ARL-TR-9536 ● AUG 2022

DEVCOM ARMY RESEARCH LABORATORY

A Detailed, Finite-Rate Chemical Kinetic Mechanism for Modeling the Thermal Decomposition and Combustion of Gaseous Nitroglycerin

by Chiung-Chu Chen and Michael J McQuaid

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REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*	2. REPORT TYPE	3. DATES COVERED (From - To)
August 2022	Technical Report	October 2021–July 2022

4. TITLE AND SUBTITLE
A Detailed, Finite-Rate Chemical Kinetic Mechanism for Modeling the Thermal Decomposition and Combustion of Gaseous Nitroglycerin

5a. CONTRACT NUMBER

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)
Chiung-Chu Chen and Michael J McQuaid

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
DEVCOM Army Research Laboratory
ATTN: FCDD-RLW-WC
Aberdeen Proving Ground, MD 21005

8. PERFORMING ORGANIZATION REPORT NUMBER
ARL-TR-9536

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release: distribution unlimited.

13. SUPPLEMENTARY NOTES
ORCID ID: Michael McQuaid, 0000-0001-5523-7468

14. ABSTRACT
As a step toward developing a state-of-the-art capability for modeling the decomposition and combustion of minimum-smoke rocket propellants and double-base gun propellants, a detailed, finite-rate chemical kinetics mechanism for modeling the thermal decomposition of gaseous nitroglycerin (NG_g) was developed and evaluated. Quantum mechanics-based electronic structure methods (QM-ESMs) were employed to characterize the molecular structures of stationary points of minimum energy paths for a network of elementary reactions capable of reducing the parent to small molecules. Thermodynamic properties for the stationary points were derived from the QM-ESM data, and the thermodynamic properties were employed to parameterize formulae for computing rate coefficients for elementary reactions. Those formulae were combined with a previously developed submechanism for modeling the small-molecule reaction chemistry common in the combustion of organic nitrate esters. The integration produced a mechanism comprising 1591 reactions and 229 species that is expected to be suitable for modeling NG's decomposition and combustion over wide ranges of temperature and pressure. To evaluate its validity for conditions of interest, it was integrated with models to simulate NG's deflagration as a function of pressure and its gas-phase decomposition from 150 to 160 °C. Reasonable agreement with measured data was observed. Anticipating the mechanism's use for other applications, we provide all its parameters for computing reaction-rate coefficients and species thermodynamic properties.

15. SUBJECT TERMS
Weapons Sciences, energetic materials, thermochemical kinetics, deflagration, decomposition

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Michael J McQuaid
Unclassified	Unclassified	Unclassified	UU	144	19b. TELEPHONE NUMBER (Include area code) (410) 278-6185

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Acknowledgments

Dating back to 2010, various DEVCOM ARL mission programs have been leveraged to develop the mechanism summarized herein, with the most recent being Reactive Multiscale Modeling for Energetic Materials. We are grateful to DEVCOM ARL management for their long support of mechanism development. The vast majority of the computing resources expended for the effort were provided by the DOD High Performance Computing Modernization Program.

1. Introduction

The widespread use of nitroglycerin (NG, $C_3H_5N_3O_9$) as an ingredient in propellant and explosive formulations has motivated numerous studies of its properties, decomposition, and combustion. A SciFinder search prompted by ($C_3H_5N_3O_9$ *and* combustion) yielded 745 citations, and that number does not include DOD- or Department of Energy-laboratory technical reports, Joint Army Navy NASA Air Force papers, or classified foreign research. The actual number notwithstanding, to our knowledge, a detailed, finite-rate chemical kinetics mechanism we began to build in the early 2010s was the first (and may still be the only) mechanism for modeling the decomposition and combustion of gaseous NG (NG_g) that reduces the parent to small molecules via a network of elementary covalent bond-breaking and/or formation reactions.

Lacking such a mechanism, models of phenomena in which the rate and products of NG's thermal decomposition play an important role have employed an empirically based pyrolysis law that converts NG irreversibly into a prescribed set of small molecules (Miller and Anderson 2000, 2004; Puduppakkam and Beckstead 2005; Beckstead et al. 2007). In models of phenomena in which thermal loads are relatively high, such as at the burning surface of a minimum-smoke rocket propellant or double-base gun propellant (Miller and Anderson 2004), this approach has merit and yielded insights. However, there is strong evidence that NG's condensed phase-to-gas phase conversion process is (reversible) evaporation of the parent molecule, not (irreversible) decomposition (Zeldovich 1942). Thus, such models have little potential to elucidate dynamics-controlling processes near the surface that might guide a propellant formulator interested in suppressing or increasing a burning rate. And the potential for such models to provide insight into phenomena associated lower thermal loads, such as cook-off scenarios, is even less because the decomposition of NG is slower and the products are less predictable.

Seeking to develop and apply a physics-based model for simulating the deflagration of nitrate ester-based propellant grains embedded with metal wires (Ritter and Demko 2016) and recognizing the limitations of then existing mechanisms for modeling NG's decomposition, we began in 2010 to develop a mechanism that could reduce the parent to small molecules via a network of elementary covalent bond-breaking and/or formation reactions. The starting point was a mechanism we had created to model the combustion of ethyl nitrate (Chen and McQuaid 2013). Its formulae for computing the rate coefficients of reactions involving the parent molecule ($CH_3CH_2ONO_2$) were parameterized based on minimum (electronic) energy path (MEP) characterizations produced with high-level quantum mechanics-based electronic structure methods (QM-ESMs) and the application of

statistical mechanics and transition state (TS) theories. As such, they were considered a reasonable basis for parameterizing formulae for computing the rates of analogous reactions with the potential to promulgate NG's decomposition. Coupled with a submechanism that would enable combustion to go to completion/equilibrium (Anderson et al. 2010) and incorporated into a 1-D, two-phase (CYCLOPS) model for simulating NG's steady laminar deflagration (Miller and Anderson 2000, 2004), the mechanism developed on that basis produced burning rates for NG at pressures from 1 to 13 MPa that were in good agreement with measured values (Chen et al. 2019).

Despite that success, for a subsequent investigation of liquid NG's decomposition that was undertaken to evaluate an approach we had proposed for modeling condensed-phase chemical kinetics (McQuaid et al. 2021), we wanted the mechanism to comprise formulae for computing the rates of the network's reactions that were as well founded as we could afford. Therefore, we directly applied QM-ESMs to obtain predictions for the molecular structures and thermodynamic properties of stationary points of the MEPs for reactions involving NG and other large molecules, and those data were employed to parameterize formulae for computing the reactions' rate coefficients.

Integrated with the starting mechanism, the newly developed formulae produced a network comprising 1591 reactions and 229 species that was expected to be suitable for modeling NG's decomposition and combustion over wide ranges of temperature and pressure. To evaluate its validity for conditions of interest, it was integrated with models to simulate NG's deflagration as a function of pressure and its gas-phase decomposition at temperatures from 150 to 160 °C. Comparisons with measured data are presented and discussed. Establishing a benchmark, we provide for reference all the coefficients of its formulae for computing reaction rate coefficients and species thermodynamic properties.

2. Computational Methods

2.1 Minimum Energy Path Characterizations

Various QM-ESMs were employed to obtain predictions for the molecular structures and relative energies of MEP stationary points. All were implemented with Gaussian 16 (Frisch et al. 2016*). The molecular geometries and normal modes of stationary points were obtained from results produced by models based

*For the origins and specifics of QM-ESMs for which citations are not provided, the interested reader should consult Frisch et al. (2016).

on density functional theory (DFT). They included B3LYP/6-31G(d,p), MPWB1K/6-31+G(d,p) (Zhao and Truhlar 2004), and M06-2X/6-31G(d,p) (Zhao and Truhlar 2008). Hereafter, those models are referred to as B3DP, B1K, and M06, respectively. For structures with di-radical character, the highest occupied molecular orbital and lowest unoccupied molecular orbital were mixed to properly account for it. We confirmed that MEP local minima had no normal modes with an imaginary frequency, and that TS structures had one and only one such mode. Intrinsic reaction coordinate calculations were performed to confirm the identities of the reactant(s) and product(s) connected by a TS.

As many as six different "high-level" QM-ESMs were employed to obtain estimates for the relative energies of the stationary points of MEPs with a "classic" TS/saddle point. They included CBS-QB3, G3MP2B3, G4, G3(MP2)//B3LYP/6-31G(d,p), G3(MP2)//MPWB1K/6-31+G(d,p), and G3(MP2)//M06-2X/6-31G(d,p). Hereafter, the latter three are referred to as G3MP2//B3DP, G3MP2//B1K, and G3MP2//M06, respectively. A QCISD(T)/6-31G(d)//B3LYP/6-311+G(d,p) model was employed to map the (barrierless) MEP for nitrogen dioxide (NO_2) elimination from NG.

2.2 Thermochemical Properties and Reaction Rate Coefficients

Gas-phase enthalpies of formation at 298 K [$\Delta_f H_g^o(298)$] were derived from enthalpy-of-reaction [$\Delta H_r(298)$] predictions for (hypothetical) isodesmic reaction schemes. The schemes were designed such that all species except the species of interest had a "trusted" $\Delta_f H_g^o(298)$ value. For small molecules, the $\Delta_f H_g^o(298)$ values were derived from results produced by CBS-APNO, CBS-QB3, G3, and G4 models. The programs SMCPS (Sheng 2002) and ROTATOR (Lay et al. 1996) were employed to estimate species' entropies at 298 K [$S°(298)$] and their heat capacities from 300 to 1500 K [$c_p(T)$].

For MEPs with saddle points, reaction rate coefficients [k] were calculated as a function of temperature (T) per,

$$k(T) = \frac{k_b T}{h} exp\left(\frac{\Delta S^{\ddagger}(T)}{R}\right) exp\left(\frac{\Delta H^{\ddagger}(T)}{RT}\right), \quad (1)$$

where $\Delta S^{\ddagger}$ was the difference between the entropies of the reactant asymptote and the TS, $\Delta H^{\ddagger}$ was the difference between the enthalpy of the reactant asymptote and the TS's, k_B was Boltzmann's constant, h was Planck's constant, and R was the universal gas constant. $\Delta H^{\ddagger}(T)$ was calculated from the integral of $c_p(T)$ with respect to $\log(T)$ for temperatures from 300 to 2000 K. The Wigner formalism (Wigner 1932) and an asymmetric Eckart barrier for H-atom tunneling (Eckart 1930) were

used to calculate the tunneling factor for reactions involving the transfer of a hydrogen (H) atom. The $k(T)$ data produced by Eq. 1 for individual reactions (i) are represented in the mechanism by

$$k_i(T) = A_i' T^{n_i} exp\left(\frac{-E_{a,i}}{RT}\right), \quad (2)$$

where A_i', n_i, and $E_{a,i}$ are constants. The constants' values were obtained from a least-squares fit of Eq. 2 to the Eq. 1-calculated data.

For reactions in which the reactant(s) and product(s) were not separated by a saddle point, variational transition state theory (VTST) was employed to compute $k(T)$, viz.

$$k(T) = \frac{k_b T}{h} exp\left(\frac{-\Delta G^{\ddagger}(T)}{RT}\right), \quad (3)$$

where $\Delta G^{\ddagger}(T)$ was the difference between the path's Gibbs free energy maximum and the reactant asymptote's. A protocol developed by Da Silva and Bozzelli (2008) was employed to establish the maximum. Like the parameterizations of $k(T)$ for MEPs having a saddle point, the $k(T)$ data produced via Eq. 3 are represented in the mechanism by Eq. 2, with the values for A_i', n_i, and $E_{a,i}$ obtained from a least-squares fit.

To obtain $k(T)$ estimates for reactions involving chemically activated adducts, we applied multi-channel, multi-frequency, quantum Rice–Ramsperger–Kassel (QRRK) theory for $k(E)$ and master equation analysis for falloff and stabilization (Dean 1985; Dean et al. 1991; Chang et al. 2000). Based on those results, parameterizations of Eq. 2 were established for selected pressures from 0.001 to 2000 atm.

2.3 The NG Mechanism

All the thermochemical kinetics-related data composing the NG mechanism are listed in the Appendix. Included are listings of the species, elementary reactions, and coefficients for computing the reactions' $k(T)$ and the species' thermodynamic properties. A look-up table for establishing the molecular structures of the species is also provided.

2.4 Burning-Rate Calculations

The NG mechanism was integrated with a CYCLOPS model to calculate NG's linear burning rate (r_b) as function of pressure. The CYCLOPS framework is described in detail elsewhere (Miller and Anderson 2000, 2004). Briefly, it involves

solving steady laminar 1-D premixed flame problems and finding values for the mass flux ($\dot{m} = r_b \rho_l$, where ρ_l is the liquid's density) and temperature (T^0) at the inlet/surface ($x = 0$) such that two conditions are satisfied. One is the conservation of energy (flux) at the condensed-phase–gas-phase interface, viz.

$$\lambda_g \left(\frac{dT}{dx}\right)^{+0} = \dot{m} \sum_k^K (Y_k^{-0} h_k^{+0} - Y_k^{-\infty} h_k^{-\infty}), \quad (4)$$

where, for a mechanism comprising K gas-phase species, λ_g is the thermal conductivity of the gas at the surface, Y_k^{-0} are the mass fractions of the nascent gas-phase products (k) of the condensed phase's decomposition, h_k^{+0} are their enthalpies at T^0, $Y_k^{-\infty}$ are the mass fractions of the condensed-phase's ingredients, and $h_k^{-\infty}$ are their enthalpies at the condensed phase's (bulk) temperature ($T^{-\infty}$).

The other condition that had to be satisfied was a relationship between $\dot{m}$ and T^0. Two different formulations for the relationship were employed in this study. One was a Hertz–Langmuir–Knudson (HLK) relationship (Li et al. 1990; Miller 1997; Galwey and Brown 1999), viz.

$$\dot{m}_{NG} = (W_{NG}/2\pi R T^0)^{\frac{1}{2}} (P_{sat}^0 - X_{NG}^{+0} P), \quad (5)$$

where W_{NG} was NG's molecular weight, X_{NG}^{+0} was the mole fraction of NG_g on the gas-phase side of the interface, P was the system's pressure, and P_{sat}^0 was NG's saturated vapor pressure at T^0. To calculate P_{sat}^0, the model employed

$$P_{sat}^0 = A exp\left(-\frac{B}{T^0}\right), \quad (6)$$

where A and B were constants. The values of all the parameters employed for these formulae are shown in Table 1.

Table 1 Properties of NG employed to calculate burning rates

Property	Units	Value
W_{NG}.	g/mol	227.1
ρ_l	g/cc	1.59
$\Delta_f H_l(298)$	kcal/mol	–89.6
A	dynes/cm^2	2.846E14[a]; 1.023E12[b]
B	K	13195[a]; 8467.2[b]
A_s	g/cm^{2}s	1.8E3
E_s	cal/mol	9935

[a]McQuaid et al. 2021. [b]Tunnell and Tod 2016.

For comparison with prior CYCLOPS-based studies of NG's deflagration (Miller and Anderson 2000, 2004; Chen et al. 2019), we performed a second set of calculations in which the relationship between $\dot{m}$ and T^0 was dictated by a pyrolysis law (PL):

$$\dot{m}_{NG} = A_s exp\left(\frac{-E_s}{RT_0}\right) \tag{7}$$

where A_s and E_s were constants. As in the prior studies, the values specified for A_s (1.8×10^3 g/cm^2-s) and E_s (9935 cal/mol) followed from Zenin (1995), who found them to be representative for a wide range of nitrate ester–based propellants.

The computation of diffusion coefficients, viscosities, thermal conductivities, and thermal diffusion coefficients was based on estimates for the species' Lennard–Jones potential well depth, Lennard–Jones collision diameter, dipole moment, polarizability, and rotational relaxation collision number (Kee et al. 1986). For species for which these properties had not (to our knowledge) been previously established, we assumed (based on our experience) that first-order approximations would be adequate and employed for them values for a relatively small nonpolar molecule (namely CH_3CHO).

2.5 Homogeneous Reactor Model

As has been discussed previously (McQuaid et al. 2021), we developed and applied a homogeneous reactor (HR) model to simulate NG_g's decomposition at temperatures from 150 to 160 °C in a closed, constant-volume (V), constant-temperature reactor (Waring and Krastins 1970). The model's species' conservation equations were formulated in terms of species mass fractions (Y_k), viz.

$$\frac{dY_k}{dt} = \dot{\omega}_k W_k / \rho_g, \tag{8}$$

where $\dot{\omega}_k$ was the molar production rate of the k^{th} species, W_k was its molecular weight, and ρ_g was the gas's density. The relationship between ρ_g, P, V, and T was based on the ideal gas law. The system of equations was solved with DASPK (Li and Petzold 2000). To identify reactions (i) with the greatest impact on the global rate of NG's decomposition, normalized first-order sensitivity coefficients ($\widehat{\omega}_{NG,i}$) were computed per

$$\widehat{\omega}_{NG,i} = \frac{A_i'}{Y_{NG}} \frac{\delta Y_{NG}}{\delta A_i'}, \tag{9}$$

where A_i' was the pre-exponential factor of reaction i's rate coefficient.

3. Results

3.1 Enthalpy-of-Formation Estimates

The lowest energy conformer we found for NG is shown in Fig. 1. It was stabilized by a combination of (noncovalent) electrostatic attractions between nitrogen (N) atoms and terminal oxygen (O) atoms of neighboring nitroxy groups and (noncovalent) interactions between terminal O atoms and H atoms bonded to nearest neighbor carbon (C) atoms. The M06-based optimization of this conformer's geometry yielded N(1)—O(2), N(2)—O(3), and N(3)—O(1) separations that were 2.79, 4.71, and 4.17 Å, respectively. The O(1)—H(1), O(2)—H(2), and O(3)—H(3) separations were 2.35, 2.22, and 2.23 Å, respectively.

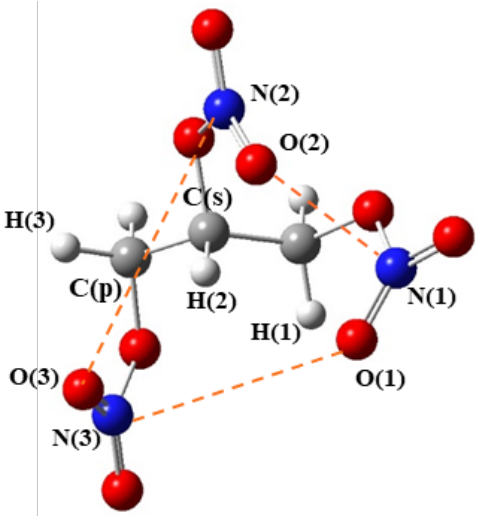


Fig. 1 The lowest energy conformer of NG

NG's $\Delta_f H_g^o(298)$ was calculated based on results produced for this conformer. Two different isodesmic reactions were formulated for that purpose. Listed in Table 2, estimates based on the results produced by high-level QM-ESMs ranged from –72.7 to –75.2 kcal/mol. (Estimates based on the results produced with the B3DP and B1K models were significantly higher, confirming the need to obtain single point electronic energies from results produced with higher-level models.) Combined with a measured value for NG's enthalpy of vaporization at 298 K (16.8 kcal/mol) (Tunnell and Tod 2016), these results produced $\Delta_f H_l^o(298)$ estimates ranging from –89.5 to –91.3 kcal/mol. The upper limit is nearly identical to the (–89.6 kcal/mol) value Handrick (1956) derived from a measured enthalpy of combustion.

