82 6530./
troe/ 0.7187 103. 1291. 4160./
h2o/5.0/
ch3o+ch3=ch2o+ch4         1.20E+13  0.0       0.0   !Tsang  1986
ch3o+h=ch2o+h2            2.00E+13  0.0       0.0   !Miller 1992
ch2oh+h=ch2o+h2           2.00E+13  0.0       0.0   !Miller 1992
ch3o+oh=ch2o+h2o          1.00E+13  0.0       0.0   !Miller 1992
ch2oh+oh=ch2o+h2o         1.00E+13  0.0       0.0   !Miller 1992
ch3o+o=ch2o+oh            1.00E+13  0.0       0.0   !Miller 1992
ch2oh+o=ch2o+oh           1.00E+13  0.0       0.0   !Miller 1992
ch3o+o2=ch2o+ho2          6.30E+10  0.0    2600.0   !Miller 1992
ch3o+co=ch3+co2           4.68E+02  3.16   5380.0   !Wantuck 1987
ch2oh+o2=ch2o+ho2         1.57E+15  -1.0      0.0   !Baulch 1992
 dup
ch2oh+o2=ch2o+ho2         7.23E+13  0.0    3577.0   !Baulch 1992
 dup
hcoh+oh=hco+h2o           2.00E+13  0.0       0.0   !Marinov 1996
hcoh+h=ch2o+h             2.00E+14  0.0       0.0   !Marinov 1996
hcoh+o=co2+h+h            5.00E+13  0.0       0.0   !Marinov 1996
hcoh+o=co+oh+h            3.00E+13  0.0       0.0   !Marinov 1996
hcoh+o2=co+oh+oh          1.00E+13  0.0       0.0   !Marinov 1998
hcoh+o2=co2+h2o           1.00E+13  0.0       0.0   !Marinov 1998
hcoh=ch2o                 2.10E+19 -3.07 31700.0    !Marinov 1998
```

```
ch2+oh=ch+h2o              1.13E+07  2.0    3000.0   !Miller 1992
ch2+oh=ch2o+h              2.50E+13  0.0       0.0   !Miller 1992
ch2+co2=ch2o+co            1.10E+11  0.0    1000.0   !Miller 1992
ch2+o=co+h+h               5.00E+13  0.0       0.0   !Miller 1992
ch2+o=co+h2                3.00E+13  0.0       0.0   !Miller 1992
ch2+o2=ch2o+o              3.29E+21 -3.3    2868.0   !Marinov 1996
ch2+o2=co2+h+h             3.29E+21 -3.3    2868.0   !Marinov 1996
ch2+o2=co2+h2              1.01E+21 -3.3    1508.0   !Marinov 1996
ch2+o2=co+h2o              7.28E+19 -2.54   1809.0   !Marinov 1996
ch2+o2=hco+oh              1.29E+20 -3.3     284.0   !Marinov 1996
ch2+ch3=c2h4+h             4.00E+13  0.0       0.0   ! Miller 1992
ch2+ch2=c2h2+h+h           4.00E+13  0.0       0.0   ! Miller 1992
ch2+hcco=c2h3+co           3.00E+13  0.0       0.0   ! Miller 1992
ch2+c2h2=h2ccch+h          1.20E+13  0.0    6600.0   ! Miller 1992
ch2(s)+m=ch2+m             1.00E+13  0.0       0.0   ! Miller 1992
h /12.0/ c2h2 /4.0/ h2o/3.0/
ch2(s)+ch4=ch3+ch3         4.00E+13  0.0       0.0   ! Miller 1992
ch2(s)+c2h6=ch3+c2h5       1.20E+14  0.0       0.0   ! Miller 1992
ch2(s)+o2=co+oh+h          7.00E+13  0.0       0.0   ! Miller 1992
ch2(s)+h2=ch3+h            7.00E+13  0.0       0.0   ! Miller 1992
ch2(s)+c2h2=h2ccch+h       1.50E+14  0.0       0.0   ! Canosa-Mas85
ch2(s)+c2h4=ac3h5+h        1.30E+14  0.0       0.0   ! Canosa-Mas85
ch2(s)+o=co+h+h            3.00E+13  0.0       0.0   ! Miller 1992
ch2(s)+oh=ch2o+h           3.00E+13  0.0       0.0   ! Miller 1992
ch2(s)+h=ch+h2             3.00E+13  0.0       0.0   ! Miller 1992
ch2(s)+co2=ch2o+co         3.00E+12  0.0       0.0   ! Miller 1992
ch2(s)+ch3=c2h4+h          2.00E+13  0.0       0.0   ! Miller 1992
ch2(s)+ch2co=c2h4+co       1.60E+14  0.0       0.0   ! Miller 1992
ch+o2=hco+o                3.30E+13  0.0       0.0   ! Miller 1992
ch+o=co+h                  5.70E+13  0.0       0.0   ! Miller 1992
ch+oh=hco+h                3.00E+13  0.0       0.0   ! Miller 1992
ch+co2=hco+co              3.40E+12  0.0     690.0   ! Miller 1992
ch+h2o=ch2o+h              1.17E+15  -0.75     0.0   ! Miller 1992
ch+ch2o=ch2co+h            9.46E+13  0.0    -515.0   ! Miller 1992
ch+c2h2=c3h2+h             1.00E+14  0.0       0.0   ! Miller 1992
ch+ch2=c2h2+h              4.00E+13  0.0       0.0   ! Miller 1992
ch+ch3=c2h3+h              3.00E+13  0.0       0.0   ! Miller 1992
ch+ch4=c2h4+h              6.00E+13  0.0       0.0   ! Miller 1992
ch2o+oh=hco+h2o            3.43E+09  1.18   -447.0   ! Tsang  1986
ch2o+h=hco+h2              2.19E+08  1.77   3000.0   ! Miller 1992
ch2o+m=hco+h+m             3.31E+16  0.0   81000.0   ! Miller 1992
ch2o+o=hco+oh              1.80E+13  0.0    3080.0   ! Miller 1992
hco+o2=ho2+co              7.58E+12  0.0     410.0   ! Timonen 1988
hco+m=h+co+m               1.86E+17  -1.0 17000.0   ! Timonen 1987
h2o/5.0/ h2/1.87/ co2/3.0/ co/1.87/ ch4/2.81/
hco+oh=h2o+co              1.00E+14  0.0       0.0   ! Miller 1992
hco+h=co+h2                1.19E+13  0.25      0.0   ! Miller 1992
hco+o=co+oh                3.00E+13  0.0       0.0   ! Miller 1992
hco+o=co2+h                3.00E+13  0.0       0.0   ! Miller 1992
co+oh=co2+h                9.42E+03  2.25 -2351.0   !Marinov 1996
co+o+m=co2+m               6.17E+14  0.0    3000.0   ! Miller 1992
co+o2=co2+o                2.53E+12  0.0   47688.0   ! Miller 1992
co+ho2=co2+oh              5.80E+13  0.0   22934.0   ! Miller 1992
c2h6+ch3=c2h5+ch4          5.50E-01  4.0    8300.0   ! Miller 1992
c2h6+h=c2h5+h2             5.40E+02  3.5    5210.0   ! Miller 1992
c2h6+o=c2h5+oh             3.00E+07  2.0    5115.0   ! Miller 1992
c2h6+oh=c2h5+h2o           7.23E+06  2.0     864.0   ! Baulch 1992
c2h5+h=c2h4+h2             1.25E+14  0.0    8000.0   ! Marinov 1995
c2h5+h=ch3+ch3             3.00E+13  0.0       0.0   ! Warnatz 1984