Table 2 $\Delta_f H_g^o(298)$ **and** $\Delta_f H_l^o(298)$ **estimates (in kcal/mol) for NG based on** $\Delta H_r(298)$ **estimates for isodesmic reaction schemes**[a]

	CBS-QB3	G3MP2B3	G4	G3MP2//B3DP	G3MP2//B1K	G3MP2//M06	B3DP	B1K	M06	b
$O_2NOCH_2CH(ONO_2)CH_2ONO_2 + CH_3CH_2OH + 2\ C_2H_6 = 3\ CH_3CH_2ONO_2 + (CH_3)_2CHOH$										
$\Delta H_r(298)$	–7.5	–7.7	–8.3	–7.8	–7.6	–7.8	–9.4	–11.4	–7.8	. . .
$\Delta_f H_g^o(298)$	–75.2	–75.1	–74.4	–75.0	–75.1	–75.0	–73.4	–71.4	–75.0	–75.0[c]
$\Delta_f H_l^o(298)$	–92.0	–91.9	–91.2	–91.8	–91.9	–91.8	–90.2	–88.2	–91.8	–91.8
$O_2NOCH_2CH(ONO_2)CH_2ONO_2 + 4\ CH_4 = 3\ CH_3ONO_2 + 2\ C_2H_6$										
$\Delta H_r(298)$	16.5	16.9	16.2	15.9	16.7	17.3	9.9	9.8	15.0	. . .
$\Delta_f H_g^o(298)$	–73.4	–73.7	–73.1	–72.7	–73.6	–74.1	–66.7	–66.6	–71.8	–73.4
$\Delta_f H_l^o(298)$	–90.2	–90.1	–89.9	–89.5	–90.4	–90.9	–83.5	–83.4	–88.6	–90.2

[a] $\Delta_f H_g^o(298)$ values for reference compounds: CH_4 = –17.9 kcal/mol; C_2H_6 = –20.0 kcal/mol; CH_3CH_2OH = –56.2 kcal/mol; $(CH_3)_2CHOH$ = –65.5 kcal/mol; CH_3ONO_2 = –29.4 kcal/mol; $CH_3CH_2ONO_2$ = –37.9 kcal/mol. [b] Nominal value for the given isodesmic reaction. [c] Value employed for thermochemical property estimation.

Isodesmic reaction schemes were also formulated to obtain $\Delta_f H_g^o(298)$ estimates for other large molecules in the mechanism. Results are presented in Table 3. We could find no results in the open literature to which they could be compared. However, for each molecule, the estimates produced by the high-level models fell within a relatively narrow (±2 kcal/mol) range, indicating they were trustworthy.

Table 3 $\Delta_f H_g^o(298)$ **estimates (in kcal/mol) for large molecules in the mechanism**[a]

Species	CBS-QB3	G3MP2B3	G4	G3MP2//B3DP	G3MP2//B1K	G3MP2//M06	b
$O_2NOCH_2CH(ONO_2)CH_2O\bullet$ [CACACOJ]	–46.8	–43.5	–44.5	–43.1	–44.5	–44.8	–44.1
$O_2NOCH_2CH(ONO_2)CHO$ [CACACDO]	–76.2	–76.1	–75.5	–75.4	–75.6	–76.2	–75.9
$O_2NOC\bullet HCH(ONO_2)CH_2OH$ [CJACACOH]	. . .	. . .	. . .	. . .	–49.0	–50.2	–49.6
$OCHCH(ONO_2)CH_2OH$ [CDOCACOH]	–96.4	–96.0	–95.6	–95.3	–95.0	–95.8	–95.8
$O_2NOCH_2C\bullet HONO_2$ [ACCJA]	. . .	. . .	. . .	–4.8	–4.9	–4.9	–4.9
$(CH_2ONO_2)_2CHO\bullet$ [DICACOJ]	–45.7	–42.5	–43.7	–42.7	–43.3	–43.2	–43.1
$(CH_2ONO_2)_2CO$ [DICACDO]	–77.6	–79.1	–78.0	–77.6	–77.0	–78.4	–78.1
$HCOCH_2ONO_2$ [HCOCONO2]	–52.4	–52.3	–52.3	–51.7	–51.6	–52.3	–52.1

[a] The isodesmic reactions employed were $\mathbf{O_2NOCH_2CH(ONO_2)CH_2O\bullet}$ + 2 C_2H_6 = $(CH_3)_2CHONO_2$ + $CH_3CH_2ONO_2$ + $CH_3CH_2O\bullet$; $\mathbf{O_2NOCH_2CH(ONO_2)CHO}$ + 2 C_2H_6 = $(CH_3)_2CHONO_2$ + $CH_3CH_2ONO_2$ + CH_3CHO; $\mathbf{O_2NOC\bullet HCH(ONO_2)CH_2OH}$ + 2 C_2H_6 = $(CH_3)_2CHONO_2$ + $CH_3CH_2ONO_2$ + $CH_3CH_2O\bullet$**;** $\mathbf{CHOCONO_2COH}$ + 2 C_2H_6 = CH_3CHO + CH3CH2OH + $(CH_3)_2CHONO_2$; $\mathbf{O_2NOCH_2C\bullet HONO_2}$ + 2 C_2H_6 = C_2H_5 + 2 $CH_3CH_2ONO_2$; $\mathbf{(CH_2ONO_2)_2CHO\bullet}$ + 2 C_2H_6 = $(CH_3)_2CHO$ + 2 $CH_3CH_2ONO_2$; $\mathbf{(CH_2ONO_2)_2CO}$ + 2 C_2H_6 = $(CH_3)_2CHO$ + 2 $CH_3CH_2ONO_2$; $\mathbf{OCHCH_2ONO_2}$ + C_2H_6 = $CH_3CH_2ONO_2$ + CH_3CHO. $\Delta_f H_g^o(298)$ for reference compounds: CH_3CH_3 = –20.0 kcal/mol; CH_3CH_2 = 28.0 kcal/mol; CH_3CHO = –39.7 kcal/mol; CH_3CH_2OH = –56.2 kcal/mol; $CH_3CH_2O\bullet$ = –4.2 kcal/mol; $(CH_3)_2CHO$ = –51.96 kcal/mol; $CH_3CH_2ONO_2$ = 37.9 kcal/mol; $(CH_3)_2CHONO_2$ = –46.8 kcal/mol. [b] Value employed for thermochemical property estimation.

3.2 Bond Dissociation Energy Estimates

Estimates for the bond dissociation energies (BDEs) of NG's C–C, C–H, C–O, and O–N (single) bonds are presented in Table 4. The BDE estimates for the C–C bonds (87.5 kcal/mol) were found to be 1–2 kcal/mol lower than the BDEs of C–C bonds in saturated aliphatic hydrocarbons. BDEs for C–H bonds associated with primary [C(p)] and secondary [C(s)] C atoms were 98.0 and 96.7 kcal/mol, respectively. Those values are 2–3 kcal/mol higher than BDEs for analogous C–H bonds in alkyl ethers. The BDE estimates for breaking C(p)–ONO_2 bonds and C(s)–ONO_2 bonds were 80.4 and 79.4 kcal/mol, respectively.

Table 4 BDE estimates

Bond type	BDE (kcal/mol)
C–C bonds	
O_2NOCH_2–$CH(ONO_2)CH_2ONO_2$	87.5
CH_3–CH_3	89.7
CH_3CH_2–CH_3	88.6
C–H bonds	
O_2NOCH(–H)$CH(ONO_2)CH_2ONO_2$	98.0
O_2NOCH_2C–$H(ONO_2)CH_2ONO_2$	96.7
CH_3CH(–H)OCH_3	96.0
$(CH_3)_2C$(–H)OCH_3	94.0
C–O bonds	
O_2NO–$CH(CH_2ONO_2)_2$	79.4
$O_2NOCH_2CH(ONO_2)CH_2$–ONO_2	80.4
O–N bonds	
$O_2NOCH_2CH(ONO_2)CH_2O$–NO_2	38.9
$O_2NOCH_2CH(O$–$NO_2)CH_2ONO_2$	39.9

Table 5 compares BDE estimates for breaking C(p)O–NO_2 and/or C(s)O–NO_2 bonds in ethyl nitrate, isopropyl nitrate, ethylene glycol dinitrate (EGDN), propylene glycol dinitrate (PGDN), and NG. The BDEs for NG's O–NO_2 bonds were non-negligibly lower than those of the analogous bonds in the smaller nitrate esters, validating our decision to compute them directly. The BDE of NG's C(s)O–NO_2 bond was higher than the BDE of its C(p)O–NO_2 bonds, because the electrostatic attractions between N atoms and O atoms of neighboring nitroxy groups were greater in the case of the secondary nitroxy group.

Table 5 BDE estimates (in kcal/mol) for C(p)O–NO_2 and C(s)O–NO_2 bonds in various nitrate esters

Bond type	CBS -QB3	G3MP2 B3	G4	G3MP2 //B3DP	G3MP2 //B1K	G3MP2 //M06	a
C(p)O–NO_2							
$CH_3CH_2ONO_2$	42.3	39.8	40.2	40.4	40.5	41.4	41.5
$O_2NOCH_2CH_2ONO_2$	40.6	39.6	39.4	40.1	39.2	40.3	40.6
$CH_3CH(ONO_2)CH_2ONO_2$	40.3	39.3	38.8	39.8	40.0	40.2	40.5
$O_2NOCH_2CH(ONO_2)CH_2ONO_2$	37.5	38.1	36.9	38.5	37.4	38.5	38.9
C(s)O–NO_2							
$CH_3CH(ONO_2)CH_3$	44.1	41.6	41.7	42.2	41.5	42.5	43.4
$CH_3CH(ONO_2)CH_2ONO_2$	41.5	40.4	40.1	41.0	41.1	41.2	41.7
$O_2NOCH_2CH(ONO_2)CH_2ONO_2$	38.0	38.7	37.6	39.1	37.8	38.9	39.9

[a] Value employed for thermochemical property estimation.

3.3 MEP Characterizations for Reactions on the $C_3H_5N_3O_9$ Potential Energy Surface

Table 6 lists all the reactions on the $C_3H_5N_3O_9$ potential energy surface for which MEPs were characterized. For paths with saddle points, as many as six different high-level QM-ESMs were employed to obtain relative zero-point corrected energies for their stationary points. Figure 2 provides an overview of the structures and relative energies of stationary points of MEPs for reactions following the breaking of a C(p)O–NO_2 bond. Figure 3 does the same for reactions following the breaking of the C(s)O–NO_2 bond. Tables 7 and 8 list the relative energies of all the local minima in the figures on a QM-ESM-by-QM-ESM basis. Based on those results, "nominal" values were selected for estimating the species' thermochemical properties. The tables also list them.

Table 9 lists the relative energies of all the transition states in Figs. 2 and 3. The consistency of the results produced by different models for each stationary point suggests their reliability. The subsections that follow discuss noteworthy results.

Table 6 Reactions on the $C_3H_5N_3O_9$ potential energy surface

R1	NG ↔ $O_2NOCH_2CH(ONO_2)CH_2O$• [CACACOJ] + NO_2
R2	NG ↔ $(CH_2ONO_2)_2CHO$• [DICACOJ] + NO_2
R3	NG ↔ $O_2NOCH_2CH(ONO_2)CHO$ [CACACDO] + *trans*-HONO (via TSR3)
R4	NG ↔ $(CH_2ONO_2)_2CO$ [DICACDO] + *trans*-HONO (via TSR4)
R5	$O_2NOCH_2CH(ONO_2)CH_2O$• ↔ O_2NOC•$HCH(ONO_2)CH_2OH$ (via TSR5) [CACACOJ ↔ CJACACOH]
R6	O_2NOC•$HCH(ONO_2)CH_2OH$ ↔ $OCHCH(ONO_2)CH_2OH$ + NO_2 (via TSR6) [CJACACOH ↔ CDOCACOH + NO_2]
R7	$O_2NOCH_2CH(ONO_2)CH_2O$• ↔ $O_2NOCH_2CH(ONO_2)CHO$ + H (via TSR7) [CACACOJ ↔ CACACDO + H]
R8	$O_2NOCH_2CH(ONO_2)CH_2O$• ↔ O_2NOCH_2C•$HONO_2$ + CH_2O (via TSR8) [CACACOJ ↔ ACCJA + CH_2O]
R9	O_2NOCH_2C•$HONO_2$ ↔ $HCOCH_2ONO_2$ + NO_2 (via TSR9) [ACCJA ↔ HCOCONO2 + NO_2]
R10	$O_2NOCH_2CH(ONO_2)CH_2O$• + NO_2 ↔ $O_2NOCH_2CH(ONO_2)CH_2OONO$ (via TSR10) [CACACOJ + NO_2 ↔ CACACOONO]
R11	$O_2NOCH_2CH(ONO_2)CH_2OONO$ ↔ $O_2NOCH_2CH(ONO_2)CH_2OO$• + NO (via TSR11) [CACACOONO ↔ CACACQJ + NO]
R12	$O_2NOCH_2CH(ONO_2)CH_2OONO$ ↔ $O_2NOCH_2CH(ONO_2)CHO$ + HNO (via TSR12) [CACACOONO ↔ CACACDO + HNO]
R13	$O_2NOCH_2CH(ONO_2)CH_2O$• + NO_2 ↔ $O_2NOCH_2CH(ONO_2)CHO$ + *cis*-HONO (via TSR13) [CACACOJ ↔ CACACDO + *cis*-HONO]
R14	$O_2NOCH_2CH(ONO_2)CH_2O$• + NO_2 ↔ $O_2NOCH_2CH(ONO_2)CHO$ + HNO_2 (via TSR14) [CACACOJ ↔ CACACDO + HNO_2]
R15	$(CH_2ONO_2)_2CHO$• + NO_2 ↔ $(CH_2ONO_2)_2CHOONO$ (via TSR15) [DICACOJ + NO_2 ↔ DICACOONO]
R16	$(CH_2ONO_2)_2CHOONO$ ↔ $(CH_2ONO_2)_2CHOO$• + NO (via TSR16) [DICACOONO ↔ DICACQJ+ NO]
R17	$(CH_2ONO_2)_2CHOONO$ ↔ $(CH_2ONO_2)_2CO$ + HNO_2 (via TSR17) [DICACOONO ↔ DICACDO + HNO_2]
R18	$(CH_2ONO_2)_2CHO$• + NO_2 ↔ $(CH_2ONO_2)_2CO$ + *cis*-HONO (TSR18) [DICACOJ + NO_2 ↔ DICACDO + *cis*-HONO]
R19	$(CH_2ONO_2)_2CHO$• + NO_2 ↔ $(CH_2ONO_2)_2CO$ + HNO_2 (TSR19) [DICACOJ + NO_2 ↔ DICACDO + HNO_2]
R20	$(CH_2ONO_2)_2CHO$• ↔ $HCOCH_2ONO_2$ + CH_2O + NO_2 (via TSR20) [DICACOJ ↔ HCOCONO2 + CH_2O + NO_2]
R21	$(CH_2ONO_2)_2CHO$• ↔ $(CH_2ONO_2)_2CO$ + H (via TSR21) [DICACOJ ↔ DICACDO + H]

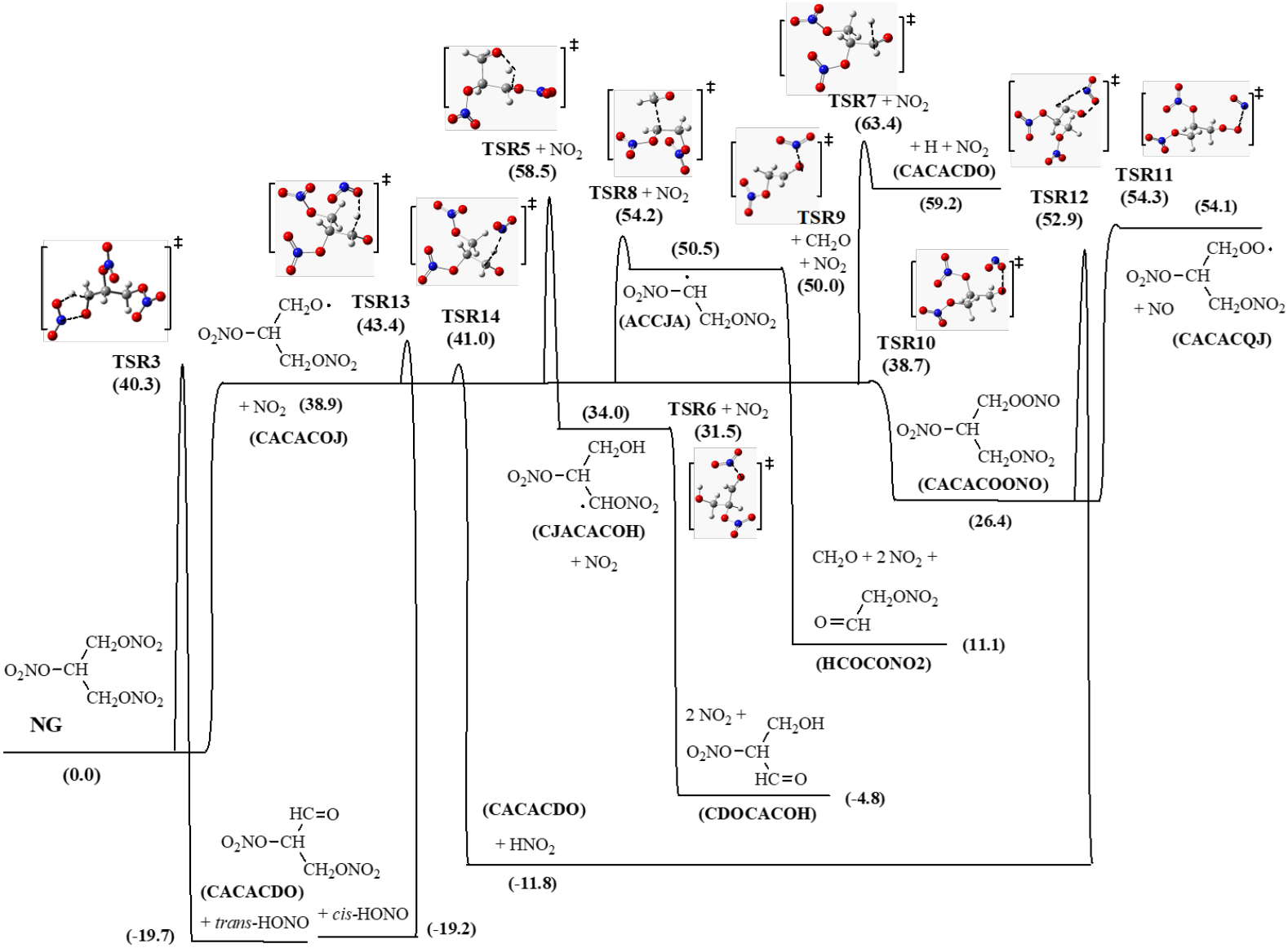


Fig. 2 MEPs for breaking one of NG's C(p)O–NO_2 bonds and unimolecular dissociations that can follow (energy units: kcal/mol)

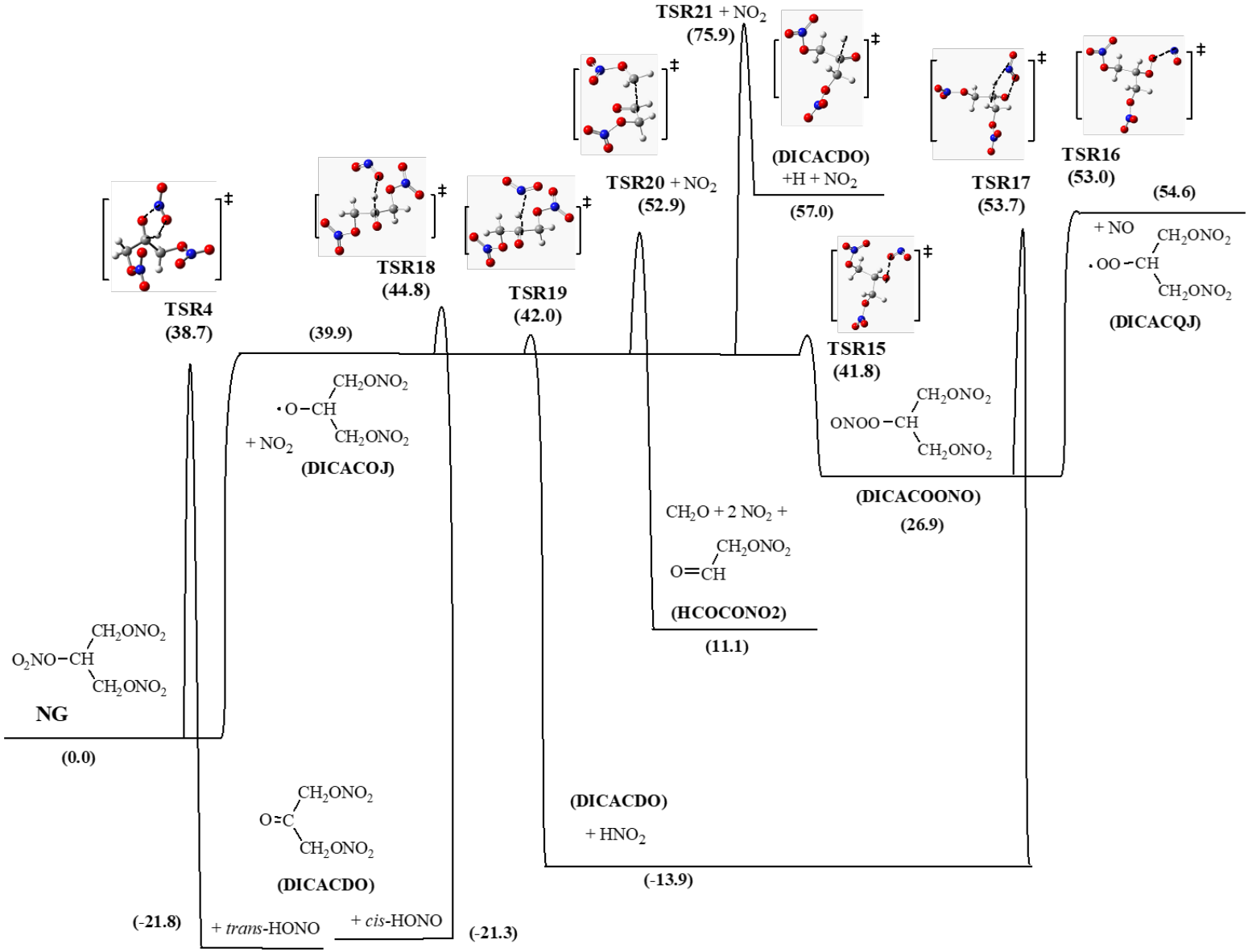


Fig. 3 MEPs for breaking NG's C(s)O–NO_2 bond and unimolecular dissociations that can follow (energy units: kcal/mol)

Table 7 Relative zero-point corrected energies (in kcal/mol) for local minima in Fig. 2

Local minimum	CBS -QB3	G3MP2 B3	G4	G3MP2 //B3DP	G3MP2 //B1K	G3MP2 //M06	a
NG	0.0	0.0	0.0	0.0	0.0	0.0	0.0
$O_2NOCH_2CH(ONO_2)CH_2O\bullet + NO_2$ [CACACOJ + NO_2]	37.5	38.1	36.9	38.5	37.4	38.5	38.9
$O_2NOCH_2CH(ONO_2)CHO$ + *trans*-HONO [CACACDO + *trans*-HONO]	–18.7	–21.0	–19.9	–20.3	–20.3	–20.2	–19.7
$O_2NOCH_2CH(ONO_2)CHO$ + *cis*-HONO [CACACDO+ *cis*-HONO]	–18.4	–20.4	–19.3	–20.2	–20.4	–19.6	–19.2
$O_2NOCH_2CH(ONO_2)CHO + HNO_2$ [CACACDO+ HNO_2]	–10.9	–12.2	–12.0	–11.5	–12.0	–11.5	–11.8
$O_2NOC\bullet HCH(ONO_2)CH_2OH + NO_2$ [CJACACOH + NO_2]	. . .	. . .	. . .	. . .	32.9	33.1	34.0
$OCHCH(ONO_2)CH_2OH + 2NO_2$ [CDOCACOH + $2NO_2$]	–4.7	. . .	–6.8	–6.9	–7.7	–5.8	–4.8
$O_2NOCH_2C\bullet HONO_2 + CH_2O + NO_2$ [ACCJA + CH_2O + NO_2]	. . .	. . .	. . .	48.7	48.0	49.9	50.5
$HCOCH_2ONO_2 + CH_2O + 2NO_2$ [HCOCONO2 + CH_2O + $2NO_2$]	11.0	6.8	8.3	8.3	7.1	9.9	11.1
$O_2NOCH_2CH(ONO_2)CHO + H + NO_2$ [CACACDO + H + NO_2]	58.9	56.7	. . .	56.2	55.3	56.5	59.2
$O_2NOCH_2CH(ONO_2)CH_2OONO$ [CACACOONO]	27.6	26.9	27.8	26.9	27.5	27.4	26.4
$O_2NOCH_2CH(ONO_2)CH_2OO\bullet + NO$ [CACACQJ + NO]	59.4	52.4	59.8	52.9	50.9	51.6	54.1

[a] Value employed for thermochemical property estimation.

Table 8 Relative zero-point corrected energies (in kcal/mol) for local minima in Fig. 3

Local minimum	CBS-QB3	G3MP2-B3	G4	G3MP2 //B3DP	G3MP2 //B1K	G3MP2 //M06	a
NG	0.0	0.0	0.0	0.0	0.0	0.0	0.0
$(CH_2ONO_2)_2CHO\bullet + NO_2$ [DICACOJ + NO_2]	38.0	38.7	37.6	39.1	37.8	38.9	39.9
$(CH_2ONO_2)_2CO$ + *trans*-HONO [DICACDO + *trans*-HONO]	–21.4	–23.5	–22.9	–22.9	–22.6	–22.8	–21.8
$(CH_2ONO_2)_2CO$ + *cis*-HONO [DICACDO + *cis*-HONO]	–21.0	–22.9	–22.3	–22.8	–22.8	–22.3	–21.3
$(CH_2ONO_2)_2CO + HNO_2$ [DICACDO + HNO_2]	–13.5	–14.7	–15.0	–14.0	–14.4	–14.1	–13.9
$(CH_2ONO_2)_2CO + H + NO_2$ [DICACDO + H + NO_2]	56.3	54.2	54.6	53.6	53.0	53.9	57.0
$(CH_2ONO_2)_2CHOONO$ [DICACOONO]	28.3	27.4	. . .	27.4	28.2	28.0	26.9
$(CH_2ONO_2)_2CHOO\bullet + NO$ [DICACQJ + NO]	55.7	52.4	. . .	52.6	59.9	51.9	54.6

[a] Value employed for thermochemical property estimation.

Table 9 Relative zero-point corrected energies (in kcal/mol) for TSs in Figs. 2 and 3

Saddle point	CBS-QB3	G3MP2B3	G4	G3MP2 //B3DP	G3MP2 //B1K	G3MP2 //M06	a
TSR3	40.4	39.8	. . .	39.8	39.4	40.5	40.3
TSR4	38.6	38.1	. . .	38.0	37.8	38.5	38.7
TSR5 + NO_2	54.5	57.2	. . .	58.2	56.2	59.4	58.5
TSR6 + NO_2	. . .	. . .	. . .	. . .	29.3	30.7	31.5
TSR7 + NO_2	. . .	61.3	. . .	61.8	60.2	62.7	63.4
TSR8 + NO_2	54.1	63.9	51.4	52.8	51.6	52.8	54.2
TSR9 + CH_2O + NO_2	47.5	47.9	. . .	. . .	46.8	49.0	50.0
TSR10	. . .	. . .	. . .	40.8	36.9	38.3	38.7
TSR11	. . .	. . .	. . .	. . .	53.9	52.9	54.3
TSR12	54.3	53.2	. . .	53.4	52.6	53.6	52.9
TSR13	. . .	. . .	. . .	45.1	44.0	44.1	43.4
TSR14	. . .	. . .	. . .	40.8	39.7	40.7	41.0
TSR15	. . .	. . .	. . .	43.7	39.3	41.8	41.8
TSR16	. . .	. . .	. . .	. . .	53.0	. . .	53.0
TSR17	54.8	53.8	. . .	54.0	53.3	54.1	53.7
TSR18	. . .	. . .	. . .	. . .	43.4	43.8	44.8
TSR19	. . .	. . .	. . .	41.6	40.8	41.8	42.0
TSR20 + NO_2	55.8	50.4	47.3	51.2	50.6	50.6	52.9
TSR21 + NO_2	71.3	75.5	. . .	73.2	70.3	76.2	75.9

[a] Value employed for thermochemical property estimation.

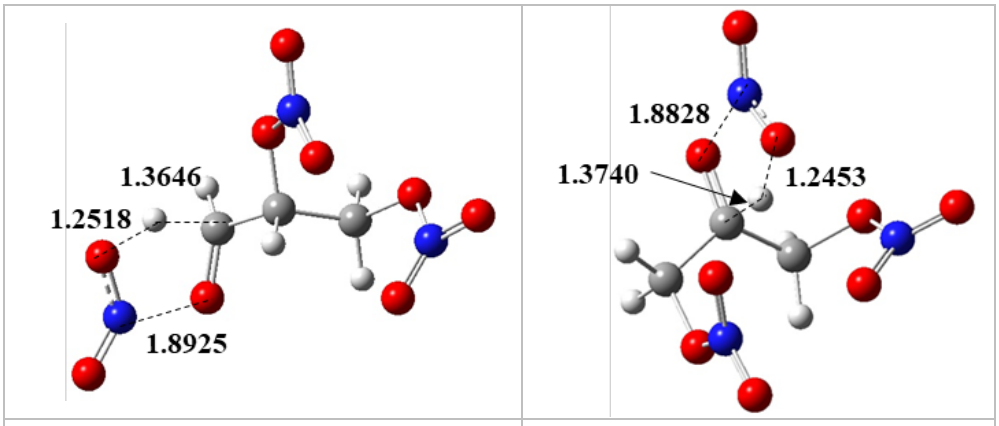
3.3.1 Unimolecular Decomposition of NG (R1–R4)

As discussed in Section 3.2, the BDEs of NG's RO–NO_2 bonds (R = C(p) or C(s)) were significantly lower than those of all its other bonds, indicating that the potential for any of the others to be an important first unimolecular step in NG's decomposition was negligible. Therefore, only MEPs for NO_2 loss (R1 and R2) and nitrous acid (HONO) elimination (R3 and R4) were characterized.

Like the MEPs for analogous reactions in smaller organic nitrate esters we have characterized, the DFT-based MEPs for R1 and R2 did not have a saddle point. As such, the derivation of $k_{R1/R2}(T)$ required that $\Delta G^{\ddagger}(T)$ be computed for a range of O–NO_2 bond lengths. Due to NG's size, the highest-level QM-ESM that could be afforded for single-point energy calculations was a QCISD(T)/6-31G(d)//B3LYP/ 6-311+G(d,p) model.

The geometries of the TSs for *trans*-HONO elimination (TSR3 and TSR4) are shown in Fig. 4. (The direct elimination of *cis*-HONO is prevented by the $-NO_2$ groups' orientations relative to the H atoms in the molecule.) Table 10 compares the relative energies of the barriers to *trans*-HONO elimination from NG and those

found for analogous reactions involving smaller organic nitrate esters (Chen et al. 2020). Nominally, TSR3 and TSR4 were, respectively, 40.3 and 38.7 kcal/mol higher in energy than the NG (reactant) asymptote, and R3 and R4 were, respectively, 19.7 and 21.8 kcal/mol exothermic. The TSs were 1.0 to 3.5 kcal/mol lower in energy than those for analogous reactions in ethyl nitrate, isopropyl nitrate, EGDN, and PGDN. From the standpoint of parameterizing $k_{R3}(T)$ and $k_{R4}(T)$, these differences are non-negligible, indicating the limitations of using results for smaller molecules for that purpose.



TSR3 TSR4

Fig. 4 TS structures for HONO elimination from NG: M06-based results (bond length unit: Å)

Table 10 Barriers (in kcal/mol) for *trans*-HONO elimination from various nitrate esters

Reaction	CBS-QB3	G3MP2-B3	G4	G3MP2//B3DP	G3MP2//B1K	G3MP2//M06	a
ethyl nitrate: $CH_3CH_2ONO_2 \leftrightarrow CH_3CHO$ + *trans*-HONO							
	42.3	41.4	42.1	42.0	41.7	42.2	42.2
EGDN: $O_2NOCH_2CH_2ONO_2 \leftrightarrow O_2NOCH_2CHO$ + *trans*-HONO							
	41.5	40.7	41.4	40.7	40.5	41.6	41.3
isopropyl nitrate: $CH_3CH(ONO_2)CH_3 \leftrightarrow CH_3C(O)CH_3$ + *trans*-HONO							
	41.5	40.8	41.4	41.4	41.1	41.6	41.8
PGDN: $CH_3CH(ONO_2)CH_2ONO_2 \leftrightarrow CH_3CH(ONO_2)CHO$ + *trans*-HONO							
	41.8	41.0	41.8	41.0	41.7	41.8	41.8
PGDN: $CH_3CH(ONO_2)CH_2ONO_2 \leftrightarrow CH_3C(O)CH_2ONO_2$ + *trans*-HONO							
	41.4	40.8	41.5	40.7	41.5	41.6	41.6
$O_2NOCH_2CH(ONO_2)CH_2ONO_2 \leftrightarrow O_2NOCH_2CH(ONO_2)CHO$ + *trans*-HONO (R3)							
	40.4	39.8		39.8	39.4	40.5	40.3
$O_2NOCH_2CH(ONO_2)CH_2ONO_2 \leftrightarrow O_2NOCH_2C(O)CH_2ONO_2$+ *trans*-HONO (R4)							
	38.6	38.1		38.0	37.8	38.5	38.7

[a] Value employed for thermochemical property estimation.

3.3.2 Unimolecular Decomposition of $O_2NOCH_2CH(ONO_2)CH_2O\bullet$ (R5–R9)

Three paths for the unimolecular decomposition of $O_2NOCH_2CH(ONO_2)CH_2O\bullet$ (CACACOJ) were postulated and characterized: 1) a 1,4 H-atom shift (R5 via TSR5), 2) a simple H-atom elimination (R7 via TSR7), and 3) a C–C bond scission (R8). Of these three steps, R8 had the lowest barrier (15.3 kcal/mol) and proved to have the largest $k(T)$ at high temperatures. Producing $O_2NOC\bullet H_2CH_2ONO_2$ (ACCJA), which via R9 could decompose to $CH_2O + 2NO_2 + OCHCH_2ONO_2$ with little to no barrier, the path initiated by R8 was 27.8 kcal/mol exothermic. R5, which had a 19.6-kcal/mol barrier and was 4.9 kcal/mol exothermic, proved to have the largest $k(T)$ at low temperatures. In addition, it produced $HOCH_2CH(ONO_2)C\bullet HONO_2$ (CJACACOH), which could decompose with little to no barrier via R6 to form $HOCH_2CH(ONO_2)CHO$ (CDOCACOH) + NO_2. This reaction was 38.8 kcal/mol exothermic. R7 had a relatively high barrier (24.5 kcal/mol) and its $k(T)$ was only significant at relatively high temperatures. However, its reverse direction (viz. H-atom addition to a carbonyl group) proved to be one of the most important reactions involving such moieties.

3.3.3 NO_2 Reacting with $O_2NOCH_2CH(ONO_2)CH_2O\bullet$ (R10–R14) or $(O_2NOCH_2)_2CHO\bullet$ (R15–R19)

Informed by our study of ethyl nitrate (Chen and McQuaid 2013), we characterized MEPs for the formation of the peroxynitrates (viz. $O_2NOCH_2CH(ONO_2)CH_2OONO$ via R10 and $(O_2NOCH_2)_2CHOONO$ via R15) and their unimolecular decomposition. The latter included 1) dissociation of the OO–NO bond, which produced a peroxide radical (viz. $O_2NOCH_2CH(ONO_2)$-$CH_2OO\bullet$ via R11 or $(O_2NOCH_2)_2CHOO\bullet$ via R16), and 2) abstraction of an H atom from the C atom adjacent to O•, which produced HNO_2 and an aldehyde (viz. $O_2NOCH_2CH(ONO_2)CHO$ via R12 or $(O_2NOCH_2)_2CO$ via R17).

As shown in Fig. 5, the TS structures for peroxynitrite formation (TSR10 and TSR15) were "loose," with the O–ONO bond distances being approximately 1.82 Å. R10 was approximately 12.5 kcal/mol exothermic and R15 was approximately 13.0 kcal/mol exothermic. The nominal value for TSR10's energy was slightly less than the $O_2NOCH_2CH(ONO_2)CH_2O\bullet$ + NO_2 asymptote's. TSR15's energy was approximately 0.9 kcal/mol higher than the $(O_2NOCH_2)_2CHO\bullet$ + NO_2 asymptote's.

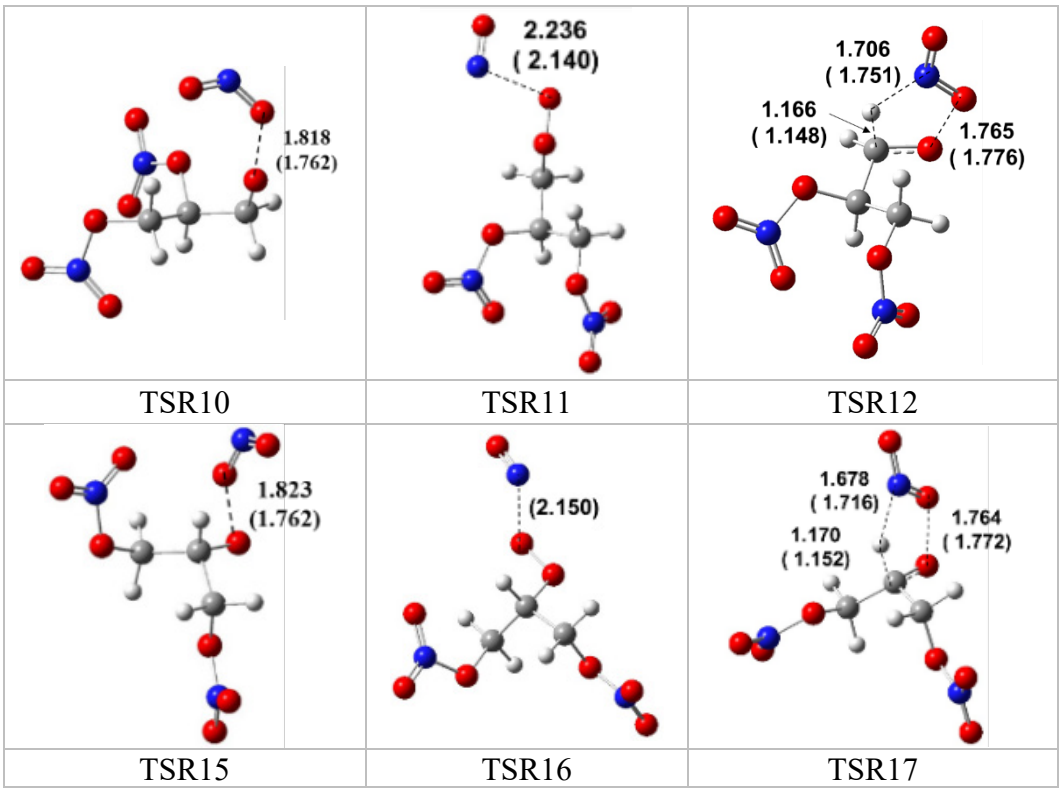


Fig. 5 Transition state structures for R10–12 and R15–17: M06- and B1K-based results. B1K-based results are in parentheses (bond length unit: Å)

The TSs for peroxynitrite decomposition to a peroxide radical (TSR11 or TSR16) were also loose, with OO–NO bond distances being approximately 2.15 Å. Both R11 and R16 were approximately 27.7 kcal/mol endothermic, and the TSs were only slightly higher in energy than the product asymptote. Nominally, the barriers to HONO elimination from the peroxynitrates (via R12 and R17) were 26.5 and 26.8 kcal/mol, respectively. Both TSR12 and TSR17 were approximately 15 kcal/mol higher in energy than their respective RO• + NO_2 asymptote.