c2h5+h=c2h6                3.00E+13  0.0       0.0   ! Marinov 1998
c2h5+oh=c2h4+h2o           4.00E+13  0.0       0.0   ! Marinov 1995
c2h5+o=ch3+ch2o            1.00E+14  0.0       0.0   ! Herron 1988
c2h5+ho2=c2h6+o2           3.00E+12  0.0       0.0   ! Marinov 1998
c2h5+ho2=ch3ch2o+oh        3.00E+13  0.0       0.0   ! Tsang 1986
c2h5+o2=c2h4+ho2           2.89E+28  -5.4   7585.0   ! This Study
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c2h5+o2=ch3hco+oh        4.90E+11 -0.48  8357.0   ! This Study
c2h5+o2=ch2ch2ooh        5.18E+42 -10.72 8576.0   ! This Study
c2h5o2=ch2ch2ooh         2.96E+55 -14.24 37892.0  ! This Study
c2h5o2=c2h4+ho2          7.37E+54 -13.55 41070.0  ! This Study
c2h5o2+ho2=c2h5ooh+o2    2.29E+11  0.0   -1550.0  ! This Study
c2h5ooh=ch3ch2o+oh       6.00E+14  0.0   42300.0  ! This Study
ch2ch2ooh=c2h4+ho2       6.87E+45 -11.09 23227.0  ! This Study
ch2ch2ooh+o2=hooc2h4o2   1.00E+12  0.0   -1100.0  ! This Study
hooc2h4o2=cqc*o+oh       6.00E+10  0.0   24500.0  ! This Study
cqc*o=ch2o+hco+oh        6.00E+14  0.0   42300.0  ! This Study
c2h4+oh=c2h4oh           1.29E+12  0.0    -817.0  ! Atkinson 1986
c2h4oh+o2=hoc2h4o2       1.00E+12  0.0   -1100.0  ! This Study
hoc2h4o2=ch2o+ch2o+oh    6.00E+10  0.0   24500.0  ! This Study
c2h4+oh=c2h3+h2o         2.02E+13  0.0   5936.0   ! Miller 1992
c2h4+o=ch3+hco           1.02E+07  1.88   179.0   ! Baulch 1994
c2h4+o=ch2hco+h          3.39E+06  1.88   179.0   ! Baulch 1994
c2h4+ch3=c2h3+ch4        6.62E+00  3.7   9500.0   ! Marinov 1995
c2h4+h=c2h3+h2           3.36E-07  6.0   1692.0   ! Dagaut 1990
c2h4+h(+m)=c2h5(+m)      1.08E+12  0.454 1822.0   ! Feng  1993
low / 1.112E+34  -5.0    4448.0 /                 ! Marinov 1996
troe / 1.0   1.0E-15   95.0  200.0 /
h2o /5.0/ h2/2.0/ co2/3.0/ co/2.0/
c2h4(+m)=c2h2+h2(+m)     1.80E+13  0.0   76000.   ! Marinov 1997
low / 1.50E+15 0.0  55443. /
c2h3+h(+m)=c2h4(+m)      6.10E+12  0.27    280.   !GRI-Mech2.11
low/9.80E+29 -3.86 3320./
troe/ 0.782 208. 2663. 6095./
h2o/5.0/
c2h3+h=c2h2+h2           4.00E+13  0.0       0.0  ! Miller 1992
c2h3+o=ch2co+h           3.00E+13  0.0       0.0  ! Miller 1992
c2h3+o2=ch2o+hco         1.70E+29  -5.312 6500.0  ! Marinov 1997
c2h3+o2=ch2hco+o         5.50E+14  -0.611 5260.0  ! Marinov 1997
c2h3+o2=c2h2+ho2         2.12E-06  6.0    9484.0  !cfm/nmm 1996
c2h3+oh=c2h2+h2o         2.00E+13  0.0       0.0  ! Miller 1992
c2h3+c2h=c2h2+c2h2       3.00E+13  0.0       0.0  ! Miller 1992
c2h3+ch=ch2+c2h2         5.00E+13  0.0       0.0  ! Miller 1992
c2h3+ch3=ac3h5+h         4.73E+02  3.7    5677.0  ! Marinov 1996
c2h3+ch3=c3h6            4.46E+56 -13.0 13865.0   ! Marinov 1996
c2h3+ch3=c2h2+ch4        2.00E+13  0.0       0.0  ! Fahr  1991
c2h2+oh=c2h+h2o          3.37E+07  2.0  14000.0   ! Miller 1992
c2h2+oh=hccoh+h          5.04E+05  2.3  13500.0   ! Miller 1992
c2h2+oh=ch2co+h          2.18E-04  4.5  -1000.0   ! Miller 1992
c2h2+oh=c2h2oh           1.02E+12  0.0     463.0  ! This Study
c2h2+oh=ch3+co           4.83E-04  4.0  -2000.0   ! Miller 1992
hccoh+h=ch2co+h          1.00E+13  0.0       0.0  ! Miller 1992
c2h2oh+o2=chocho+oh      2.00E+12  0.0       0.0  ! This Study
c2h2oh+h=ch2hco+h        1.00E+14  0.0       0.0  ! This Study
c2h2+o=ch2+co            6.12E+06  2.0    1900.0  ! Marinov 1996
c2h2+o=hcco+h            1.43E+07  2.0    1900.0  ! Marinov 1996
c2h2+o=c2h+oh            3.16E+15 -0.6   15000.0  ! Miller 1992
c2h2+ch3=c2h+ch4         1.81E+11  0.0   17289.0  ! Tsang  1986
c2h2+o2=hcco+oh          4.00e+07  1.5   30100.0  ! Marinov 1997
c2h2+m=c2h+h+m           4.20E+16  0.0  107000.0  ! Miller 1992
c2h2+h (+m)=c2h3(+m)     3.11E+11  0.58   2589.0  ! Knyazev 1995
low / 2.25E+40  -7.269   6577.0 /                 ! Marinov 1996
troe /1.0 1.0E-15  675.0 1.0E+15 /
h2o /5.0/ h2/2.0/ co2/3.0/ co/2.0/
c2h5oh(+m)=ch3+ch2oh(+m) 5.71E+23 -1.68 94405.0  !Marinov 1998
low /3.11E+85 -18.84 113095./
troe/0.5 550. 825.  6100./
h2o/5./ h2/2.0/ co2/3.0/ co/2.0/
c2h5oh(+m)=c2h5+oh(+m)   2.40E+23 -1.62 99535.0   !Marinov 1998
low /5.11E+85 -18.80 118768./
troe/0.5 650. 800. 1.e15/
h2o/5./ h2/2.0/ co2/3.0/ co/2.0/
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low/6.68E+82 -18.7 85500./
troe/6.7 1.e-15 460. 1.e15/
h2o/5./
c2h5oh(+m)=ch3hco+h2(+m) 1.67E+9  1.0  90820.0   !Marinov 1998
low /2.04e82 -17.94 111674./
troe/0.9 900. 1120. 7500./
h2o/5./
c2h5oh+oh=c2h4oh+h2o      1.74E+11   0.27     600.0 !Marinov 1998
c2h5oh+oh=ch3choh+h2o     4.64E+11   0.15       0.0 !Marinov 1998
c2h5oh+oh=ch3ch2o+h2o     7.46E+11   0.30    1634.0 !Marinov 1998
c2h5oh+h=c2h4oh+h2        1.23E+7    1.8     5098.0 !Marinov 1998
c2h5oh+h=ch3choh+h2       2.58E+7    1.65    2827.0 !Marinov 1998
c2h5oh+h=ch3ch2o+h2       1.50E+7    1.60    3038.0 !Marinov 1998
c2h5oh+o=c2h4oh+oh        9.41E+7    1.70    5459.0 !Marinov 1998
c2h5oh+o=ch3choh+oh       1.88E+7    1.85    1824.0 !Marinov 1998
c2h5oh+o=ch3ch2o+oh       1.58E+7    2.00    4448.0 !Marinov 1998
c2h5oh+ch3=c2h4oh+ch4     1.33E+2    3.18    9362.0 !Marinov 1998
c2h5oh+ch3=ch3choh+ch4    4.44E+2    2.90    7690.0 !Marinov 1998