We also characterized MEPs for the abstractions of an H atom from the C atom adjacent to O•. They produced *cis*-HONO (R13/R18) or HNO_2 (R14/R19) and an aldehyde. The TS structures for the four possibilities are shown in Fig. 6. The barriers to HNO_2 formation (via TSR14 and TSR19) were lower than those for *cis*-HONO formation (via TSR13 and TSR18). TSR14 was nominally 2.4 kcal/mol lower in energy than TSR13. TSR19 was nominally 2.8 kcal/mol lower in energy than TSR18.

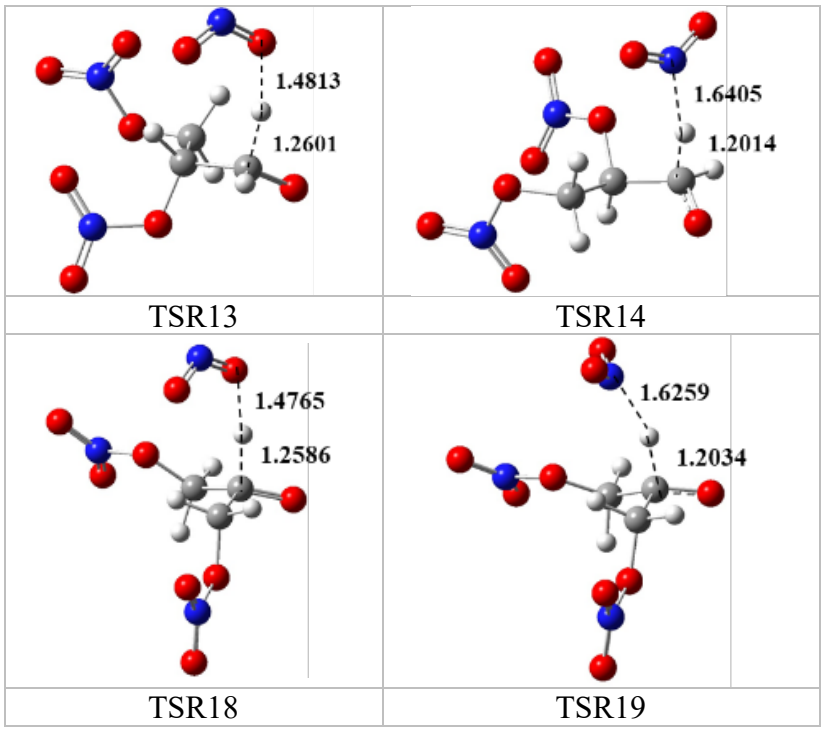


Fig. 6 TS structures for NO_2-mediated H-atom abstraction reactions (R13, R14, R18, and R19): M06-based results (bond length unit: Å)

3.3.4 Unimolecular Decomposition of $(O_2NOCH_2)_2CHO\bullet$ (R20 and R21)

Two paths for the unimolecular decomposition of $(O_2NOCH_2)_2CHO\bullet$ (DICACOJ) were postulated and characterized. One was the β-scission of a C–C bond (R20 via TSR20). It produced acetyl nitrate ($HCOCH_2ONO_2$) and a radical ($\bullet CH_2ONO_2$) that decomposed with little to no barrier to CH_2O and NO_2. The barrier to R20 was 13.0 kcal/mol. The other was a simple C–H bond dissociation (R21 via TSR21) that formed $(O_2NOCH_2)_2CO$ (DICACDO). The barrier to this reaction was 36.0 kcal/mol, and it was 17.1 kcal/mol endothermic. As such, its contribution to the decomposition process was expected to be negligible.

3.4 MEP Characterizations for Reactions on the $C_3H_5N_3O_9 + NO_2$ Potential Energy Surface

Because NO_2 loss is the dominant first step in NG's decomposition, NO_2 is a prominent labile oxidizer in decomposing systems and we expected it to react with NG. Table 11 lists the reactions that were postulated and characterized. Figure 7 provides an overview of the stationary point structures and relative energies of their MEPs.

Table 11 Reactions on the $C_3H_5N_3O_9$ + NO_2 potential energy surface

R22	NG + NO_2 ↔ $O_2NOCH_2CH(ONO_2)C•HONO_2$ [NG1J] + *cis*-HONO (via TSR22)
R23	NG + NO_2 ↔ $O_2NOCH_2CH(ONO_2)C•HONO_2$ [NG1J] + HNO_2 (via TSR23)
R24	NG + NO_2 ↔ $(CH_2ONO_2)_2C•ONO_2$ [NG2J] + *cis*-HONO (via TSR24)
R25	NG + NO_2 ↔ $(CH_2ONO_2)_2C•ONO_2$ [NG2J] + HNO_2 (via TSR25)
R26	$O_2NOCH_2CH(ONO_2)C•HONO_2$ ↔ $O_2NOCH_2CH(ONO_2)CHO$ + NO_2 (via TSR26) [NG1J ↔ CACACDO + NO_2]
R27	$(CH_2ONO_2)_2C•ONO_2$ ↔ $(CH_2ONO_2)_2CO$ + NO_2 (via TSR27) [NG2J ↔ DICACDO + NO_2]
R28	NG + NO_2 ↔ $O_2NOCH_2CH(ONO_2)CH_2O•$ [CACACOJ] + O_2NNO_2 (via TSR28)
R29	NG + NO_2 ↔ $(CH_2ONO_2)_2CHO•$ [DICACDO] + O_2NNO_2 (via TSR29)

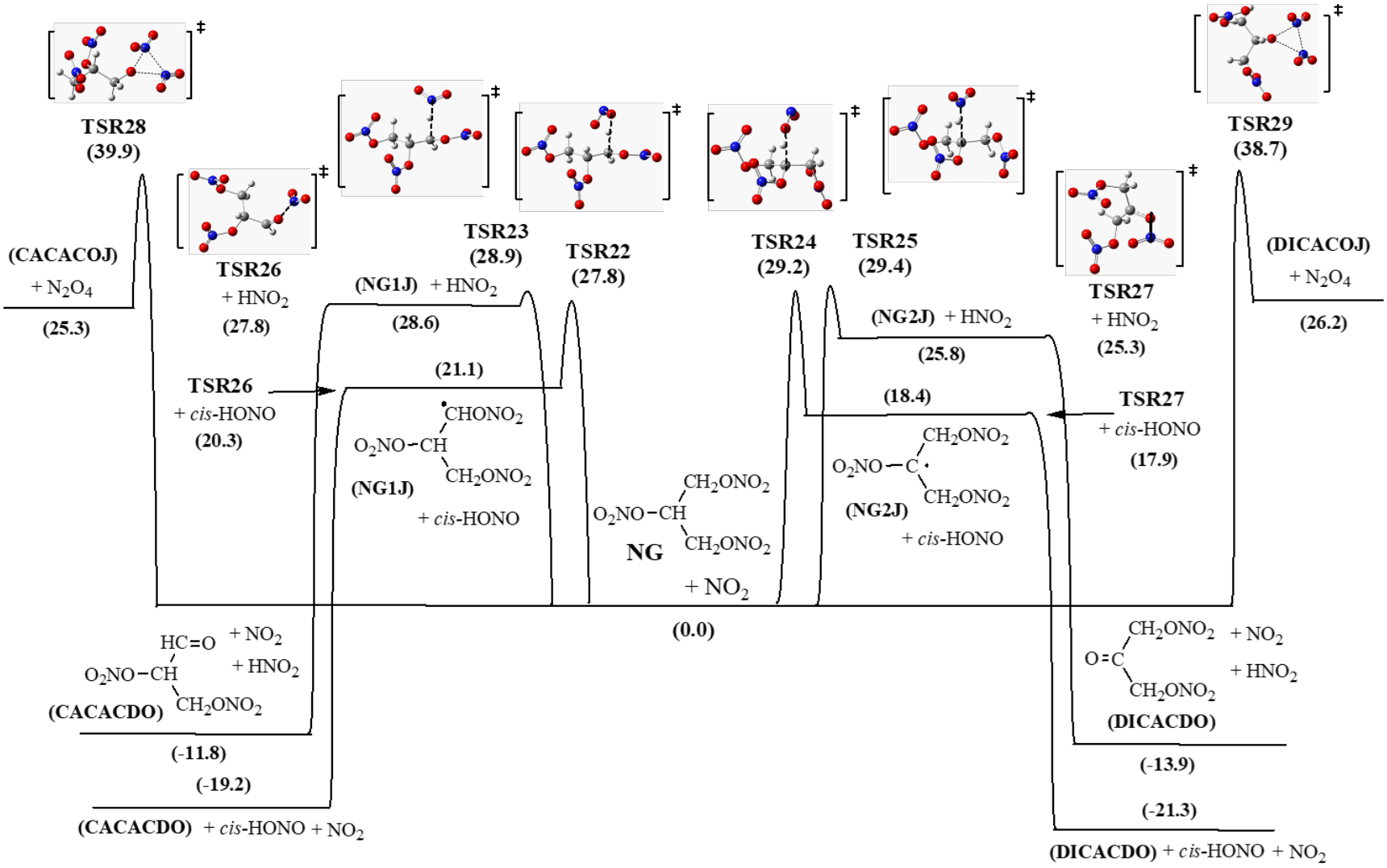


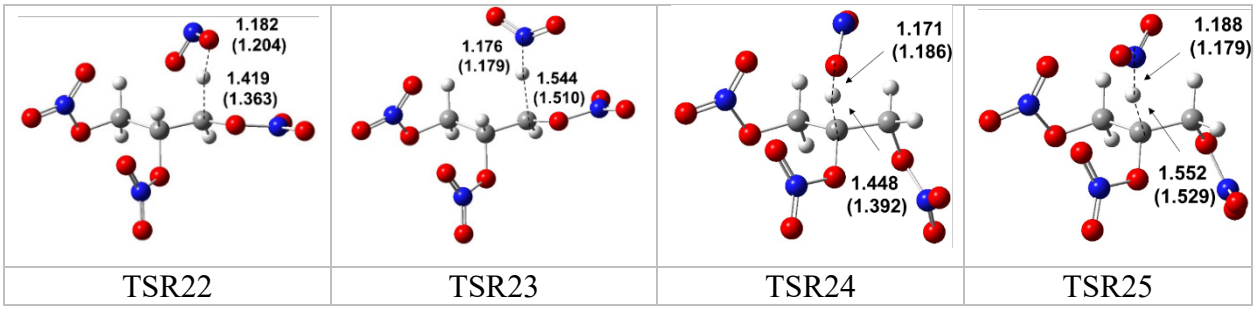
Fig. 7 MEPs on the $C_3H_5N_3O_9$ + NO_2 potential energy surface (energy units: kcal/mol)

3.4.1 H-Atom Abstraction Reactions (R22–R27)

Based on prior studies (McQuaid and Ishikawa 2006; Chen and McQuaid 2014), it was considered likely that the abstraction of H atoms from NG by NO_2 would play an important role in NG's decomposition and combustion. Therefore, we characterized four possibilities: abstraction from a C(p) atom and the formation of *cis*-HONO (R22) or HNO_2 (R23), and abstraction from the C(s) atom and the formation of *cis*-HONO (R24) or HNO_2 (R25). We did not characterize H-atom abstractions that produced *trans*-HONO because the prior studies suggested the barriers to them would be significantly higher than those for *cis*-HONO or HNO_2 formation.

Depictions of the molecular structures of TSR22, TSR23, TSR24, and TSR25 are shown in Fig. 8. Their energies relative to the NG + NO_2 asymptote are listed in Table 12. Nominally, TSR22, TSR23, TSR24, and TSR25 were 27.8, 28.9, 29.2, and 29.4 kcal/mol higher in energy than the NG + NO_2 asymptote. The relative energies of the transition states for HNO_2 formation (TSR23 and TSR25) were slightly higher than those for *cis*-HONO formation (TSR22 and TSR24).

The other products of H-atom abstraction reactions were $O_2NOCH_2CH(ONO_2)C\bullet HONO_2$ [NG1J] and $(CH_2ONO_2)_2C\bullet ONO_2$ [NG2J]. They proved to be relatively unstable. Indeed, geometry optimizations performed with the B3DP model did not produce a stable structure for either. Geometry optimizations performed with the M06 and B1K models did, but other results produced by those models indicated both NG1J and NG2J would readily lose one of their NO_2 groups. (The O–NO_2 bond lengths in the transition states for those reactions were less than 0.1 Å longer than that in the corresponding radical.) Moreover, based on single-point energies produced with the G3MP2 model, the energies of the transition states (TSR26 or TSR27) were slightly lower in energy than their corresponding radical.



TSR22	TSR23	TSR24	TSR25

Fig. 8 The molecular structures for TSR22, TSR23, TSR24, and TSR25. B3DP- and M06-based results. M06-based results are in parentheses (bond length unit: Å)

Table 12 Relative zero-point corrected energies (in kcal/mol) of stationary points shown in Fig. 7

Stationary point	G3MP2B3	G3MP2/ /B3DP	G3MP2// B1K	G3MP2// M06	a
NG + NO_2	. . .	0.0	0.0	0.0	. . .
TSR22	. . .	28.3	27.5	27.2	27.8
TSR23	. . .	29.3	29.3	29.1	28.9
TSR24	. . .	29.9	28.7	28.3	29.2
TSR25	. . .	30.2	29.7	29.2	29.4
NG1J + *cis*-HONO	. . .	. . .	21.3	21.3	21.1
TSR26 + *cis*-HONO	. . .	. . .	19.9	20.0	20.3
NG2J + *cis*-HONO	. . .	. . .	18.5	18.6	18.4
TSR27 + *cis*-HONO	. . .	. . .	17.3	17.5	17.9
TSR28	40.9	40.3	. . .	. . .	39.9
CACACOJ + O_2NNO_2	27.0	26.5	. . .	. . .	25.3
TSR29	39.5	38.9	. . .	. . .	38.7
DICACOJ + O_2NNO_2	27.6	27.1	. . .	. . .	26.2

[a] Value employed for thermochemical property estimation.

3.4.2 O_2NNO_2 Formation (R28–R29)

MEPs for O_2NNO_2 formation via R30 and R31 were characterized based on results produced with G3MP2B3 and G3MP2//B3DP models. TS structures (TSR28 and TSR29) for these reactions are shown in Fig. 9. Their energies relative to the NG + NO_2 asymptote are listed in Table 12. Because their barriers are more than 10 kcal/mol higher than those of the H-atom abstraction reactions, R28 and R29 are expected to be significantly less important than them at temperatures of interest.

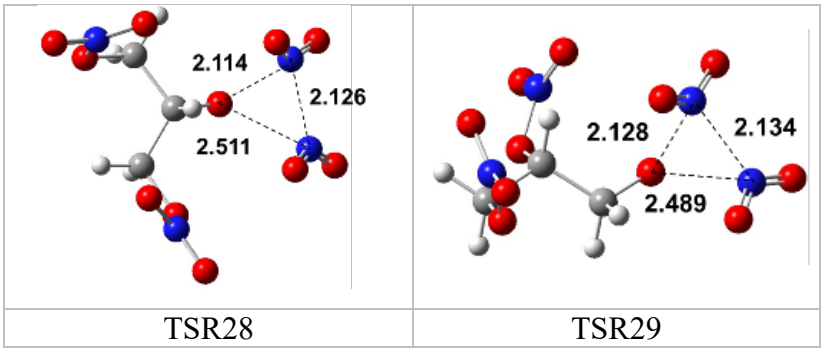


Fig. 9 The geometries of TSR28 and TSR29: B3DP-based results (bond length unit: Å)

3.5 MEP Characterizations for Reactions on the $C_3H_5N_2O_7$ + NO Potential Energy Surface

As discussed in Section 3.3, R11 and R16 produced nitric oxide (NO). Therefore, we considered it prudent to characterize MEPs for two types of reaction between NO and either $O_2NOCH_2CH(ONO_2)CH_2O$• or $(O_2NOCH_2)_2CHONO$•. Listed in Table 13 and shown schematically in Fig. 10, they included 1) N-atom-led addition to O•, producing a nitrite (RONO via R30 or R33) and 2) direct abstraction of an H atom from the C atom adjacent to O•, producing HNO and an aldehyde (via R32 or R35). In addition, MEPs for HNO elimination from the nitrites $O_2NOCH_2CH(ONO_2)CH_2ONO$ and $(O_2NOCH_2)_2CHONO$ were also characterized. Selected bond lengths for TSR31, TSR32, TSR34, and TSR35 are shown in Fig. 11.

Table 13 Reactions on the $C_3H_5N_2O_7$ + NO potential energy surface

R30	$O_2NOCH_2CH(ONO_2)CH_2O$• + NO ↔ $O_2NOCH_2CH(ONO_2)CH_2ONO$ [CACACOJ + NO ↔ CACACONO]
R31	$O_2NOCH_2CH(ONO_2)CH_2ONO$ ↔ $O_2NOCH_2CH(ONO_2)CHO$ + HNO (via TSR31) [CACACONO ↔ CACACDO + HNO]
R32	$O_2NOCH_2CH(ONO_2)CH_2O$• + NO ↔ $O_2NOCH_2CH(ONO_2)CHO$ + HNO (via TSR32) [CACACOJ + NO ↔ CACACDO + HNO]
R33	$(CH_2ONO_2)_2CHO$• + NO ↔ $(CH_2ONO_2)_2CHOONO$ [DICACOJ + NO ↔ DICACONO]
R34	$(CH_2ONO_2)_2CHONO$ ↔ $(CH_2ONO_2)_2CO$ + HNO (via TSR34) [DICACONO ↔ DICACDO + HNO]
R35	$(CH_2ONO_2)_2CHO$•+ NO ↔ $(CH_2ONO_2)_2CO$ + HNO (via TSR35) [DICACOJ + NO ↔ DICACDO + HNO]

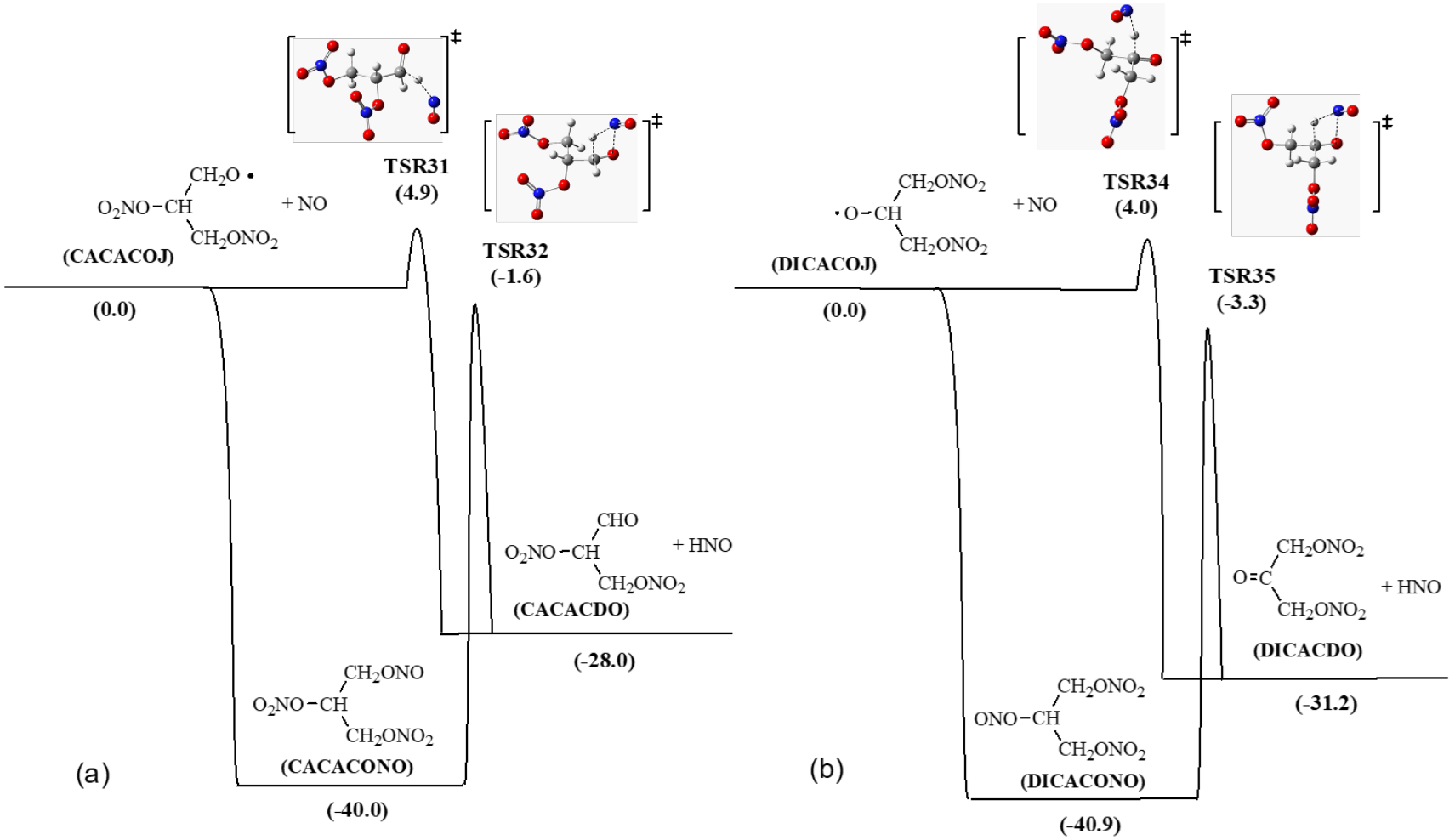


Fig. 10 MEPs for NO reacting with (a) $O_2NOCH_2CH(ONO_2)CH_2O\bullet$ and (b) $(O_2NOCH_2)_2CHONO\bullet$ (energy units: kcal/mol)

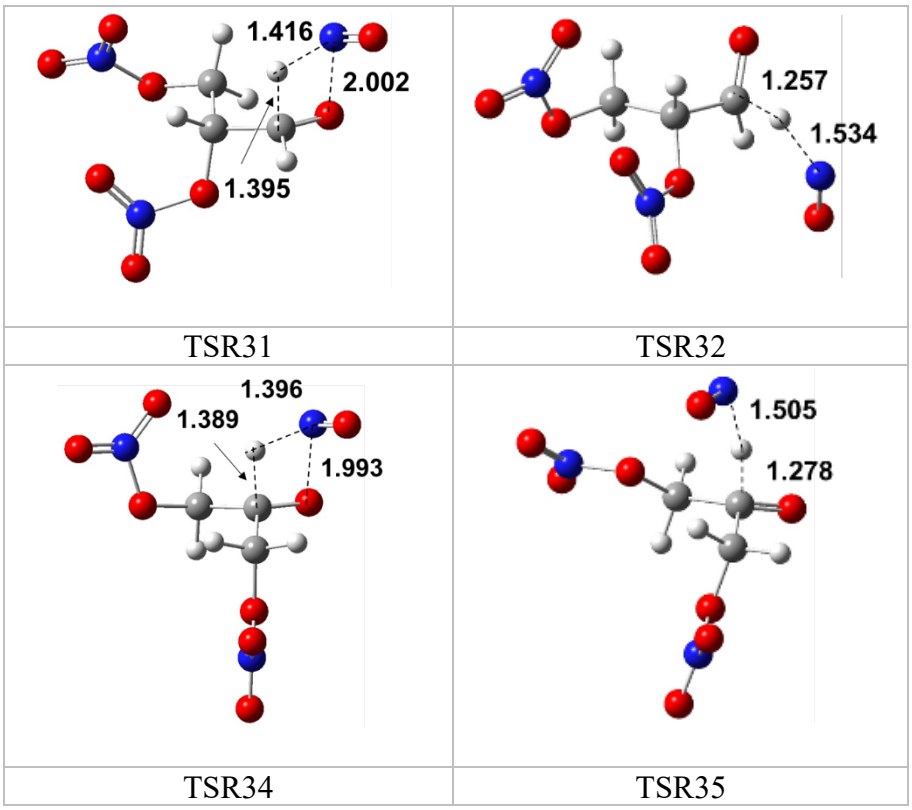


Fig. 11 TS structures for NO reacting with $O_2NOCH_2CH(ONO_2)CH_2O$• (R31 and R34) and $(O_2NOCH_2)_2CHONO$• (R32 and R35): M06-based results (bond length unit: Å)

The relative energies of all the stationary points for the MEPs depicted in Fig. 10 are listed in Table 14. We observed them to be very comparable to results for analogous reactions involving C_2H_5O• (Chen and McQuaid 2013). For example, the formation of ethyl nitrite (CH_3CH_2ONO) was previously found to be barrierless and 40.9 kcal/mol exothermic. $O_2NOCH_2CH(ONO_2)CH_2ONO$ formation (via R30) was 40.0 kcal/mol exothermic and $(CH_2ONO_2)_2CHONO$ formation (via R33) was 40.9 kcal/mol exothermic. The barrier to HNO elimination from CH_3CH_2ONO was 39.0 kcal/mol. The barriers to HNO elimination from $O_2NOCH_2CH(ONO_2)CH_2ONO$ and $(CH_2ONO_2)_2CHONO$ were 38.4 and 37.6 kcal/mol, respectively. The barriers to the direct abstraction from an H atom from C_2H_5O• was 7.0 kcal/mol. The barriers to the direct abstraction from an H atom from $O_2NOCH_2CH(ONO_2)CH_2O$• and $(O_2NOCH_2)_2CHONO$• were 4.9 and 4.0 kcal/mol, respectively.

Table 14 Relative energies (in kcal/mol) for stationary points shown in Fig. 10

Stationary point	CBS-QB3	G3MP2B3	G3MP2 //B3DP	G3MP2 //B1K	G3MP2 //M06	a
$O_2NOCH_2CH(ONO_2)CH_2O$•+NO [CACACOJ + NO]	0.0	0.0	0.0	0.0	0.0	. . .
$O_2NOCH_2CH(ONO_2)CH_2ONO$ [CACACONO]	–38.0	–40.0	–40.2	–38.5	–39.3	–40.0
$O_2NOCH_2CH(ONO_2)CHO$+HNO [CACACDO + HNO]	–26.2	–29.1	–28.5	–27.7	–28.0	–28.0
TSR31	0.6	5.8	5.6	3.6	4.8	4.9
TSR32	0.8	–2.1	–2.3	–1.4	–1.3	–1.6
$(CH_2ONO_2)_2CHO$+NO_2 [DICACOJ + NO_2]	0.0	0.0	0.0	0.0	0.0	. . .
$(CH_2ONO_2)_2CHONO$ [DICACONO]	–38.3	–40.5	–40.7	–38.8	–39.5	–40.9
$(O_2NOCH_2)_2CHO$+HNO [DICACDO + HNO]	–29.4	–32.2	–31.7	–30.5	–31.0	–31.2
TSR34	. . .	. . .	4.9	3.3	4.5	4.0
TSR35	–0.8	–3.7	–3.9	–2.8	–2.7	–3.3

[a] Value employed for thermochemical property estimation.

3.6 Rate Coefficient Parameterizations for R1–R4

To compute $\Delta G^{\ddagger}_{R1/R2}(T)$, and therefrom $k_{R1/R2}(T)$, relaxed potential energy scans were performed with a QCISD(T)/6-31G(d)//B3LYP/6-311+G(d,p) model. Values were computed at 0.05-Å intervals. To produce $\Delta G^{\ddagger}_{R1/R2}(T)$ values that were consistent with nominal values chosen to represent the difference between the reactant and product asymptotes—see Tables 7 and 8—the QCISD(T)/6-31G(d)//B3LYP/6-311+G(d,p)-based values were scaled by the ratio of the latter to the former. For R1, the scaling factor was 0.99 (38.4/39.1). For R2, the scaling factor was 0.97 (38.6/39.9). The $k(T)$ derived on this basis are listed in Table 15 as function of temperature (from 300 to 2000 K) and O–NO_2 bond length (between 1.90 and 2.34 Å). Fitting Eq. 2 to these data yielded $k_{\infty,R1}(T) = 4.11 \times 10^{15} T^{-0.04933}$ exp(-37,439/RT) and $k_{\infty,R2}(T) = 1.82 \times 10^{16} T^{-0.5192}$ exp(-38,520/RT).

Table 15 Rate coefficients (in s^{-1}) for R1 and R2 as a function of temperature and O–NO_2 bond length[a]

Temp (K)	C(p)O–NO_2 bond length (Å)							
	1.99	**2.04**	**2.09**	**2.14**	**2.19**	**2.24**	**2.29**	**2.34**
300	6.84×10^{-7}	1.30×10^{-9}	7.32×10^{-11}	8.55×10^{-12}	1.84×10^{-12}	5.68×10^{-13}	**4.10×10^{-13}**	4.50×10^{-13}
400	1.11×10^{-1}	6.41×10^{-4}	8.48×10^{-5}	1.93×10^{-5}	6.87×10^{-6}	3.10×10^{-6}	**2.89×10^{-6}**	3.49×10^{-6}
500	1.66×10^{2}	1.79×10^{0}	3.97×10^{-1}	1.36×10^{-1}	6.59×10^{-2}	**3.76×10^{-2}**	4.06×10^{-2}	5.20×10^{-2}
600	2.35×10^{4}	3.73×10^{2}	1.17×10^{2}	5.25×10^{1}	3.14×10^{1}	**2.12×10^{1}**	2.51×10^{1}	3.35×10^{1}
800	1.32×10^{7}	3.21×10^{5}	1.56×10^{5}	9.85×10^{4}	7.69×10^{4}	**6.43×10^{4}**	8.49×10^{4}	1.19×10^{5}
1000	6.55×10^{8}	1.97×10^{7}	1.24×10^{7}	9.67×10^{6}	8.86×10^{6}	**8.49×10^{6}**	1.19×10^{7}	1.73×10^{7}
1200	9.43×10^{9}	3.17×10^{8}	2.38×10^{8}	**2.12×10^{8}**	2.17×10^{8}	2.28×10^{8}	3.31×10^{8}	4.90×10^{8}
1500	1.45×10^{11}	5.23×10^{9}	**4.67×10^{9}**	4.78×10^{9}	5.43×10^{9}	6.28×10^{9}	9.45×10^{9}	1.43×10^{10}
2000	2.45×10^{12}	**8.89×10^{10}**	9.42×10^{10}	1.11×10^{11}	1.40×10^{11}	1.78×10^{11}	2.76×10^{11}	4.25×10^{11}
Temp (K)	**C(s)O–NO_2 bond length (Å)**							
	1.90	**1.95**	**2.00**	**2.05**	**2.10**	**2.15**	**2.20**	**2.25**
300	3.59×10^{-7}	8.99×10^{-10}	6.87×10^{-11}	4.14×10^{-12}	1.19×10^{-12}	2.32×10^{-13}	**8.98×10^{-14}**	1.29×10^{-13}
400	5.77×10^{-2}	4.14×10^{-4}	6.80×10^{-5}	9.23×10^{-6}	4.06×10^{-6}	1.32×10^{-6}	**6.75×10^{-7}**	1.06×10^{-6}
500	8.25×10^{1}	1.06×10^{0}	2.74×10^{-1}	6.08×10^{-2}	3.46×10^{-2}	1.53×10^{-2}	**9.44×10^{-3}**	1.55×10^{-2}
600	1.09×10^{4}	1.99×10^{2}	7.00×10^{1}	2.17×10^{1}	1.47×10^{1}	7.97×10^{0}	**5.61×10^{0}**	9.42×10^{0}
800	5.22×10^{6}	1.40×10^{5}	7.26×10^{4}	3.40×10^{4}	2.87×10^{4}	2.03×10^{4}	**1.71×10^{4}**	2.92×10^{4}
1000	2.23×10^{8}	7.21×10^{6}	4.71×10^{6}	2.84×10^{6}	2.73×10^{6}	2.26×10^{6}	**2.14×10^{6}**	3.67×10^{6}
1200	2.81×10^{9}	9.95×10^{7}	7.59×10^{7}	5.42×10^{7}	5.69×10^{7}	**5.24×10^{7}**	5.37×10^{7}	9.21×10^{7}
1500	3.67×10^{10}	1.37×10^{9}	1.22×10^{9}	**1.03×10^{9}**	1.18×10^{9}	1.21×10^{9}	1.35×10^{9}	2.30×10^{9}
2000	5.06×10^{11}	**1.86×10^{10}**	1.95×10^{10}	1.95×10^{10}	2.44×10^{10}	2.78×10^{10}	3.38×10^{10}	5.73×10^{10}

[a]The variational rate coefficient at each temperature is in bold text.

The MEPs for *trans*-HONO elimination had a saddle point. Formulae for computing the high-pressure limit rate coefficients ($k_{\infty,i}$) for eliminations involving the primary and secondary nitroxy groups were $k_{\infty,R3}(T) = 3.0 \times 10^{18} T^{-0.9538} \exp(-40{,}727/RT)$ and $k_{\infty,R4}(T) = 5.99 \times 10^{16} T^{-1.0655} \exp(-39{,}081/RT)$, respectively.

As shown in Fig. 12, $k_{\infty,R1}(T)$ was greater than $k_{\infty,R2}(T)$, $k_{\infty,R3}(T)$, and $k_{\infty,R4}(T)$ for all T, and $k_{\infty,R4}(T)$ was significantly lower than the other three. $k_{\infty,R2}(T)$ was slightly greater than $k_{\infty,R3}(T)$ for 300 K $\leq T \leq$ 500 K. For $T >$ 500 K, $k_{\infty,R3}(T)$ was greater than $k_{\infty,R2}(T)$, and the difference increased with increase in T.

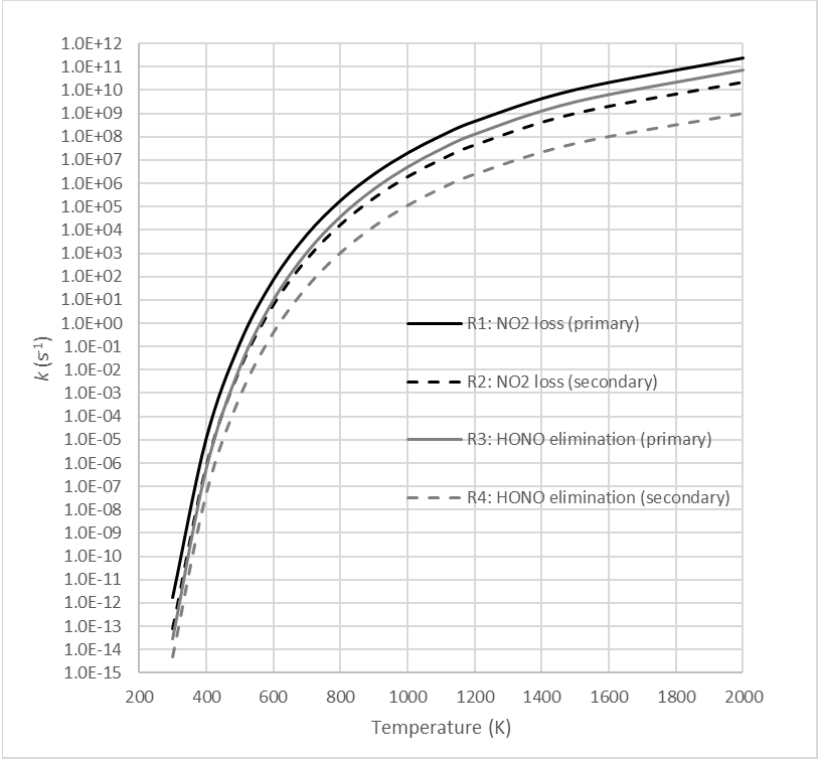


Fig. 12 Comparison of high-pressure rate coefficients for NO_2 loss and HONO elimination from NG as a function of temperature

Table 16 and Fig. 13 compare the $k(T)$ for R1–R4 for $300 \leq T \leq 1200$ K and $0.001 \leq \mathrm{P} \leq 100$ atm. For any given (T, P) pair, k_{R1} was the largest of the four, and k_{R4} was the smallest. k_{R2} and k_{R3} were very similar for $300\ \mathrm{K} \leq T \leq 600$ K. Above 600 K, k_{R2} became noticeably larger and continued to increase relative to k_{R3} as T increased.

Table 16 Logarithms of QRRK-derived rate coefficients (in s^{-1}) for R1, R2, R3, and R4

Temperature (K)	$\log_{10} k_{R1}$	$\log_{10} k_{R2}$	$\log_{10} k_{R3}$	$\log_{10} k_{R4}$
P = 1E-3 atm				
300	–11.8	–13.1	–13.6	–14.3
400	–5.0	–6.2	–6.3	–7.4
500	–1.0	–2.2	–2.2	–3.4
600	1.3	0.2	0.3	–1.0
700	2.7	1.6	1.7	0.3
800	3.5	2.4	2.4	1.1
900	4.0	2.8	2.9	1.5
1000	4.3	3.1	3.1	1.8
P = 1 atm				
300	–11.8	–13.1	–13.6	–14.3
400	–5.0	–6.1	–6.3	–7.4
500	–0.9	–2.0	–1.9	–3.2
600	1.8	0.8	1.0	–0.4
700	3.7	2.7	3.0	1.5
800	5.0	4.0	4.3	2.7
900	5.9	4.8	5.1	3.6
1000	6.4	5.3	5.7	4.1
P = 100 atm				
300	–11.8	–13.1	–13.6	–14.3
400	–5.0	–6.1	–6.3	–7.4
500	–0.9	–2.0	–1.9	–3.2
600	1.8	0.8	1.0	–0.4
700	3.8	2.8	3.1	1.5
800	5.2	4.2	4.6	3.0
900	6.3	5.3	5.7	4.1
1000	7.1	6.1	6.6	4.9

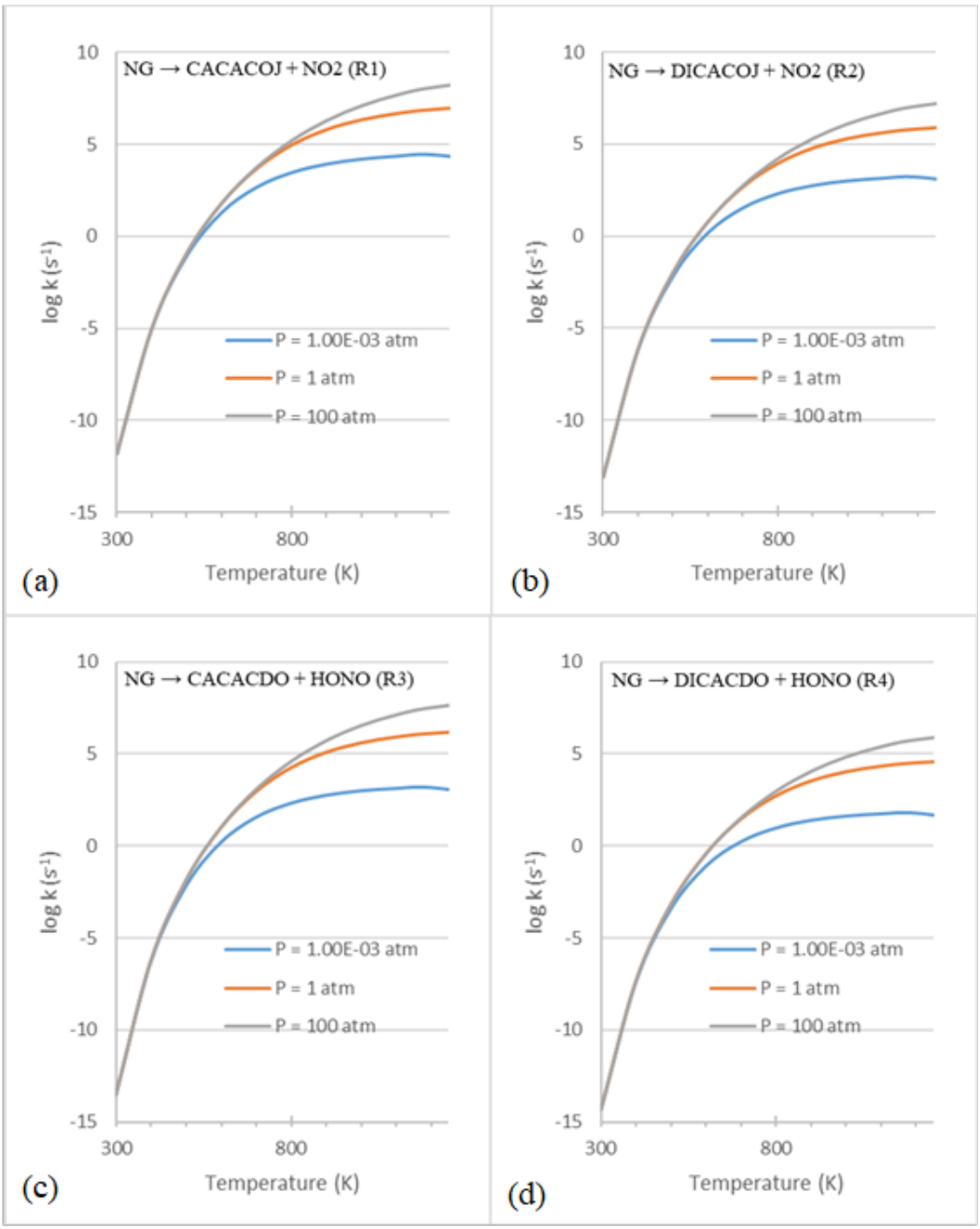


Fig. 13 QRRK-based $k(T)$ for R1, R2, R3, and R4 as a function of temperature and pressure

3.7 Burning-Rate Predictions

Figure 14 compares CYCLOPS-based burning-rate predictions to measured values found in the open literature (Andreev 1940, 1957; Andreev et al. 1959). The burning rates predicted based on the HLK- and PL-based prescriptions for the relationship between $\dot{m}$ and T^0 were very similar and in good agreement with the measurement-based data.