c2h5oh+ch3=ch3ch2o+ch4    1.34E+2    2.92    7452.0 !Marinov 1998
c2h5oh+ho2=ch3choh+h2o2   7.20E+3    2.55   10750.0 !Marinov 1998
c2h5oh+ho2=c2h4oh+h2o2    1.00E+4    2.55   15750.0 !Marinov 1998
c2h5oh+ho2=ch3ch2o+h2o2   2.50E+12   0.0    24000.0 !Marinov 1998
ch3ch2o+m=ch3hco+h+m      1.16E+35  -5.89   25274.0 !Marinov 1998
ch3ch2o+m=ch3+ch2o+m      1.35E+38  -6.96   23800.0 !Marinov 1998
ch3ch2o+o2=ch3hco+ho2     4.00E+10   0.0     1100.0 !Hartmann 1990
ch3ch2o+co=c2h5+co2       4.68E+2    3.16    5380.0 !Marinov 1998
ch3ch2o+h=ch3+ch2oh       1.00E+13   0.0        0.0 !Marinov 1998
ch3ch2o+h=ch3hco+h2       1.00E+13   0.0        0.0 !Marinov 1998
ch3ch2o+oh=ch3hco+h2o     1.00E+13   0.0        0.0 !Marinov 1998
ch3choh+o2=ch3hco+ho2     4.82E+14   0.0     5017.0 !Marinov 1998
dup
ch3choh+o2=ch3hco+ho2     8.43E+15  -1.2        0.0 !Marinov 1998
dup
ch3choh+ch3=ic3h7+oh      2.00E+13   0.0        0.0 !Marinov 1998
ch3choh+o=ch3hco+oh       1.00E+14   0.0        0.0 !Marinov 1998
ch3choh+h=ch3hco+h2       1.00E+13   0.0        0.0 !Marinov 1998
ch3choh+h=ch3+ch2oh       1.00E+13   0.0        0.0 !Marinov 1998
ch3choh+ho2=ch3hco+oh+oh  4.00E+13   0.0        0.0 !Marinov 1998
ch3choh+oh=ch3hco+h2o     5.00E+12   0.0        0.0 !Marinov 1998
ch3choh+m=ch3hco+h+m      1.00E+14   0.0    25000.0 !Marinov 1998
ch3hco+oh=ch3co+h2o       9.24E+6    1.5     -962.0 !Taylor 1996
ch3hco+oh=ch2hco+h2o      1.72E+5    2.4      815.0 !Taylor 1996
ch3hco+oh=ch3+hcooh       3.00E+15  -1.076      0.0 !Marinov 1998
ch3hco+o=ch3co+oh         1.77E+18  -1.9     2975.0 !Marinov 1998
ch3hco+o=ch2hco+oh        3.72E+13  -0.2     3556.0 !Marinov 1998
ch3hco+h=ch3co+h2         4.66E+13  -0.35    2988.0 !Marinov 1998
ch3hco+h=ch2hco+h2        1.85E+12   0.40    5359.0 !Marinov 1998
ch3hco+ch3=ch3co+ch4      3.90E-7    5.8     2200.0 !Marinov 1998
ch3hco+ch3=ch2hco+ch4     2.45E+1    3.15    5727.0 !Marinov 1998
ch3hco+ho2=ch3co+h2o2     2.40E+19  -2.2    14030.0 !Marinov 1998
ch3hco+ho2=ch2hco+h2o2    2.32E+11   0.40   14864.0 !Marinov 1998
hcooh+m=co+h2o+m          2.09E+14   0.0    40400.0 !Saito 1984
hcooh+m=co2+h2+m          1.35E+15   0.0    60600.0 !Saito 1984
hcooh+oh=co2+h2o+h        2.62E+6    2.056    916.0 !Marinov 1998
hcooh+oh=co+h2o+oh        1.85E+7    1.5     -962.0 !Marinov 1998
hcooh+h=co2+h2+h          4.24E+6    2.1     4868.0 !Marinov 1998
hcooh+h=co+h2+oh          6.06E+13  -0.35    2988.0 !Marinov 1998
hcooh+ch3=ch4+co+oh       3.90E-7    5.8     2200.0 !Marinov 1998
hcooh+ho2=co+h2o2+oh      2.40E+19  -2.2    14030.0 !Marinov 1998
hcooh+o=co+oh+oh          1.77E+18  -1.9     2975.0 !Marinov 1998
ch2hco+h=ch3+hco          5.00E+13   0.0        0.0 !Marinov 1998
ch2hco+h=ch2co+h2         2.00E+13   0.0        0.0 !Marinov 1998
ch2hco+o=ch2o+hco         1.00E+14   0.0        0.0 !Marinov 1996
ch2hco+oh=ch2co+h2o       3.00E+13   0.0        0.0 !Marinov 1996
ch2hco+o2=ch2o+co+oh      3.00E+10   0.0        0.0 !Baulch  1992
ch2hco+ch3=c2h5+co+h      4.90E+14  -0.50       0.0 !Marinov 1998
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ch2hco+ho2=ch2o+hco+oh    7.00E+12   0.0        0.0 !Marinov 1998
ch2hco+ho2=ch3hco+o2      3.00E+12   0.0        0.0 !Marinov 1998
ch2hco=ch3+co             1.17E+43  -9.83   43756.0 !Marinov 1998
ch2hco=ch2co+h            1.81E+43  -9.61   45868.0 !Marinov 1998
chocho(+m)=ch2o+co(+m)   4.27E+12  0.0   50600.0  ! Marinov 1995
low /  8.91E+16    0.0    49200.0 /               ! Marinov 1995
chocho=co+co+h2          4.07E+42 -8.5   69278.0  ! Marinov 1996
chocho+oh=hco+co+h2o     1.00E+13  0.0       0.0  ! Marinov 1995
chocho+o=hco+co+oh       7.24E+12  0.0    1970.0  ! Marinov 1995
chocho+h=ch2o+hco        1.00E+12  0.0       0.0  ! Marinov 1995
chocho+ho2=hco+co+h2o2   1.70E+12  0.0   10700.0  ! Marinov 1995
chocho+ch3=hco+co+ch4    1.74E+12  0.0    8440.0  ! Marinov 1995
chocho+o2=hco+co+ho2     1.00E+14  0.0   37000.0  ! Marinov 1995
ch3co(+m)=ch3+co(+m)     3.00E+12  0.0   16722.0  ! Warnatz 1984
low / 1.20E+15    0.0     12518.0 /               ! Warnatz 1984
ch2co+o=co2+ch2          1.75E+12  0.0    1350.0  ! Marinov 1995
ch2co+h=ch3+co           2.71E+4   2.75    714.0  ! Marinov 1996
ch2co+h=hcco+h2          2.00E+14  0.0    8000.0  ! Marinov 1996
ch2co+o=hcco+oh          1.00E+13  0.0    8000.0  ! Miller 1992
ch2co+oh=hcco+h2o        1.00E+13  0.0    2000.0  ! Marinov 1996
ch2co+oh=ch2oh+co        3.73E+12  0.0   -1013.0  ! Brown 1989
ch2co(+m)=ch2+co(+m)     3.00E+14  0.0   70980.0  ! Miller 1992
low /  3.60E+15    0.0    59270.0 /               ! Miller 1992
c2h+h2=c2h2+h            4.09E+05  2.39    864.3  ! Miller 1992
c2h+o=ch+co              5.00E+13  0.0       0.0  ! Miller 1992
c2h+oh=hcco+h            2.00E+13  0.        0.0  ! Miller 1992
c2h+o2=co+co+h           9.04E+12  0.0    -457.0  ! Opansky 1993
hcco+c2h2=h2ccch+co      1.00E+11  0.0    3000.0  ! Miller 1992
hcco+h=ch2(s)+co         1.00E+14  0.0       0.0  ! Miller 1992
hcco+o=h+co+co           8.00E+13  0.0       0.0  ! Peeters 1995
hcco+o=ch+co2            2.95E+13  0.0    1113.0  ! Peeters 1995
hcco+o2=hco+co+o         2.50E+8   1.0       0.0  ! Marinov 1997
hcco+o2=co2+hco          2.40E+11  0.0    -854.0  ! Marinov 1997
hcco+ch=c2h2+co          5.00E+13  0.0       0.0  ! Miller 1992
hcco+hcco=c2h2+co+co     1.00E+13  0.0       0.0  ! Miller 1992
hcco+oh=c2o+h2o          3.00E+13  0.0       0.0  ! Miller 1992
c2o+h=ch+co              1.00E+13  0.0       0.0  ! Miller 1992
c2o+o=co+co              5.00E+13  0.0       0.0  ! Miller 1992
c2o+oh=co+co+h           2.00E+13  0.0       0.0  ! Miller 1992
c2o+o2=co+co+o           2.00E+13  0.0       0.0  ! Miller 1992
c3h8(+m)=c2h5+ch3(+m)    7.90E+22 -1.8   88629.0  ! Tsang 1988
low / 7.237E+27 -2.88 67448.0 /                   ! Al-Alami 1983
troe /1.0 1.0E-15 1500.0 1.0E+15/
h2o/5.0/ co2/3.0/ co/2.0/ h2/2.0/
ic3h7+ho2=c3h8+o2        3.00E+12  0.0       0.0  !Marinov 1998
nc3h7+ho2=c3h8+o2        3.00E+12  0.0       0.0  !Marinov 1998
c3h8+ho2=nc3h7+h2o2      4.76E+04  2.55  16492.0  ! Tsang 1988
c3h8+ho2=ic3h7+h2o2      9.64E+03  2.6   13909.0  ! Tsang 1988
c3h8+oh=nc3h7+h2o        3.16E+07  1.8     934.0  ! Cohen 1991
c3h8+oh=ic3h7+h2o        7.08E+06  1.9    -159.0  ! Cohen 1991
c3h8+o=nc3h7+oh          3.73E+06  2.4    5504.0  ! Cohen 1986
c3h8+o=ic3h7+oh          5.48E+05  2.5    3139.0  ! Cohen 1986
c3h8+h=ic3h7+h2          1.30E+06  2.4    4471.0  ! Tsang 1988
c3h8+h=nc3h7+h2          1.33E+06  2.54   6756.0  ! Tsang 1988
c3h8+ch3=nc3h7+ch4       9.04E-01  3.65   7153.0  ! Tsang 1988
c3h8+ch3=ic3h7+ch4       1.51E+00  3.46   5480.0  ! Tsang 1988
c3h8+c2h3=ic3h7+c2h4     1.00E+03  3.1    8830.0  ! Tsang 1988
c3h8+c2h3=nc3h7+c2h4     6.00E+02  3.3   10500.0  ! Tsang 1988
c3h8+c2h5=ic3h7+c2h6     1.51E+00  3.46   7470.0  ! Tsang 1988
c3h8+c2h5=nc3h7+c2h6     9.03E-01  3.65   9140.0  ! Tsang 1988
c3h8+ac3h5=c3h6+nc3h7    2.35E+02  3.3   19842.0  ! Tsang 1988
c3h8+ac3h5=c3h6+ic3h7    7.83E+01  3.3   18169.0  ! Tsang 1988
nc3h7(+m)=c2h4+ch3(+m)   1.23E+13  -0.1  30202.0  ! Bencsura 1992
low / 5.485E+49  -10.0  35766.0 /                 ! Bencsura 1992
troe / 2.17   1.0E-15   251.0   1185.0 /
h2o /5.0/ h2/2.0/ co2/3.0/ co/2.0/
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c3h6+h(+m)=ic3h7(+m)    5.70E+09   1.16    874.0  ! Seakins 1993
low / 1.64E+54   -11.1   9364.0 /                 ! Marinov 1996
troe / 1.0   1.0E-15   260.0   3000.0 /
h2o /5.0/ h2/2.0/ co2/3.0/ co/2.0/
ic3h7+o2=c2coo           1.75E+58 -14.89  12608.0 !This Study
ic3h7+o2=c2jcq           7.06E+27 -5.91    4802.0 !This Study
ic3h7+o2=c3h6+ho2        1.88E+20 -2.69    7109.0 !This Study
ic3h7+o2=ccyc2o+oh       4.54E+4   1.55    5000.0 !This Study
c2coo=c2jcq              6.18E+61 -16.03  43008.0 !This Study
c2coo=c3h6+ho2           1.51E+72 -18.69  51699.0 !This Study
c2coo=ccyc2o+oh          1.95E+57 -14.99  49595.0 !This Study
c2coo+ho2=c2cq+o2        2.29E+11   0.0   -1550.0 !This Study
c2cq=c2coj+oh            6.00E+14   0.0   42300.0 !This Study
c2coj=acetone+h          2.00E+14   0.0   21500.0 !Batt 1979
c2coj=ch3+ch3hco         4.00E+14   0.0   17200.0 !Batt 1979
c2coj+o2=acetone+ho2     4.90E+10   0.0    1590.0 !Heicklen 1988
c2coj+co=ic3h7+co2       4.68E+2    3.16   5380.0 !This Study
c2jcq=ch2hco+ch3+oh      8.19E+7    0.46  29230.0 !This Study
c2jcq+o2=ccqcoo          1.08E+31  -6.04   5019.0 !This Study
c2jcq+o2=cc*ocq+oh       1.15E+27  -4.61  10312.0 !This Study
c2jcq+o2=cjcqcq          6.98E+30  -6.14  11470.0 !This Study
c2jcq+o2=c*ccq+ho2       1.41E+42  -9.22  20724.0 !This Study
ccqcoo=cc*ocq+oh         2.46E+23  -3.95  24702.0 !This Study
ccqcoo=cjcqcq            4.72E+25  -4.89  26209.0 !This Study
cjcqcq=cc*ocq+oh         1.17E+24  -4.71  21921.0 !This Study
cjcqcq=c*ccq+ho2         3.53E+20  -2.8   18874.0 !This Study
cc*ocq=ch3co+ch2o+oh     6.00E+14   0.0   42300.0 !This Study
acetone+oh=ch2co+ch3+h2o 7.23E+6    2.0     864.0 !This Study
acetone+o=ch2co+ch3+oh   3.00E+7    2.0    5115.0 !This Study
acetone+h=ch2co+ch3+h2   5.40E+2    3.5    5210.0 !This Study
nc3h7+o2=cccoo           8.57E+46  -10.79 11555.0 !This Study
nc3h7+o2=cccho+oh        2.04E+16  -1.29  18186.0 !This Study
nc3h7+o2=ccjcq           1.45E+36  -7.61  13874.0 !This Study
nc3h7+o2=c3h6+ho2        3.83E+26  -4.44   7724.0 !This Study
nc3h7+o2=cjccq           3.47E+45  -10.05 19704.0 !This Study
cccoo=c3h6+ho2           1.88E+61  -14.94 49716.0 !This Study
cccoo=cjccq              4.18E+34  -7.33  31801.0 !This Study
cccoo=ccjcq              1.61E+42  -9.75  35783.0 !This Study
ccjcq=c3h6+ho2           2.19E+30  -6.11  18849.0 !This Study
ccjcq=ccyc2o+oh          1.01E+20  -3.36  20038.0 !This Study
cjccq=c3h6+ho2           1.22E+57  -13.84 43391.0 !This Study
cjccq=cyccco+oh          2.23E+14  -1.26  18153.0 !This Study
ccjcq+o2=ccoocq          1.00E+36  -7.67   6314.0 !This Study
ccjcq+o2=cjcqcq          5.00E+34  -7.22  13951.0 !This Study
ccjcq+o2=c*ccq+ho2       8.54E+43  -9.53  22551.0 !This Study
ccjcq+o2=ccqc*o+oh       6.13E+28  -5.05  11272.0 !This Study
ccqc*o=ch3hco+hco+oh     6.00E+14   0.0   42300.0 !This Study
cqcc*o=ch2hco+ch2o+oh    6.00E+14   0.0   42300.0 !This Study