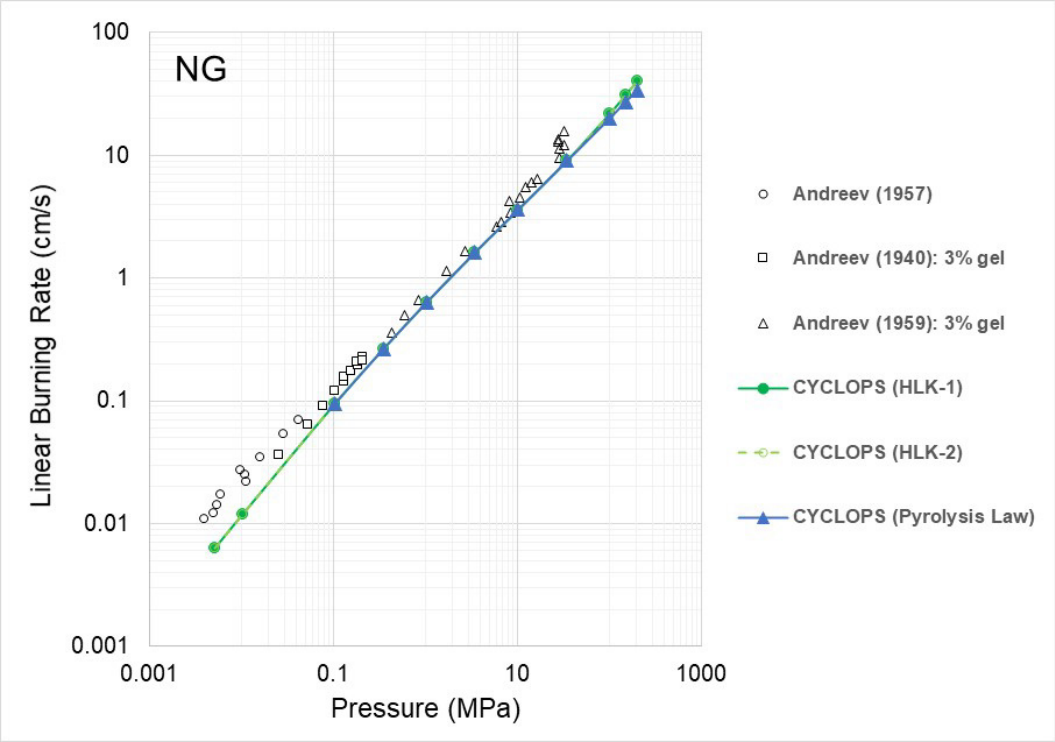


Fig. 14 Comparison of measured and predicted burning rates (HLK-1: McQuaid et al. 2021; HLK-2: Tunnell and Tod 2016)

Given the historical use of PLs for specifying the relationship between $\dot{m}$ and T^0, we were curious how the relationships established via the HLK-based simulations and the PL prescribed by Zenin (1995) would compare. The results are shown in Fig. 15. Given that the burning-rate predictions for the three cases were nearly identical over the entire range of P considered, the range of T^0 capable of producing a given $\dot{m}$ indicates the relationship between $\dot{m}$ and T^0 is far less constrained than the PL implies. We have found this to be the case for other energetic materials as well (McQuaid et al. 2015).

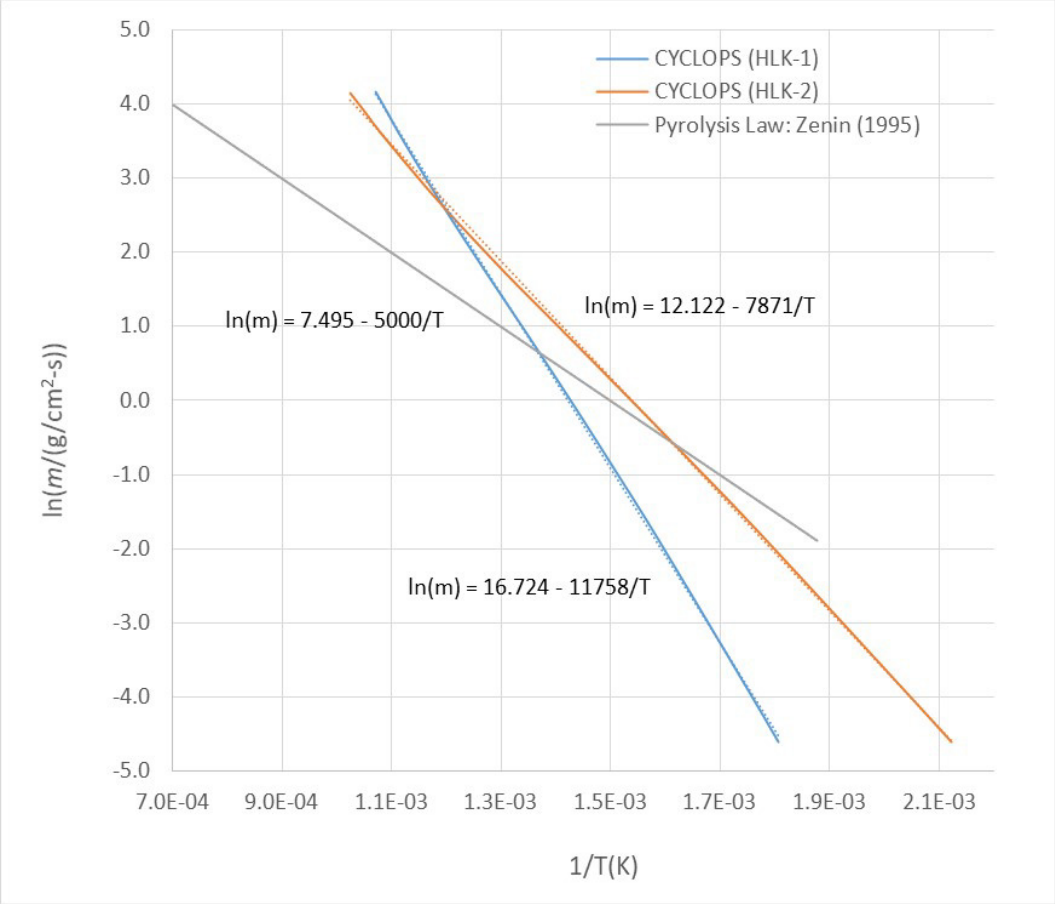


Fig. 15 Comparison of pyrolysis laws derived from measurements and model-generated results

3.8 Products of NG_g's Pyrolysis

In a previous study (McQuaid et al. 2021), the NG mechanism was integrated with the HR model to simulate experiments performed by Waring and Krastins (1970). In that study, measured and predicted values for the global rate at which NG_g decomposed when held at a constant temperature in the range 150–160 °C were compared. Predicted rates were observed to be approximately a factor of 3 lower than measured values, and good agreement could be obtained by introducing a scaling factor that by thermodynamic standards was relatively small.

In addition to measuring global rates for NG_g's decomposition, Waring and Krastins performed experiments in which the partial pressures of carbon monoxide (CO), carbon dioxide (CO_2), NO, NO_2, and formic acid (HCOOH) were measured as a function of time following the immersion of a flask containing neat NG_g in a bath held at 160 °C. The HR model's predictions for the process are compared to the measurement-based data in Fig. 16. The model's predictions for [CO] and [NO]

were greater than the measured values while its predictions for [NO_2] and [CO_2] were less than measured values. Nonetheless, the transients for these species' concentrations were reasonably reproduced, and the predictions for [HCOOH] were in reasonable agreement with the measured values. Thus, we believe the mechanism offers considerable potential to provide fundamental insight into NG's reaction chemistry at conditions established in standard calorimetric experiments.

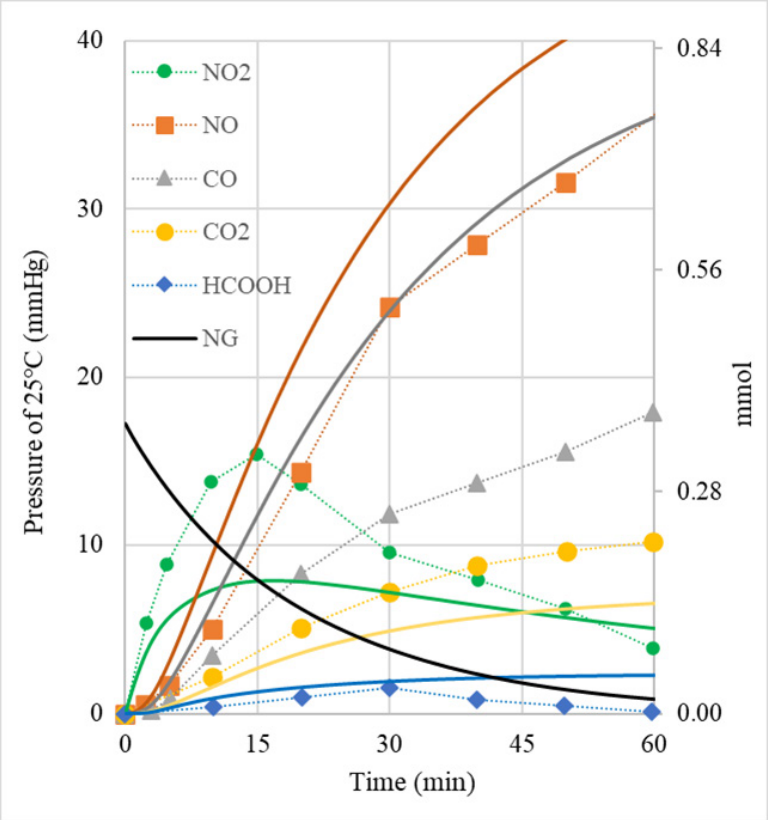


Fig. 16 Simulation of an experiment performed by Waring and Krastins (M/V = 2 × 10^{-4} g/cm^3 at 433 K)

3.9 Sensitivity Analysis

To identify reactions in the mechanism with the most potential to impact the rate at which neat NG_g decomposes, $\widehat{\omega}_{NG,i}(t)$ were computed for a simulation corresponding to a Waring and Krastins' experiment at 160 °C in which ρ_g was 1.2 × 10^{-4} g/cm^3. Plots for the 15 reactions that produced at some point a $\left|\widehat{\omega}_{NG,i}(t)\right|$ value exceeding 0.001 are shown in Fig. 17. They suggest that the 10 reactions with the greatest influence on the rate at which NG_g decomposed under these conditions were 1) dissociation of NG's C(p)O-NO_2 bond via R1; 2) β-scission of R1-produced $O_2NOCH_2CH(ONO_2)CH_2O$•, generating CH_2O and an unstable radical (O_2NOCH_2C•$HONO_2$) via R8; 3) a 1,4-H-atom shift on $O_2NOCH_2CH(ONO_2)CH_2O$•

via R5; 4) dissociation of NG's C(s)O–NO_2 bond via R2; 5) HONO elimination involving a primary nitroxy group via R3; 6) HCO reacting with NO_2 via R1217 or R1218; 7) CH_2O reacting with NO_2 via R1216, 8) CH_2O reacting with OH via R1051; and 9) HCO reacting with NO to form CO and HNO (R992).

We note that, experimentally, the global rate of NG_g's decomposition displayed first-order character at 150, 155, and 160 °C out to decomposition levels of approximately 55%. The results presented in Fig. 17 show that that result was a consequence of a complex interplay between competing reactions.

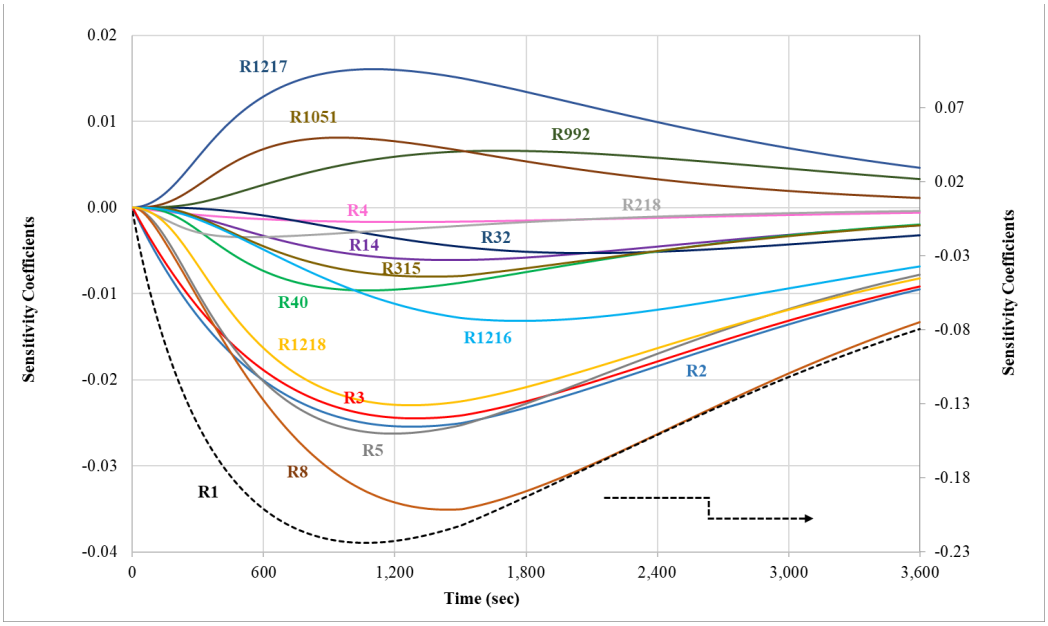


Fig. 17 $\hat{\omega}_{NG,i}$ **vs.** t **plots for reactions producing the largest** $|\hat{\omega}_{NG,i}|$

4. Summary and Conclusions

As a step toward developing a state-of-the-art capability for modeling the response of nitrate ester-based gun and rocket-propellant formulations to thermal loads they will or might experience over the course of their life cycle, we created and evaluated a detailed finite-rate chemical kinetics mechanism for modeling NG_g's decomposition and combustion. High-level QM-ESMs were employed to characterize the molecular structure and normal modes of stationary points of MEPs for a network of covalent bond breaking and/or formation reactions capable of reducing the parent to small molecules. Statistical mechanics was employed to translate the stationary point characterizations into formulae for computing their thermodynamic properties, and transition state theories were employed to translate those properties into formulae for computing the reactions' rate coefficients. Combined with a (sub)mechanism comprising reactions and species common to the

combustion chemistry of nitrate esters, the new formulae were employed in a CYCLOPS deflagration model to predict NG's linear burning rate at pressures from 1 to 13 MPa. Good agreement between measured and predicted values was observed. The mechanism was also employed as a basis for modeling NG_g's decomposition in a closed, constant-volume, constant-temperature reactor. Overall, agreement with measured data suggested the mechanism has significant potential to reveal fundamental insights into the reaction chemistry underlying NG's response to various thermal loads. As such, it is expected to prove helpful in designing and screening NG-containing formulations. Establishing a benchmark, all the mechanism's parameters for computing reaction rate coefficients and species thermodynamic properties are provided.

5. References

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Appendix. Data Composing a Detailed Finite-Rate Chemical Kinetics Mechanism for Modeling the Decomposition and Combustion of Gaseous Nitroglycerin

Table A-1 lists the elementary reactions and species composing the current version of the mechanism we created to model the decomposition and combustion of nitroglycerin (NG). For each reaction, constants employed in formulae for computing the rate coefficients (k) of the steps as a function of temperature (T) and (if applicable) pressure (P) are provided. Except for two formularies employed for computing the rates of fall-off reactions, standard CHEMKIN notation and usage apply.[1]

The nonstandard formularies for computing rate coefficients are the "T&H" method[2] and an interpolation method.[3] Reactions whose rate coefficients are calculated via the T&H method are identified by "auxiliary data" that include the string "T&H". This string prompts a calculation of "F_{cent}"[1] per

$$F_{cent} = a_0 + a_1 T + a_2 T^2 \,, \tag{A-1}$$

where the polynomial's coefficients (a_i) are given in order after the string. (If there is only one number after the string, a_1 and a_2 are zero. If there are only two numbers after the string, a_2 is zero.)

Per the interpolation formulary, rate coefficients are calculated by logarithmically interpolating between those at pressures that bound the one of interest.[3] That is, given formulae,

$$k_1(T) = A_1 T^{b_1} exp(E_1/RT) \tag{A-2}$$

and

$$k_2(T) = A_2 T^{b_2} exp(E_2/RT) \tag{A-3}$$

for pressures P_1 and P_2, respectively, the rate coefficient at an intermediate pressure ($P_1 < P < P_2$) is computed per

$$\log k(T,P) = \log k_1(T) + (\log k_2(T) - \log k_1(T)) \frac{\log P - \log P_1}{\log P_2 - \log P_1}. \tag{A-4}$$

Reactions whose rate coefficients are calculated via this method are identified by auxiliary data that include strings led with "Imn", where mn is a two-digit number.

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[1] Kee RJ, Rupley FM, Miller JA, Coltrin ME, Grcar JF, Meeks E, Moffat HK, Lutz AE, Dixon-Lewis G, Smooke MD, et al. CHEMKIN Collection, release 3.7. Reaction Design, Inc.; 2002.

[2] Tsang W, Herron JT. Chemical kinetic data base for propellant combustion: I. reactions involving NO, NO_2, HNO, HNO_2, HCN and N_2O. J Phys Chem Ref Data. 1991;20:609–623.

[3] Goodwin DG, Speth RL, Moffat HK, Weber BW. Cantera: an object-oriented software toolkit for chemical kinetics, thermodynamics, and transport processes. Version 2.4.0. Zenodo; 2018. doi:10.5281/zenodo.1174508.

Each Imn string is followed by four numbers. They correspond to A_i, b_i, E_i, and P_i (in atmospheres), respectively. The numbers on the line that define such reactions are dummy variables; they serve no function in computing the reaction's rate coefficient.

Table A-1 also provides information about the species involved, including their elemental composition, molecular weight, and the temperature range over which the coefficients for estimating their thermodynamic properties were fit.

Coefficients for computing the species' thermodynamic properties as a function of temperature are provided in Table A-2. Also, due to (CHEMKIN) preprocessor-imposed restrictions on the number of characters and character types that can be employed to label molecules, it was not possible to assign to most species a label that could be unambiguously translated into a molecular structure. Table A-3 provides that information.