ccoocq=cjcqcq            3.21E+37  -8.25  34660.0 !This Study
ccoocq=ccqc*o+oh         1.21E+30  -5.85  28978.0 !This Study
cjcqcq=ccqc*o+oh         1.41E+33  -7.14  28454.0 !This Study
c*ccq=ch2chch2o+oh       6.00E+14   0.0   42300.0 !This Study
cjccq+o2=cooccq          6.92E+28  -5.32   4441.0 !This Study
cjccq+o2=cqcc*o+oh       1.46E+29  -5.5   10127.0 !This Study
cjccq+o2=cqcjcq          4.81E+32  -6.71  12303.0 !This Study
cjccq+o2=c*ccq+ho2       1.76E+41  -8.76  20150.0 !This Study
cooccq=cqcc*o+oh         1.81E+18  -2.68  20340.0 !This Study
cooccq=cqcjcq            4.08E+30  -6.24  30612.0 !This Study
cooccq=c*ccq+ho2         1.06E+38  -7.99  40074.0 !This Study
cqcjcq=cqcc*o+oh         2.37E+30  -6.77  27650.0 !This Study
cqcjcq=c*ccq+ho2         1.44E+24  -4.03  19130.0 !This Study
cccoo+ho2=cccq+o2        2.29E+11   0.00  -1550.0 !This Study
cccq=cccoj+oh            6.00E+14   0.0   42300.0 !This Study
cccoj+o2=cccho+ho2       1.95E+11   0.0    1980.0 !This Study
cccoj+co=nc3h7+co2       4.68E+2    3.16   5380.0 !This Study
cccoj+m=c2h5+ch2o+m      1.35E+38  -6.96  23800.0 !This Study
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cccoj+m=cccho+h+m       1.16E+35  -5.89  25274.0 !This Study
cccho+oh=c2h5+co+h2o    1.00E+10   1.0       0.0 !This Study
cccho+o=c2h5+co+oh      7.24E+12   0.0    1970.0 !This Study
cccho+h=c2h5+co+h2      3.98E+13   0.0    4200.0 !This Study
ic3h7+h=c2h5+ch3        5.00E+13   0.0       0.0 ! Tsang 1988
nc3h7+h=c2h5+ch3        1.00E+14   0.0       0.0 ! Tsang 1988
c3h6=c2h2+ch4           2.50E+12   0.0   70000.0 ! Hidaka 1992
c3h6=ac3h4+h2           3.00E+13   0.0   80000.0 ! Hidaka 1992
pc3h5+h=c3h6            1.00E+14   0.0       0.0 !Marinov 1998
sc3h5+h=c3h6            1.00E+14   0.0       0.0 !Marinov 1998
c3h6+ho2=ac3h5+h2o2     9.64E+03   2.6   13910.0 ! Tsang 1991
c3h6+oh=hoc3h6          2.92E+12   0.0   -1000.0 ! Atkinson 1986
hoc3h6+o2=hoc3h6o2      1.00E+12   0.0   -1100.0 !This Study
hoc3h6o2=ch3hco+ch2o+oh 6.00E+10   0.0   26000.0 !This Study
hoc3h6o2+ho2=hoccqc+o2  2.29E+11   0.0   -1550.0 !This Study
hoccqc=ch2oh+ch3hco+oh  6.00E+14   0.0   42300.0 !This Study
c3h6+oh=ac3h5+h2o       2.60E+06   2.0    -298.0 !Tsang 1991
c3h6+oh=sc3h5+h2o       1.11E+06   2.0    1451.0  ! Tsang 1991
c3h6+oh=pc3h5+h2o       2.11E+06   2.0    2778.0  ! Tsang 1991
c3h6+o=ch3co+ch3        5.00E+7    1.76     76.0  ! This Study
c3h6+o=c2h5+hco        1.58E+07   1.76  -1216.0   ! Tsang 1991
c3h6+o=ac3h5+oh        5.24E+11   0.7     5884.0   ! Tsang 1991
c3h6+o=pc3h5+oh        1.20E+11   0.7     8959.0   ! Tsang 1991
c3h6+o=sc3h5+oh        6.03E+10   0.7     7632.0   ! Tsang 1991
c3h6+h=c2h4+ch3        4.00E+13   0.0     1302.0   ! This Study
c3h6+h=ac3h5+h2        1.73E+05   2.5     2492.0   ! Tsang 1991
c3h6+h=sc3h5+h2        4.09E+05   2.5     9794.0   ! Tsang 1991
c3h6+h=pc3h5+h2        8.04E+05   2.5    12284.0   ! Tsang 1991
c3h6+ch3=ac3h5+ch4     2.22E+00   3.5     5675.0   ! Tsang 1991
c3h6+ch3=sc3h5+ch4     8.43E-01   3.5    11656.0   ! Tsang 1991
c3h6+ch3=pc3h5+ch4     1.35E+00   3.5    12848.0   ! Tsang 1991
c3h6+hco=ac3h5+ch2o    1.08E+07   1.9    17010.0   ! Tsang 1991
c3h6+o2=ac3h5+ho2      1.0e14     0.0    40000.0   ! This Study
ch3chco+oh=ch2chco+h2o 4.00E+06   2.0        0.0   ! Marinov 1996
ch3chco+o=ch2chco+oh   7.60E+08   1.5     8500.0   ! Marinov 1996
ch3chco+h=ch2chco+h2   2.00E+05   2.5     2500.0   ! Marinov 1996
ch3chco+h=c2h5+co      2.00E+13   0.0     2000.0   ! Marinov 1996
ch3chco+o=ch3+hco+co   3.00E+07   2.0        0.0   ! Marinov 1996
ch2chcho+oh=hoc3h4o    2.92E+12   0.0    -1000.0   ! This Study
ch2chcho+oh=chchcho+h2o 1.01e13   0.0     5936.0   ! This Study
chchcho+o2=c2h2+co+ho2  2.00e12   0.0        0.0   ! This Study
chchcho=c2h2+hco       1.00e14    0.0    33000.0   ! This Study
hoc3h4o+o2=hoc3h4o3    1.00E+12   0.0    -1100.0   ! This Study
hoc3h4o3=ch2o+chocho+oh 6.00E+10  0.0    26000.0   ! This Study
hoc3h4o3+ho2=hoccqcho+o2 2.29E+11 0.0    -1550.0   ! This Study
hoccqcho=ch2oh+chocho+oh 6.00E+14 0.0    42300.0   ! This Study
ch2chcho+oh=ch2chco+h2o 9.24E+6   1.5     -962.0   ! Marinov 1996
ch2chcho+o=ch2chco+oh   7.24E+12  0.0     1970.0   ! Marinov 1996
ch2chcho+o=ch2hco+hco   5.01E+07  1.76      76.0   ! Marinov 1996
ch2chcho+h=ch2chco+h2   3.98E+13  0.0     4200.0   ! Marinov 1996
ch2chcho+h=c2h4+hco     2.00E+13  0.0     1500.0   ! Marinov 1996
ch2chcho+o2=ch2chco+ho2 3.00E+13  0.0    36000.0   ! Marinov 1996
ch2chco=c2h3+co         1.00E+14  0.0    34000.0   ! Marinov 1996
ch2chco+o=c2h3+co2      1.00E+14  0.0        0.0   ! Marinov 1996
ac3h5+o2=ac3h5o2        6.98E+22 -4.38   -5119.0   ! Bozzelli 1993
ac3h5+o2=ch2chcho+oh    1.82E+13 -0.41   22859.0   ! Bozzelli 1993
ac3h5+o2=ac3h4+ho2      4.99E+15 -1.4    22428.0   ! Bozzelli 1993
ac3h5+o2=ch2hco+ch2o    1.06E+10  0.34   12838.0   ! Bozzelli 1993
ac3h5+o2=c2h2+ch2o+oh   2.78E+25 -4.8    15468.0   ! Bozzelli 1993
ac3h5o2+ac3h5=ch2chch2o+ch2chch2o 2.40E+13 0.0 0.0 !This Study
ac3h5o2+ho2=ac3h5o2h+o2    2.29E+11  0.0 -1550.0  !This Study
ac3h5o2h=ch2chch2o+oh      6.00E+14  0.0 42300.0  !This Study