Table A-1 Species data and rate coefficient parameterizations for elementary reactions in the NG mechanism

ELEMENTS CONSIDERED	ATOMIC WEIGHT
1. C	12.0112
2. H	1.00797
3. N	14.0067
4. O	15.9994
5. HE	4.00260
6. AR	39.9480

SPECIES CONSIDERED	PHASE	CHARG E	MOLECULAR WEIGHT	TEMPERATURE LOW	TEMPERATURE HIGH	ELEMENT COUNT C	H	O	N	HE	AR
1. NG	G	0	227.08800	300	5000	3	5	3	9	0	0
2. CO	G	0	28.01055	300	5000	1	0	0	1	0	0
3. CO2	G	0	44.00995	300	5000	1	0	0	2	0	0
4. H2O	G	0	18.01534	300	5000	0	2	0	1	0	0
5. NO	G	0	30.00610	200	6000	0	0	1	1	0	0
6. NO2	G	0	46.00550	300	5000	0	0	1	2	0	0
7. H2	G	0	2.01594	300	5000	0	2	0	0	0	0
8. N2	G	0	28.01340	300	5000	0	0	2	0	0	0
9. O2	G	0	31.99880	300	5000	0	0	0	2	0	0
10. HOCHO	G	0	46.02589	300	4000	1	2	0	2	0	0
11. HE	G	0	4.00260	300	5000	0	0	0	0	1	0
12. AR	G	0	39.94800	300	5000	0	0	0	0	0	1
13. NG1J	G	0	226.08003	300	5000	3	4	3	9	0	0
14. NG2J	G	0	226.08003	300	5000	3	4	3	9	0	0
15. DICACOJ	G	0	181.08250	300	5000	3	5	2	7	0	0
16. CACACOJ	G	0	181.08250	300	5000	3	5	2	7	0	0
17. CACACDO	G	0	180.07453	300	5000	3	4	2	7	0	0
18. DICACDO	G	0	180.07453	300	5000	3	4	2	7	0	0
19. HCOCDOCA	G	0	133.06106	300	5000	3	3	1	5	0	0
20. CDJOCA	G	0	104.04254	300	5000	2	2	1	4	0	0
21. DICDOCA	G	0	133.06106	300	5000	3	3	1	5	0	0
22. HCOCOJCA	G	0	134.06903	300	5000	3	4	1	5	0	0
23. HCOCACOJ	G	0	134.06903	300	5000	3	4	1	5	0	0
24. HCOCDOCJA	G	0	132.05309	300	5000	3	2	1	5	0	0
25. CDJOCDOCA	G	0	132.05309	300	5000	3	2	1	5	0	0
26. DICDOCJA	G	0	132.05309	300	5000	3	2	1	5	0	0
27. DICDJOCA	G	0	132.05309	300	5000	3	2	1	5	0	0
28. HCOCONO2	G	0	105.05051	300	5000	2	3	1	4	0	0
29. CJACACOH	G	0	181.08250	300	5000	3	5	2	7	0	0
30. CDOCACOH	G	0	135.07700	300	5000	3	5	1	5	0	0
31. CACDOCOJ	G	0	134.06903	300	5000	3	4	1	5	0	0
32. DICJACDO	G	0	179.06656	300	5000	3	3	2	7	0	0
33. CJACDOCOH	G	0	134.06903	300	5000	3	4	1	5	0	0
34. ODCCDOCOH	G	0	88.06353	300	5000	3	4	0	3	0	0
35. CACACDJO	G	0	179.06656	300	5000	3	3	2	7	0	0

36. CACJACDO	G	0	179.06656	300	5000	3	3	2	7	0	0
37. CJACACDO	G	0	179.06656	300	5000	3	3	2	7	0	0
38. ODCJCACOH	G	0	134.06903	300	5000	3	4	1	5	0	0
39. COHCDO	G	0	60.05298	300	5000	2	4	0	2	0	0
40. ODCICDO2	G	0	86.04759	300	5000	3	2	0	3	0	0
41. ODCCDOCOJ	G	0	87.05556	300	5000	3	3	0	3	0	0
42. DICDOCOJ	G	0	87.05556	300	5000	3	3	0	3	0	0
43. HCOCJONO2	G	0	104.04254	300	5000	2	2	1	4	0	0
44. CDOCOJCOH	G	0	89.07150	300	5000	3	5	0	3	0	0
45. CDOCJACOH	G	0	134.06903	300	5000	3	4	1	5	0	0
46. ODCCDJO	G	0	57.02907	300	5000	2	1	0	2	0	0
47. OCJCDOCOH	G	0	87.05556	300	5000	3	3	0	3	0	0
48. COHCDJO	G	0	59.04501	300	5000	2	3	0	2	0	0
49. ODCJKIDO	G	0	85.03962	300	5000	3	1	0	3	0	0
50. ODCKCJOH	G	0	87.05556	300	5000	3	3	0	3	0	0
51. COHONOKK	G	0	133.06106	300	5000	3	3	1	5	0	0
52. COHOJKK	G	0	103.05496	300	5000	3	3	0	4	0	0
53. COHONOK	G	0	105.05051	300	5000	2	3	1	4	0	0
54. COHOJK	G	0	75.04441	300	5000	2	3	0	3	0	0
55. KIDOCDOOJ	G	0	101.03902	300	5000	3	1	0	4	0	0
56. CDOOHA	G	0	121.04991	300	5000	2	3	1	5	0	0
57. CDOOJA	G	0	122.05788	300	5000	2	4	1	5	0	0
58. CACACDOOH	G	0	196.07393	300	5000	3	4	2	8	0	0
59. CACACDOOJ	G	0	197.08190	300	5000	3	5	2	8	0	0
60. ACCJA	G	0	151.05601	300	5000	2	3	2	6	0	0
61. Y3COCA	G	0	105.05051	300	5000	2	3	1	4	0	0
62. Y3COCOJ	G	0	59.04501	300	5000	2	3	0	2	0	0
63. HOYCCO	G	0	60.05298	300	5000	2	4	0	2	0	0
64. CJOCDO	G	0	59.04501	300	5000	2	3	0	2	0	0
65. HOYCJCO	G	0	59.04501	300	5000	2	3	0	2	0	0
66. CJCDOOH	G	0	59.04501	300	5000	2	3	0	2	0	0
67. HOYCCJO	G	0	59.04501	300	5000	2	3	0	2	0	0
68. CJOHCDO	G	0	59.04501	300	5000	2	3	0	2	0	0
69. COCDO	G	0	60.05298	300	5000	2	4	0	2	0	0
70. COCDJO	G	0	59.04501	300	5000	2	3	0	2	0	0
71. CCDOOH	G	0	60.05298	300	5000	2	4	0	2	0	0
72. C2H2OH	G	0	43.04561	300	5000	2	3	0	1	0	0
73. SC2H2OH	G	0	43.04561	300	5000	2	3	0	1	0	0
74. HOCDONO	G	0	75.02402	300	5000	1	1	1	3	0	0
75. HOCDONO2	G	0	91.02342	300	5000	1	1	1	4	0	0
76. HOCDOONO	G	0	91.02342	300	5000	1	1	1	4	0	0
77. ONOCHO	G	0	75.02402	300	5000	1	1	1	3	0	0
78. HCJOHONO	G	0	76.03199	300	5000	1	2	1	3	0	0
79. OJNHCHO	G	0	76.03199	300	5000	1	2	1	3	0	0
80. HONJOCHO	G	0	76.03199	300	5000	1	2	1	3	0	0
81. O2NCHO	G	0	75.02402	300	5000	1	1	1	3	0	0
82. DIOHCH2	G	0	48.04183	300	5000	1	4	0	2	0	0
83. O	G	0	15.99940	300	5000	0	0	0	1	0	0
84. N2O	G	0	44.01280	300	5000	0	0	2	1	0	0
85. H	G	0	1.00797	300	5000	0	1	0	0	0	0
86. HNO	G	0	31.01407	300	5000	0	1	1	1	0	0
87. OH	G	0	17.00737	300	5000	0	1	0	1	0	0
88. HONO	G	0	47.01347	300	5000	0	1	1	2	0	0
89. HCN	G	0	27.02582	200	6000	1	1	1	0	0	0
90. CN	G	0	26.01785	300	5000	1	0	1	0	0	0
91. C2N2	G	0	52.03570	300	5000	2	0	2	0	0	0
92. HNCO	G	0	43.02522	200	6000	1	1	1	1	0	0

93. NH	G	0	15.01467	200	6000	0	1	1	0	0	0
94. H2CN	G	0	28.03379	300	4000	1	2	1	0	0	0
95. NCNO	G	0	56.02395	300	4000	1	0	2	1	0	0
96. C	G	0	12.01115	300	5000	1	0	0	0	0	0
97. N	G	0	14.00670	300	5000	0	0	1	0	0	0
98. NO3	G	0	62.00490	300	5000	0	0	1	3	0	0
99. HO2	G	0	33.00677	200	6000	0	1	0	2	0	0
100. NH2	G	0	16.02264	200	6000	0	2	1	0	0	0
101. NH3	G	0	17.03061	300	5000	0	3	1	0	0	0
102. CH	G	0	13.01912	300	5000	1	1	0	0	0	0
103. HCO	G	0	29.01852	200	6000	1	1	0	1	0	0
104. HCCO	G	0	41.02967	300	4000	2	1	0	1	0	0
105. H2O2	G	0	34.01474	300	5000	0	2	0	2	0	0
106. NCN	G	0	40.02455	300	4000	1	0	2	0	0	0
107. HCNO	G	0	43.02522	250	4000	1	1	1	1	0	0
108. NCO	G	0	42.01725	200	6000	1	0	1	1	0	0
109. NNH	G	0	29.02137	250	4000	0	1	2	0	0	0
110. N2H2	G	0	30.02934	200	6000	0	2	2	0	0	0
111. N2H3	G	0	31.03731	300	5000	0	3	2	0	0	0
112. N2H4	G	0	32.04528	300	5000	0	4	2	0	0	0
113. HNC	G	0	27.02582	300	5000	1	1	1	0	0	0
114. HOCO	G	0	45.01792	300	4000	1	1	0	2	0	0
115. HNNO	G	0	45.02077	300	5000	0	1	2	1	0	0
116. HNO3	G	0	63.01287	300	5000	0	1	1	3	0	0
117. CH2	G	0	14.02709	250	4000	1	2	0	0	0	0
118. CH2(S)	G	0	14.02709	300	4000	1	2	0	0	0	0
119. CH3	G	0	15.03506	300	5000	1	3	0	0	0	0
120. CH2O	G	0	30.02649	200	3500	1	2	0	1	0	0
121. CH4	G	0	16.04303	300	5000	1	4	0	0	0	0
122. CH2OH	G	0	31.03446	250	4000	1	3	0	1	0	0
123. CH3O	G	0	31.03446	300	3000	1	3	0	1	0	0
124. CH3OH	G	0	32.04243	300	5000	1	4	0	1	0	0
125. C2H	G	0	25.03027	300	4000	2	1	0	0	0	0
126. C2H2	G	0	26.03824	300	5000	2	2	0	0	0	0
127. C2H5	G	0	29.06215	300	5000	2	5	0	0	0	0
128. C2H6	G	0	30.07012	300	4000	2	6	0	0	0	0
129. CH2CO	G	0	42.03764	300	5000	2	2	0	1	0	0
130. C2H3	G	0	27.04621	300	5000	2	3	0	0	0	0
131. C2H4	G	0	28.05418	300	5000	2	4	0	0	0	0
132. HCCOH	G	0	42.03764	300	4000	2	2	0	1	0	0
133. HNO2	G	0	47.01347	300	5000	0	1	1	2	0	0
134. HNOH	G	0	32.02204	300	5000	0	2	1	1	0	0
135. NH2O	G	0	32.02204	300	5000	0	2	1	1	0	0
136. C2H4O	G	0	44.05358	300	5000	2	4	0	1	0	0
137. CH2CHO	G	0	43.04561	300	5000	2	3	0	1	0	0
138. CH3CHO	G	0	44.05358	200	6000	2	4	0	1	0	0
139. HOCN	G	0	43.02522	300	4000	1	1	1	1	0	0
140. CH3NHNH2	G	0	46.07237	298	6000	1	6	2	0	0	0
141. CH3NH	G	0	30.04973	200	6000	1	4	1	0	0	0
142. CH3NNH2	G	0	45.06440	200	6000	1	5	2	0	0	0
143. CH3NNH	G	0	44.05643	200	6000	1	4	2	0	0	0
144. CH2NH	G	0	29.04176	300	5000	1	3	1	0	0	0
145. CH3NN	G	0	43.04846	200	6000	1	3	2	0	0	0
146. CH3NNCH3	G	0	58.08352	300	4000	2	6	2	0	0	0
147. CH3N(NH2)NO2	G	0	91.06990	200	6000	1	5	3	2	0	0
148. CH3N(NH2)ONO	G	0	91.06990	200	6000	1	5	3	2	0	0
149. N2O4	G	0	92.01100	300	5000	0	0	2	4	0	0

150. NAMMH	G	0	109.08524	200	6000	1	7	3	3	0	0
151. CH3NO2	G	0	61.04056	300	4000	1	3	1	2	0	0
152. CH3NO	G	0	45.04116	300	4000	1	3	1	1	0	0
153. H2CNO2	G	0	60.03259	300	4000	1	2	1	2	0	0
154. CH3ONO	G	0	61.04056	300	4000	1	3	1	2	0	0
155. CHOCHO	G	0	58.03704	300	5000	2	2	0	2	0	0
156. C3H8	G	0	44.09721	300	5000	3	8	0	0	0	0
157. C3H7	G	0	43.08924	300	5000	3	7	0	0	0	0
158. CH3ONO2	G	0	77.03996	300	5000	1	3	1	3	0	0
159. CH3OONO	G	0	77.03996	300	5000	1	3	1	3	0	0
160. CH3OONOI	G	0	77.03996	300	5000	1	3	1	3	0	0
161. CH3O2	G	0	47.03386	300	5000	1	3	0	2	0	0
162. CH3O2H	G	0	48.04183	300	5000	1	4	0	2	0	0
163. C2H5O	G	0	45.06155	300	5000	2	5	0	1	0	0
164. CH3CO	G	0	43.04561	300	5000	2	3	0	1	0	0
165. CDCONO2	G	0	89.05111	300	5000	2	3	1	3	0	0
166. CONOCDO	G	0	89.05111	300	5000	2	3	1	3	0	0
167. CNO2CDO	G	0	89.05111	300	5000	2	3	1	3	0	0
168. CDCJONO2	G	0	88.04314	300	5000	2	2	1	3	0	0
169. CJONOCDO	G	0	88.04314	300	5000	2	2	1	3	0	0
170. CONOCDJO	G	0	88.04314	300	5000	2	2	1	3	0	0
171. CJNO2CDO	G	0	88.04314	300	5000	2	2	1	3	0	0
172. CNO2CDJO	G	0	88.04314	300	5000	2	2	1	3	0	0
173. KDCNOHOJ	G	0	88.04314	300	5000	2	2	1	3	0	0
174. ETONO2	G	0	91.06705	300	5000	2	5	1	3	0	0
175. CJCONO2	G	0	90.05908	300	5000	2	4	1	3	0	0
176. YC2JO	G	0	43.04561	300	5000	2	3	0	1	0	0
177. COJCONO2	G	0	106.05848	300	5000	2	4	1	4	0	0
178. CQJCONO2	G	0	122.05788	300	5000	2	4	1	5	0	0
179. CDOCQ	G	0	76.05238	300	5000	2	4	0	3	0	0
180. CDOCOJ	G	0	59.04501	300	5000	2	3	0	2	0	0
181. CDJOCQ	G	0	75.04441	300	5000	2	3	0	3	0	0
182. CCOONO	G	0	91.06705	300	5000	2	5	1	3	0	0
183. CCOONO_I	G	0	91.06705	300	5000	2	5	1	3	0	0
184. C2H5O2	G	0	61.06095	300	5000	2	5	0	2	0	0
185. C2H5OH	G	0	46.06952	300	5000	2	6	0	1	0	0
186. SC2H4OH	G	0	45.06155	300	5000	2	5	0	1	0	0
187. HOCH2O	G	0	47.03386	300	5000	1	3	0	2	0	0
188. OCHO	G	0	45.01792	300	5000	1	1	0	2	0	0
189. CH3CO2	G	0	59.04501	300	5000	2	3	0	2	0	0
190. PC2H4OH	G	0	45.06155	300	5000	2	5	0	1	0	0
191. C2H4O2H	G	0	61.06095	300	5000	2	5	0	2	0	0
192. C2H5O2H	G	0	62.06892	300	5000	2	6	0	2	0	0
193. O2C2H4OH	G	0	77.06035	300	5000	2	5	0	3	0	0
194. C2H5ONO	G	0	75.06765	300	5000	2	5	1	2	0	0
195. C2H5NO2	G	0	75.06765	300	5000	2	5	1	2	0	0
196. NH2NO	G	0	46.02874	300	5000	0	2	2	1	0	0
197. NH2OH	G	0	33.03001	300	5000	0	3	1	1	0	0
198. H2NN	G	0	30.02934	300	5000	0	2	2	0	0	0
199. H2NONO	G	0	62.02814	300	5000	0	2	2	2	0	0
200. H2NNO2	G	0	62.02814	300	4500	0	2	2	2	0	0
201. HOONO	G	0	63.01287	300	5000	0	1	1	3	0	0
202. NH2QJ	G	0	48.02144	300	5000	0	2	1	2	0	0
203. HNNDOOH_Z	G	0	62.02814	300	4500	0	2	2	2	0	0
204. HNNDOOH	G	0	62.02814	300	4500	0	2	2	2	0	0
205. N2O5	G	0	108.01040	300	5000	0	0	2	5	0	0
206. HNJNO2	G	0	61.02017	300	5000	0	1	2	2	0	0

207. NJH2Q	G	0	48.02144	300	5000	0	2	1	2	0	0
208. HNOJNO2	G	0	77.01957	300	5000	0	1	2	3	0	0
209. N2O3	G	0	76.01160	300	5000	0	0	2	3	0	0
210. ONONO2	G	0	92.01100	300	5000	0	0	2	4	0	0
211. HONNH	G	0	46.02874	300	5000	0	2	2	1	0	0
212. O3	G	0	47.99820	300	5000	0	0	0	3	0	0
213. OH*	G	0	17.00737	300	5000	0	1	0	1	0	0
214. C3H3	G	0	39.05736	300	5000	3	3	0	0	0	0
215. CDCOH	G	0	44.05358	300	5000	2	4	0	1	0	0
216. H2NCHO	G	0	45.04116	300	5000	1	3	1	1	0	0
217. CDCJCDO	G	0	55.05676	300	5000	3	3	0	1	0	0
218. H2CC	G	0	26.03824	200	6000	2	2	0	0	0	0
219. VCDO	G	0	56.06473	300	5000	3	4	0	1	0	0
220. VCDJO	G	0	55.05676	300	5000	3	3	0	1	0	0
221. VJCDO	G	0	55.05676	300	5000	3	3	0	1	0	0
222. CACACOONO	G	0	227.08800	300	5000	3	5	3	9	0	0
223. CACACQJ	G	0	197.08190	300	5000	3	5	2	8	0	0
224. DICACOONO	G	0	227.08800	300	5000	3	5	3	9	0	0
225. DICACQJ	G	0	197.08190	300	5000	3	5	2	8	0	0
226. CACACONO	G	0	211.08860	300	5000	3	5	3	8	0	0
227. DICACONO	G	0	211.08860	300	5000	3	5	3	8	0	0
228. CACACOH	G	0	182.09047	300	5000	3	6	2	7	0	0
229. DICACOH	G	0	182.09047	300	5000	3	6	2	7	0	0