ac3h5+ho2=ch2chch2o+oh     1.00E+13  0.0     0.0  !Tsang 1991
ch2chch2o+o2=ch2chcho+ho2  4.00E+10  0.0  1100.0  !This Study
ch2chch2o+co=ac3h5+co2     4.68E+2   3.16 5380.0  !This Study
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low/ 1.50E+30 -4.8 5560./
troe/0.78  94.  1555. 4200./
h2o/5./
ac3h5+oh=ac3h4+h2o       1.00E+13  0.0        0.0   ! Tsang 1991
ac3h5+h=ac3h4+h2         5.00E+13  0.0        0.0   ! Marinov 1996
ac3h5+h=c3h6             1.88E+26  -3.6    5468.0   ! Marinov 1996
ac3h5+o=ch2chcho+h       1.81E+14  0.0        0.0   ! Slagle 1992
ac3h5+ch3=ac3h4+ch4      3.02E+12  -0.32   -131.0   ! Tsang 1991
ac3h5+ac3h5=c6h10        3.00E+47  -8.0   19780.0   ! Tsang 1991
c6h10+oh=c6h9+h2o        4.16E+6    2.0    -298.0   ! This Study
c6h9+ho2=ch2chcho+ac3h5+oh 5.0E+12 0.0        0.0   ! This Study
pc3h5+o2=ch3hco+hco      1.09E+23  -3.29   3892.0   ! Marinov 1996
pc3h5+o2=ch3chco+h+o     1.60E+15  -0.78   3135.0   ! Marinov 1996
pc3h5+o=ch3chco+h        1.00E+14   0.0       0.0   ! Marinov 1996
pc3h5+h=pc3h4+h2         2.00E+13   0.0       0.0   ! Marinov 1996
pc3h5+oh=pc3h4+h2o       1.00E+13   0.0       0.0   ! Marinov 1996
pc3h5+h=ac3h5+h          1.00E+14   0.0       0.0   ! Marinov 1996
sc3h5+h=ac3h5+h          1.00E+14   0.0       0.0   ! Marinov 1996
sc3h5+o2=ch3co+ch2o      1.09E+22  -3.29   3892.0   ! Marinov 1996
sc3h5+o=ch2co+ch3        1.00E+14   0.0       0.0   ! Marinov 1996
sc3h5+h=pc3h4+h2         4.00E+13   0.0       0.0   ! Marinov 1996
sc3h5+oh=pc3h4+h2o       2.00E+13   0.0       0.0   ! Marinov 1996
ac3h4+h=h2ccch+h2        2.00E+7    2.0    5000.0   ! Marinov 1997
ac3h4+o=c2h4+co          1.34E+07   1.88    179.0   ! Marinov 1996
ac3h4+oh=h2ccch+h2o      1.00E+7    2.0    1000.0   ! Marinov 1997
ac3h4+ch3=h2ccch+ch4     1.50E+0    3.5    5600.0   ! Marinov 1997
ac3h4=pc3h4              1.48E+13   0.0   60401.0   ! Marinov 1997
pc3h4+h=h2ccch+h2        2.00E+7    2.0    5000.0   ! Marinov 1997
pc3h4+o=c2h4+co          1.50E+13   0.0    2102.0   ! Marinov 1996
pc3h4+oh=h2ccch+h2o      1.00E+7    2.0    1000.0   ! Marinov 1997
pc3h4+ch3=h2ccch+ch4     1.50E+0    3.5    5600.0   ! Marinov 1997
pc3h4+h=ch3+c2h2         5.12E+10   1.0    2060.0   ! Marinov 1997
pc3h4+h(+m)=sc3h5(+m)    6.50E+12   0.0    2000.0   ! Wagner 1972
 low / 8.45E+39  -7.27    6577.0 /                  ! Marinov 1996
ac3h4+h(+m)=ac3h5(+m)    1.20E+11   0.69   3007.0   ! Tsang 1992
 low / 5.56E+33   -5.0    4448.0 /                  ! Marinov 1996
ac3h4+h(+m)=sc3h5(+m)    8.49E+12   0.0    2000.0   ! Wagner 1972
 low / 1.11E+34   -5.0    4448.0 /                  ! Marinov 1996
h2ccch+o2=ch2co+hco      3.00E+10   0.0    2868.0   ! Miller 1992
h2ccch+o=ch2o+c2h        1.40E+14   0.0       0.0   ! Pauwels 1995
h2ccch+h=c3h2+h2         5.00e+13   0.0    1000.0   ! Pauwels 1995
h2ccch+oh=c3h2+h2o       2.00E+13   0.0       0.0   ! Miller 1992
h2ccch+ch3=c3h2+ch4      2.00E+13   0.0       0.0   ! Marinov 1997
h2ccch+h(+m)=ac3h4(+m) 1.66E+15 -0.37         0.0   ! Marinov 1996
 low / 3.36E+45 -8.52  6293.0  /                    ! Kiefer 1995
h2o/5.0/ h2/2.0/ co2/3.0/ co/2.0/ o2/2.0/ c2h2/2.0/
h2ccch+h(+m)=pc3h4(+m) 1.66E+15 -0.37         0.0   ! Marinov 1996
 low / 8.78E+45 -8.9   7974.0 /                     ! Kiefer 1995
h2o /5.0/ h2/2.0/ co2/3.0/ co/2.0/ o2/2.0/ c2h2/2.0/
c3h2+o2=hcco+co+h        2.00E+12   0.0     1000.0  ! Pauwels 1995
c3h2+o=c2h2+co           1.00E+14   0.0        0.0  ! Pauwels 1995
c3h2+oh=c2h2+hco         5.00E+13   0.0        0.0  ! Miller 1992
n+no=n2+o                3.50E+13   0.00     330.0  ! GRI-Mech2.11
n+o2=no+o                2.65E+12   0.00     6400.0 ! GRI-Mech2.11
n+oh=no+h                7.33E+13   0.00     1120.0 ! GRI-Mech2.11
n2o+o=n2+o2              1.40E+12   0.00    10810.0 ! GRI-Mech2.11
n2o+o=2no                2.90E+13   0.00    23150.0 ! GRI-Mech2.11
n2o+h=n2+oh              4.40E+14   0.00    18880.0 ! GRI-Mech2.11
n2o+oh=n2+ho2            2.00E+12   0.00    21060.0 ! GRI-Mech2.11
n2o(+m)=n2+o(+m)         1.30E+11   0.00    59620.0 ! GRI-Mech2.11
 low  /   6.200e+14      .000  56100.00/
h2/2.00/ h2o/6.00/ ch4/2.00/ co/1.50/ co2/2.00/ c2h6/3.00/ ar/ .70/
no+ho2=no2+oh            2.11E+12   0.00     -480.0 ! GRI-Mech2.11
no+o+m=no2+m             1.06E+20  -1.410       0.0 ! GRI-Mech2.11
h2/2.00/ h2o/6.00/ ch4/2.00/ co/1.50/ co2/2.00/ c2h6/3.00/ ar/ .70/
no2+o=no+o2              3.90E+12   0.00     -240.0 ! GRI-Mech2.11
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no2+h=no+oh            1.32E+14   0.00      360.0 ! GRI-Mech2.11
nh+o=no+h              5.00E+13   0.00        0.0 ! GRI-Mech2.11
nh+h=n+h2              3.20E+13   0.00      330.0 ! GRI-Mech2.11
nh+oh=hno+h            2.00E+13   0.00        0.0 ! GRI-Mech2.11
nh+oh=n+h2o            2.00E+09   1.20        0.0 ! GRI-Mech2.11
nh+o2=hno+o            4.61E+05   2.00     6500.0 ! GRI-Mech2.11
nh+o2=no+oh            1.28E+06   1.50      100.0 ! GRI-Mech2.11
nh+n=n2+h              1.50E+13   0.00        0.0 ! GRI-Mech2.11
nh+h2o=hno+h2          2.00E+13   0.00    13850.0 ! GRI-Mech2.11
nh+no=n2+oh            2.16E+13  -.230        0.0 ! GRI-Mech2.11
nh+no=n2o+h            4.16E+14  -.450        0.0 ! GRI-Mech2.11
nh2+o=oh+nh            7.00e+12     .000          .00 !GRI-Mech2.11
nh2+o=h+hno            4.60e+13     .000          .00 !GRI-Mech2.11
nh2+h=nh+h2            4.00e+13     .000      3650.00 !GRI-Mech2.11
nh2+oh=nh+h2o          9.00e+07    1.500      -460.00 !GRI-Mech2.11
nnh=n2+h               3.30e+08     .000          .00 !GRI-Mech2.11
dup
nnh+m=n2+h+m           1.30e+14    -.110     4980.00 !GRI-Mech2.11
dup
h2/2.00/ h2o/6.00/ ch4/2.00/ co/1.50/ co2/2.00/ c2h6/3.00/ ar/ .70/
nnh+o2=ho2+n2          5.00e+12     .000          .00 !GRI-Mech2.11
nnh+o=oh+n2            2.50e+13     .000          .00 !GRI-Mech2.11
nnh+o=nh+no            7.00e+13     .000          .00 !GRI-Mech2.11
nnh+h=h2+n2            5.00e+13     .000          .00 !GRI-Mech2.11
nnh+oh=h2o+n2          2.00e+13     .000          .00 !GRI-Mech2.11
nnh+ch3=ch4+n2         2.50e+13     .000          .00 !GRI-Mech2.11
h+no+m=hno+m           8.95e+19   -1.320      740.00 !GRI-Mech2.11
h2/2.00/ h2o/6.00/ ch4/2.00/ co/1.50/ co2/2.00/ c2h6/3.00/ ar/ .70/
hno+o=no+oh            2.50e+13     .000          .00 !GRI-Mech2.11
hno+h=h2+no            4.50e+11     .720      660.00 !GRI-Mech2,11
hno+oh=no+h2o          1.30e+07    1.900     -950.00 !GRI-Mech2.11
hno+o2=ho2+no          1.00e+13     .000    13000.00 !GRI-Mech2.11
cn+o=co+n              7.70e+13     .000          .00 !GRI-Mech2.11
cn+oh=nco+h            4.00e+13     .000          .00 !GRI-Mech2.11
cn+h2o=hcn+oh          8.00e+12     .000     7460.00 !GRI-Mech2.11
cn+o2=nco+o            6.14e+12     .000     -440.00 !GRI-Mech2.11
cn+h2=hcn+h            2.10e+13     .000     4710.00 !GRI-Mech2.11
nco+o=no+co            2.35e+13     .000          .00 !GRI-Mech2.11
nco+h=nh+co            5.40e+13     .000          .00 !GRI-Mech2.11
nco+oh=no+h+co         2.50e+12     .000          .00 !GRI-Mech2.11
nco+n=n2+co            2.00e+13     .000          .00 !GRI-Mech2.11
nco+o2=no+co2          2.00e+12     .000    20000.00 !GRI-Mech2.11
nco+m=n+co+m           8.80e+16    -.500    48000.00 !GRI-Mech2.11
h2/2.00/ h2o/6.00/ ch4/2.00/ co/1.50/ co2/2.00/ c2h6/3.00/ ar/ .70/
nco+no=n2o+co          2.85e+17   -1.520      740.00 !GRI-Mech2.11
nco+no=n2+co2          5.70e+18   -2.000      800.00 !GRI-Mech2.11
hcn+m=h+cn+m           1.04e+29   -3.300   126600.00 !GRI-Mech2.11
h2/2.00/ h2o/6.00/ ch4/2.00/ co/1.50/ co2/2.00/ c2h6/3.00/ ar/ .70/
hcn+o=nco+h            1.11e+04    2.640     4980.00 !GRI-Mech2.11
hcn+o=nh+co            2.77e+03    2.640     4980.00 !GRI-Mech2.11
hcn+o=cn+oh            2.13e+09    1.580    26600.00 !GRI-Mech2.11
hcn+oh=hocn+h          1.10e+06    2.030    13370.00 !GRI-Mech2.11
hcn+oh=hnco+h          4.40e+03    2.260     6400.00 !GRI-Mech2.11
hcn+oh=nh2+co          1.60e+02    2.560     9000.00 !GRI-Mech2.11
h+hcn+m=h2cn+m         1.40e+26   -3.400     1900.00 !GRI-Mech2.11
h2/2.00/ h2o/6.00/ ch4/2.00/ co/1.50/ co2/2.00/ c2h6/3.00/ ar/ .70/
h2cn+n=n2+ch2          6.00e+13     .000      400.00 !GRI-Mech2.11
c+n2=cn+n              6.30e+13     .000    46020.00 !GRI-Mech2.11
ch+n2=hcn+n            2.86e+08    1.100    20400.00 !GRI-Mech2.11
ch+n2(+m)=hcnn(+m)     3.10e+12     .150          .00 !GRI-Mech2.11
low  /  1.300e+25    -3.160     740.00/
troe/    .6670  235.00  2117.00  4536.00 /
h2/2.00/ h2o/6.00/ ch4/2.00/ co/1.50/ co2/2.00/ c2h6/3.00/ ar/ .70/
ch2+n2=hcn+nh          1.00e+13     .000    74000.00 !GRI-Mech2.11
ch2(s)+n2=nh+hcn       1.00e+11     .000    65000.00 !GRI-Mech2.11
c+no=cn+o              1.90e+13     .000          .00 !GRI-Mech2.11
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```
c+no=co+n                  2.90e+13      .000          .00 !GRI-Mech2.11
ch+no=hcn+o                5.00e+13      .000          .00 !GRI-Mech2.11
ch+no=h+nco                2.00e+13      .000          .00 !GRI-Mech2.11
ch+no=n+hco                3.00e+13      .000          .00 !GRI-Mech2.11
ch2+no=h+hnco              3.10e+17    -1.380      1270.00 !GRI-Mech2.11
ch2+no=oh+hcn              2.90e+14     -.690       760.00 !GRI-Mech2.11
ch2+no=h+hcno              3.80e+13     -.360       580.00 !GRI-Mech2.11
ch2(s)+no=h+hnco           3.10e+17    -1.380      1270.00 !GRI-Mech2.11
ch2(s)+no=oh+hcn           2.90e+14     -.690       760.00 !GRI-Mech2.11
ch2(s)+no=h+hcno           3.80e+13     -.360       580.00 !GRI-Mech2.11
ch3+no=hcn+h2o             9.60e+13      .000     28800.00 !GRI-Mech2.11
ch3+no=h2cn+oh             1.00e+12      .000     21750.00 !GRI-Mech2.11
hcnn+o=co+h+n2             2.20e+13      .000          .00 !GRI-Mech2.11
hcnn+o=hcn+no              2.00e+12      .000          .00 !GRI-Mech2.11
hcnn+o2=o+hco+n2           1.20e+13      .000          .00 !GRI-Mech2.11
hcnn+oh=h+hco+n2           1.20e+13      .000          .00 !GRI-Mech2.11
hcnn+h=ch2+n2              1.00e+14      .000          .00 !GRI-Mech2.11
hnco+o=nh+co2              9.80e+07     1.410      8500.00 !GRI-Mech2.11
hnco+o=hno+co              1.50e+08     1.570     44000.00 !GRI-Mech2.11
hnco+o=nco+oh              2.20e+06     2.110     11400.00 !GRI-Mech2.11
hnco+h=nh2+co              2.25e+07     1.700      3800.00 !GRI-Mech2.11
hnco+h=h2+nco              1.05e+05     2.500     13300.00 !GRI-Mech2.11
hnco+oh=nco+h2o            4.65e+12      .000      6850.00 !GRI-Mech2.11
hnco+oh=nh2+co2            1.55e+12      .000      6850.00 !GRI-Mech2.11
hnco+m=nh+co+m             1.18e+16      .000     84720.00 !GRI-Mech2.11
h2/2.00/ h2o/6.00/ ch4/2.00/ co/1.50/ co2/2.00/ c2h6/3.00/ ar/ .70/
hcno+h=h+hnco              2.10e+15     -.690      2850.00 !GRI-Mech2.11
hcno+h=oh+hcn              2.70e+11      .180      2120.00 !GRI-Mech2.11
hcno+h=nh2+co              1.70e+14     -.750      2890.00 !GRI-Mech2.11
hocn+h=h+hnco              2.00e+07     2.000      2000.00 !GRI-Mech2.11
hcco+no=hcno+co            2.35e+13      .000         0.00 !GRI-Mech2.11
ch3+n=h2cn+h               6.10e+14     -.310       290.00 !GRI-Mech2.11
ch3+n=hcn+h2               3.70e+12      .150       -90.00 !GRI-Mech2.11
nh3+h=nh2+h2               5.40e+05     2.400      9915.00 !GRI-Mech2.11
nh3+oh=nh2+h2o             5.00e+07     1.600       955.00 !GRI-Mech2.11
nh3+o=nh2+oh               9.40e+06     1.940      6460.00 !GRI-Mech2.11
ch3no2(+m)=ch3+no2(+m) 1.78E+16      0.0       58500.0 !Glaenzer 1972
low /1.26E+17 0.0 42000./
ch3no2+oh=ch2o+no+h2o  3.00E+6       2.0        2000.0 !This Study
ch3no2+o=ch2o+no+oh    1.51E+13      0.0        5354.0 !Salter 1977
ch3no2+h=ch2o+no+h2    4.67E+12      0.0        3732.0 !Ko 1991
ch3no2+ch3=ch2o+no+ch4 7.08E+11      0.0       11140.0 !Ballod 1980
ac3h5+no2=c3h5no2      1.44E+50    -12.01      10260.0 !This Study
c3h5no2+oh=ch2chcho+no+h2o  2.08E+6 2.0         -298.0 !This Study
c3h5no2+h=ch2chcho+no+h2    1.15E+5 2.5         2492.0 !This Study
c3h5no2+ch3=ch2chcho+no+ch4 1.48E+0 3.5         5675.0 !This Study
hno2+h=no2+h2          2.40E+8       1.5        5087.0 !Dean 1997
hno2+o=no2+oh          1.70E+8       1.5        3020.0 !Dean 1997
hno2+oh=no2+h2o        1.20E+6       2.0        -596.0 !Dean 1997
hno2+ch3=no2+ch4       8.10E+5       1.87       4838.0 !Dean 1997
hno2=hono              1.30E+29     -5.47      52814.0 !Dean 1997
hono+ch3=no2+ch4       8.10E+5       1.87       5504.0 !Dean 1997
hono+oh=no2+h2o        1.26E+10      1.0         135.0 !Dean 1997
hono+o=no2+oh          1.21E+13      0.0        5962.0 !Dean 1997
hono+h=no2+h2          1.21E+13      0.0        7353.0 !Dean 1997
hono+hono=no+no2+h2o   1.02E+13      0.0        8540.0 !England 1975
no+oh(+m)=hono(+m)     2.00E+13      0.0           0.0 !Forster 1995
low /2.33E+23 -2.4 0.0/
oh+no2(+m)=hono2(+m)   2.40E+13      0.0           0.0 !Tsang 1991
low / 6.42E+32 -5.49 2351./
troe/0.525 1.0E-15 1.0E-15 1.0E+15/
h2o /5.0/
hono2+oh=no3+h2o                1.03E+10  0.0    -1240.0 !Lamb 1984
no3=no+o2                       2.50E+6   0.0    12122.0 !Johnston 1986
no2+o+m=no3+m                   2.94E+21 -2.0        0.0 !Atkinson 1989
no2+no2=no3+no                  9.60E+9   0.73   20923.0 !Tsang 1991
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dup
no2+no2=no3+no                  1.60E+12   0.0   26123.0 !Tsang 1991
dup
ch3o+no(+m)=ch3ono(+m)          1.21E+13   0.0    -322.0 !Atkinson 1992
low / 2.70E+27 -3.50 0.0/
ch3o2+no=ch3o+no2               2.53E+12   0.0    -358.0 !Atkinson 1992
c2h5o2+no=ch3ch2o+no2           2.53E+12   0.0    -358.0 !This Study
hoc2h4o2+no=ch2oh+ch2o+no2      2.53E+12   0.0    -358.0 !This Study
ac3h5o2+no=ch2chch2o+no2        2.53E+12   0.0    -358.0 !This Study
hoc3h6o2+no=ch2oh+ch3hco+no2    2.53E+12   0.0    -358.0 !This Study
hoc3h4o3+no=chocho+ch2oh+no2    2.53E+12   0.0    -358.0 !This Study
cccoo+no=cccoj+no2              2.11E+12   0.0    -358.0
c2coo+no=c2coj+no2              2.11E+12   0.0    -358.0
ch3o+no=ch2o+hno                6.00E+13  -0.6       0.0 !Frost 1990
ch3ch2o+no=ch3hco+hno           4.00E+13  -0.6       0.0 !This Study
ch2chch2o+no=ch2chcho+hno       4.00E+13  -0.6       0.0 !This Study
cccoj+no=cccho+hno              4.00E+13  -0.6       0.0 !This Study
ch3+no(+m)=ch3no(+m)            2.17E+11   0.6       0.0 !Jodkowski 1993
low /2.06E+27  -3.50 0.0/
co+no2=co2+no                   9.04E+13   0.0   33782.0 !Tsang 1991
ch3+no2=ch3o+no                 1.50E+13   0.0       0.0 !Yamada 1981
ch3o+no2(+m)=ch3ono2(+m)        1.20E+13   0.0       0.0 !Atkinson 1992
low / 1.40E+30 -4.50 0.0/
c2h5+no2=ch3ch2o+no             2.70E+13   0.0       0.0 !Park 1983
ch2hco+no2=ch2o+hco+no          1.00E+13   0.0       0.0 !Barnhard 1991
ac3h5+no2=ch2chch2o+no          2.30E+13   0.0       0.0 !Slagle 1981
c6h9+no2=ch2chcho+ac3h5+no      2.00E+13   0.0       0.0 !This Study
no2+ho2=hono+o2                 6.31E+08   1.25   5000.0 !This Study
ch3o+no2=ch2o+hono              4.00E+12   0.0    2285.0 !McCaulley 1985
ch3ch2o+no2=ch3hco+hono         2.70E+12   0.0     105.0 !This Study
ch2chch2o+no2=ch2chcho+hono     2.70E+12   0.0     105.0 !This Study
c2coj+no2=acetone+hono          2.70E+12   0.0     105.0 !This Study
cccoj+no2=cccho+hono            2.70E+12   0.0     105.0 !This Study
end
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