REACTIONS CONSIDERED	(k = A T**b exp(-E/RT)) A	b	E
1. NG(+M)=CACACOJ+NO2(+M)	1.00E+00	0.0	0.0
I01: 1.7500E+81 -2.1850E+01 5.3461E+04 1.0000E-03			
I02: 2.2200E+79 -2.0900E+01 5.4255E+04 1.0000E-02			
I03: 3.5400E+78 -2.0360E+01 5.5205E+04 1.0000E-01			
I04: 2.1000E+58 -1.3800E+01 4.9612E+04 1.0000E+00			
I05: 6.5000E+50 -1.1280E+01 4.7942E+04 1.0000E+01			
I06: 9.1000E+48 -1.0640E+01 4.7596E+04 2.5000E+01			
I07: 8.6600E+45 -9.6600E+00 4.6769E+04 5.0000E+01			
I08: 2.0600E+44 -9.1300E+00 4.6324E+04 7.5000E+01			
I09: 1.4300E+43 -8.7600E+00 4.6002E+04 1.0000E+02			
2. NG(+M)=DICACOJ+NO2(+M)	1.00E+00	0.0	0.0
I01: 2.6200E+83 -2.2880E+01 5.4695E+04 1.0000E-03			
I02: 5.3600E+81 -2.1980E+01 5.5646E+04 1.0000E-02			
I03: 1.1700E+81 -2.1460E+01 5.6720E+04 1.0000E-01			
I04: 3.0200E+60 -1.4770E+01 5.1073E+04 1.0000E+00			
I05: 6.1200E+52 -1.2180E+01 4.9391E+04 1.0000E+01			
I06: 7.4700E+50 -1.1520E+01 4.9042E+04 2.5000E+01			
I07: 5.6800E+47 -1.0500E+01 4.8193E+04 5.0000E+01			
I08: 1.1900E+46 -9.9600E+00 4.7736E+04 7.5000E+01			
I09: 7.5500E+44 -9.5700E+00 4.7405E+04 1.0000E+02			
3. NG(+M)=CACACDO+HONO(+M)	1.00E+00	0.0	0.0
I01: 3.5017E+88 -2.4421E+01 5.7103E+04 1.0000E-03			
I02: 2.3250E+87 -2.3619E+01 5.8421E+04 1.0000E-02			
I03: 1.1188E+87 -2.3156E+01 5.9789E+04 1.0000E-01			
I04: 5.5001E+65 -1.6208E+01 5.4053E+04 1.0000E+00			
I05: 4.4749E+57 -1.3464E+01 5.2354E+04 1.0000E+01			
I06: 4.0535E+55 -1.2751E+01 5.1996E+04 2.5000E+01			
I07: 1.8492E+52 -1.1662E+01 5.1101E+04 5.0000E+01			
I08: 2.9305E+50 -1.1079E+01 5.0616E+04 7.5000E+01			

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I09:   1.4791E+49 -1.0662E+01  5.0263E+04  1.0000E+02
4. NG(+M)=DICACDO+HONO(+M)                  1.00E+00    0.0        0.0
I01:   4.9300E+84 -2.3710E+01  5.5315E+04  1.0000E-03
I02:   1.3300E+83 -2.2830E+01  5.6353E+04  1.0000E-02
I03:   3.4800E+82 -2.2330E+01  5.7496E+04  1.0000E-01
I04:   5.9600E+61 -1.5570E+01  5.1825E+04  1.0000E+00
I05:   9.7200E+53 -1.2950E+01  5.0139E+04  1.0000E+01
I06:   1.1100E+52 -1.2270E+01  4.9788E+04  2.5000E+01
I07:   7.5000E+48 -1.1240E+01  4.8929E+04  5.0000E+01
I08:   1.4800E+47 -1.0690E+01  4.8465E+04  7.5000E+01
I09:   8.9200E+45 -1.0300E+01  4.8129E+04  1.0000E+02
5. CACACOJ=CJACACOH                         5.08E+19   -1.5    19715.0
6. CJACACOH=CDOCACOH+NO2                    4.99E+11    0.2    -1712.8
7. CACACDO+H=CACACOJ                        4.61E+07    1.7     7090.0
8. CACACOJ=ACCJA+CH2O                       1.98E+13    0.3    15826.0
9. ACCJA=HCOCONO2+NO2                       6.64E+12    0.3      442.1
10. CACACOJ+NO2(+M)=CACACOONO(+M)           1.00E+00    0.0        0.0
I01:   8.2500E+98 -3.2650E+01  1.4640E+04  1.0000E-03
I02:   1.0600+102 -3.3250E+01  1.5929E+04  1.0000E-02
I03:   1.6500+106 -3.4170E+01  1.7848E+04  1.0000E-01
I04:   4.7700+111 -3.5450E+01  2.0522E+04  1.0000E+00
I05:   1.4600+118 -3.7020E+01  2.3902E+04  1.0000E+01
I06:   6.8200+120 -3.7670E+01  2.5365E+04  2.5000E+01
I07:   6.5100+122 -3.8140E+01  2.6485E+04  5.0000E+01
I08:   8.7200+123 -3.8410E+01  2.7139E+04  7.5000E+01
I09:   5.2600+124 -3.8600E+01  2.7601E+04  1.0000E+02
11. CACACOONO(+M)=>CACACQJ+NO(+M)           1.00E+00    0.0        0.0
I01:   1.2200E-01 -1.5700E+00  1.7301E+04  1.0000E-03
I02:   3.3600E+02 -2.2600E+00  1.5951E+04  1.0000E-02
I03:   5.6900E+07 -3.4300E+00  1.4345E+04  1.0000E-01
I04:   8.2900E+20 -6.8000E+00  1.5636E+04  1.0000E+00
I05:   3.0400E+43 -1.2610E+01  2.3447E+04  1.0000E+01
I06:   5.5700E+50 -1.4330E+01  2.6900E+04  2.5000E+01
I07:   1.6600E+55 -1.5310E+01  2.9401E+04  5.0000E+01
I08:   1.3700E+57 -1.5660E+01  3.0742E+04  7.5000E+01
I09:   2.5800E+58 -1.5910E+01  3.1567E+04  1.0000E+02
12. CACACOONO(+M)=CACACDO+HNO2(+M)          1.00E+00    0.0        0.0
I01:   2.3900E-03 -1.6100E+00  1.6726E+04  1.0000E-03
I02:   6.9900E+00 -2.3100E+00  1.5390E+04  1.0000E-02
I03:   1.5400E+06 -3.5200E+00  1.3870E+04  1.0000E-01
I04:   4.0500E+19 -6.9600E+00  1.5468E+04  1.0000E+00
I05:   2.5300E+41 -1.2540E+01  2.3218E+04  1.0000E+01
I06:   2.1700E+48 -1.4170E+01  2.6568E+04  2.5000E+01
I07:   4.1100E+52 -1.5110E+01  2.8994E+04  5.0000E+01
I08:   2.5600E+54 -1.5430E+01  3.0281E+04  7.5000E+01
I09:   4.2800E+55 -1.5660E+01  3.1081E+04  1.0000E+02
13. CACACOJ+NO2=CACACDO+HONO                1.27E+18   -1.4     6517.4
14. CACACOJ+NO2=CACACDO+HNO2                4.09E+16   -1.4     1916.5
15. DICACOJ+NO2(+M)=DICACOONO(+M)           1.00E+00    0.0        0.0
I01:   7.2600+107 -3.4570E+01  2.2317E+04  1.0000E-03
I02:   5.2700+113 -3.5950E+01  2.5422E+04  1.0000E-02
I03:   6.6000+119 -3.7390E+01  2.8905E+04  1.0000E-01
I04:   1.1500+125 -3.8560E+01  3.2302E+04  1.0000E+00
I05:   2.5000+128 -3.9150E+01  3.5156E+04  1.0000E+01
I06:   1.0100+129 -3.9170E+01  3.6054E+04  2.5000E+01
I07:   1.4500+129 -3.9090E+01  3.6627E+04  5.0000E+01
I08:   1.3300+129 -3.9010E+01  3.6917E+04  7.5000E+01
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I09:   1.1000+129 -3.8930E+01  3.7101E+04  1.0000E+02
16. DICACOONO(+M)=>DICACQJ+NO(+M)            1.00E+00    0.0        0.0
I01:   3.0400E+23 -7.6700E+00  1.7342E+04  1.0000E-03
I02:   8.7700E+34 -1.0340E+01  2.1406E+04  1.0000E-02
I03:   9.1500E+47 -1.3380E+01  2.7930E+04  1.0000E-01
I04:   5.9400E+52 -1.4000E+01  3.2254E+04  1.0000E+00
I05:   2.8800E+48 -1.1980E+01  3.3314E+04  1.0000E+01
I06:   4.7100E+47 -1.1500E+01  3.3979E+04  2.5000E+01
I07:   8.9000E+45 -1.0800E+01  3.4049E+04  5.0000E+01
I08:   6.1200E+44 -1.0360E+01  3.4012E+04  7.5000E+01
I09:   6.6200E+43 -1.0000E+01  3.3924E+04  1.0000E+02
17. DICACOONO(+M)=DICACDO+HNO2(+M)           1.00E+00    0.0        0.0
I01:   1.6000E+21 -7.2200E+00  1.7695E+04  1.0000E-03
I02:   1.0500E+35 -1.0550E+01  2.2426E+04  1.0000E-02
I03:   8.2100E+46 -1.3250E+01  2.8253E+04  1.0000E-01
I04:   4.1200E+52 -1.4060E+01  3.3128E+04  1.0000E+00
I05:   3.0000E+48 -1.2050E+01  3.4370E+04  1.0000E+01
I06:   5.0000E+47 -1.1560E+01  3.5082E+04  2.5000E+01
I07:   9.5400E+45 -1.0860E+01  3.5186E+04  5.0000E+01
I08:   6.1500E+44 -1.0410E+01  3.5156E+04  7.5000E+01
I09:   6.6700E+43 -1.0050E+01  3.5081E+04  1.0000E+02
18. DICACOJ+NO2=DICACDO+HONO                 3.45E+16   -1.1     3349.2
19. DICACOJ+NO2=DICACDO+HNO2                 3.80E+17   -1.3     6501.3
20. DICACOJ=HCOCONO2+CH2O+NO2                1.11E+12    0.5    13982.0
21. DICACOJ=DICACDO+H                        4.16E+11    0.7    35213.0
22. NG+NO2=NG1J+HONO                         1.58E-11    7.1       17.1
23. NG+NO2=NG1J+HNO2                         6.64E-08    6.2       24.5
24. NG+NO2=NG2J+HONO                         2.20E-20    9.4    14543.0
25. NG+NO2=NG2J+HNO2                         3.23E-10    6.5    22879.0
26. NG1J=CACACDO+NO2                         6.89E+08    1.2    -2218.9
27. NG2J=DICACDO+NO2                         1.01E+12    0.3      273.4
28. NG+NO2=CACACOJ+N2O4                      1.17E+00    4.1    39013.0
29. NG+NO2=DICACOJ+N2O4                      6.93E-01    4.0    35940.0
30. CACACOJ+NO(+M)=CACACONO(+M)              1.00E+00    0.0        0.0
I01:   2.7200+136 -4.1120E+01  2.9621E+04  1.0000E-03
I02:   4.4900+138 -4.1400E+01  3.1775E+04  1.0000E-02
I03:   4.6100+139 -4.1320E+01  3.3609E+04  1.0000E-01
I04:   9.7300+138 -4.0720E+01  3.4898E+04  1.0000E+00
I05:   1.8300+136 -3.9520E+01  3.5459E+04  1.0000E+01
I06:   3.5300+134 -3.8850E+01  3.5448E+04  2.5000E+01
I07:   1.0100+133 -3.8280E+01  3.5344E+04  5.0000E+01
I08:   9.9800+131 -3.7910E+01  3.5244E+04  7.5000E+01
I09:   1.7400+131 -3.7640E+01  3.5155E+04  1.0000E+02
31. CACACONO(+M)=CACACDO+HNO(+M)             1.00E+00    0.0        0.0
I01:   1.1500E+70 -1.9720E+01  4.9929E+04  1.0000E-03
I02:   8.3500E+73 -2.0560E+01  5.2504E+04  1.0000E-02
I03:   3.3900E+75 -2.0690E+01  5.4439E+04  1.0000E-01
I04:   2.3700E+74 -1.9980E+01  5.5446E+04  1.0000E+00
I05:   1.8000E+71 -1.8700E+01  5.5704E+04  1.0000E+01
I06:   1.2600E+70 -1.8230E+01  5.5777E+04  2.5000E+01
I07:   3.8100E+69 -1.8000E+01  5.5896E+04  5.0000E+01
I08:   8.9000E+67 -1.7440E+01  5.5572E+04  7.5000E+01
I09:   3.3800E+67 -1.7280E+01  5.5550E+04  1.0000E+02
32. CACACOJ+NO=CACACDO+HNO                   1.66E+17   -1.4     3590.2
33. DICACOJ+NO(+M)=DICACONO(+M)              1.00E+00    0.0        0.0
I01:   7.7300+135 -4.0900E+01  2.9631E+04  1.0000E-03
I02:   9.4100+137 -4.1140E+01  3.1756E+04  1.0000E-02
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I03:   6.6500+138 -4.1000E+01  3.3539E+04  1.0000E-01
I04:   8.6400+137 -4.0350E+01  3.4750E+04  1.0000E+00
I05:   8.7600+134 -3.9060E+01  3.5209E+04  1.0000E+01
I06:   1.2900+133 -3.8360E+01  3.5151E+04  2.5000E+01
I07:   3.0000+131 -3.7760E+01  3.5011E+04  5.0000E+01
I08:   2.6400+130 -3.7380E+01  3.4890E+04  7.5000E+01
I09:   4.2400+129 -3.7100E+01  3.4786E+04  1.0000E+02
34. DICACONO(+M)=DICACDO+HNO(+M)             1.00E+00    0.0        0.0
I01:   2.6000E+69 -1.9360E+01  4.9420E+04  1.0000E-03
I02:   2.2500E+72 -1.9930E+01  5.1667E+04  1.0000E-02
I03:   2.6100E+73 -1.9960E+01  5.3175E+04  1.0000E-01
I04:   2.2400E+71 -1.9020E+01  5.3698E+04  1.0000E+00
I05:   2.7200E+68 -1.7830E+01  5.3902E+04  1.0000E+01
I06:   4.6400E+66 -1.7180E+01  5.3747E+04  2.5000E+01
I07:   5.9700E+65 -1.6840E+01  5.3725E+04  5.0000E+01
I08:   8.8300E+64 -1.6550E+01  5.3611E+04  7.5000E+01
I09:   1.2200E+64 -1.6250E+01  5.3437E+04  1.0000E+02
35. DICACOJ+NO=DICACDO+HNO                   5.05E+17   -1.3     3802.4
36. NG(+M)=NG2J+H(+M)                        1.00E+00    0.0        0.0
I01:   1.3600E+60 -3.3920E+01  9.8759E+04  1.0000E-03
I02:   1.1600E+86 -3.7820E+01  1.0086E+05  1.0000E-02
I03:   4.8700+119 -4.3330E+01  1.0818E+05  1.0000E-01
I04:   1.1400+109 -3.5760E+01  1.0758E+05  1.0000E+00
I05:   1.4700+114 -3.4580E+01  1.1515E+05  1.0000E+01
I06:   8.4300+116 -3.4630E+01  1.1857E+05  2.5000E+01
I07:   4.4300+113 -3.3080E+01  1.1927E+05  5.0000E+01
I08:   3.9600+111 -3.2160E+01  1.1958E+05  7.5000E+01
I09:   7.3400+109 -3.1440E+01  1.1967E+05  1.0000E+02
37. NG(+M)=NG1J+H(+M)                        1.00E+00    0.0        0.0
I01:   1.1438E+57 -3.3920E+01  1.0171E+05  1.0000E-03
I02:   1.5076E+83 -3.7870E+01  1.0360E+05  1.0000E-02
I03:   6.3195+118 -4.3840E+01  1.1033E+05  1.0000E-01
I04:   2.2014+110 -3.6510E+01  1.0941E+05  1.0000E+00
I05:   4.3920+116 -3.5390E+01  1.1736E+05  1.0000E+01
I06:   1.0965+120 -3.5550E+01  1.2109E+05  2.5000E+01
I07:   1.3326+117 -3.4060E+01  1.2202E+05  5.0000E+01
I08:   1.9239+115 -3.3180E+01  1.2246E+05  7.5000E+01
I09:   4.8286+113 -3.2481E+01  1.2265E+05  1.0000E+02
38. CACACOJ+NO2(+M)=CACACDO+HNO2(+M)         1.00E+00    0.0        0.0
I01:   1.6600E+11 -6.2000E-01  1.7255E+04  1.0000E-03
I02:   1.6600E+11 -6.2000E-01  1.7255E+04  1.0000E-02
I03:   1.6600E+11 -6.2000E-01  1.7255E+04  1.0000E-01
I04:   1.6600E+11 -6.2000E-01  1.7256E+04  1.0000E+00
I05:   3.0500E+11 -7.0000E-01  1.7396E+04  1.0000E+01
I06:   1.2900E+12 -8.8000E-01  1.7732E+04  2.5000E+01
I07:   9.5800E+12 -1.1300E+00  1.8204E+04  5.0000E+01
I08:   4.5400E+13 -1.3300E+00  1.8575E+04  7.5000E+01
I09:   1.6000E+14 -1.4900E+00  1.8879E+04  1.0000E+02
39. CACACOJ+NO2(+M)=>CACACQJ+NO(+M)          1.00E+00    0.0        0.0
I01:   6.1200E+13 -7.2000E-01  1.7939E+04  1.0000E-03
I02:   6.1200E+13 -7.2000E-01  1.7939E+04  1.0000E-02
I03:   6.1200E+13 -7.2000E-01  1.7939E+04  1.0000E-01
I04:   6.1300E+13 -7.2000E-01  1.7940E+04  1.0000E+00
I05:   9.8700E+13 -7.8000E-01  1.8050E+04  1.0000E+01
I06:   3.5200E+14 -9.4000E-01  1.8345E+04  2.5000E+01
I07:   2.2500E+15 -1.1700E+00  1.8781E+04  5.0000E+01
I08:   9.8900E+15 -1.3600E+00  1.9133E+04  7.5000E+01
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I09:   3.3300E+16 -1.5100E+00  1.9425E+04  1.0000E+02
40. DICACOJ+NO2(+M)=DICACDO+HNO2(+M)         1.00E+00    0.0         0.0
I01:   1.7900E+09  1.0000E-02  1.6544E+04  1.0000E-03
I02:   2.5900E+09 -4.0000E-02  1.6629E+04  1.0000E-02
I03:   1.6900E+11 -5.7000E-01  1.7614E+04  1.0000E-01
I04:   9.3500E+15 -1.9300E+00  2.0351E+04  1.0000E+00
I05:   1.0700E+21 -3.3600E+00  2.3832E+04  1.0000E+01
I06:   1.9900E+22 -3.7000E+00  2.5057E+04  2.5000E+01
I07:   6.7600E+22 -3.8200E+00  2.5851E+04  5.0000E+01
I08:   9.0300E+22 -3.8400E+00  2.6254E+04  7.5000E+01
I09:   9.0900E+22 -3.8300E+00  2.6511E+04  1.0000E+02
41. DICACOJ+NO2(+M)=>DICACQJ+NO(+M)          1.00E+00    0.0         0.0
I01:   4.4600E+09 -9.0000E-02  1.5438E+04  1.0000E-03
I02:   8.1000E+09 -1.7000E-01  1.5576E+04  1.0000E-02
I03:   1.1200E+12 -7.9000E-01  1.6742E+04  1.0000E-01
I04:   9.4700E+16 -2.2100E+00  1.9606E+04  1.0000E+00
I05:   9.2600E+21 -3.6100E+00  2.3091E+04  1.0000E+01
I06:   1.5300E+23 -3.9300E+00  2.4302E+04  2.5000E+01
I07:   4.7800E+23 -4.0500E+00  2.5085E+04  5.0000E+01
I08:   6.0900E+23 -4.0600E+00  2.5481E+04  7.5000E+01
I09:   5.9500E+23 -4.0400E+00  2.5734E+04  1.0000E+02
42. CACACOJ+NO(+M)=CACACDO+HNO(+M)           1.00E+00    0.0         0.0
I01:   3.4100E+13 -1.4900E+00  3.4600E+03  1.0000E-03
I02:   6.4300E+17 -2.7100E+00  6.0070E+03  1.0000E-02
I03:   5.0900E+22 -4.1100E+00  9.1120E+03  1.0000E-01
I04:   2.2000E+27 -5.4100E+00  1.2414E+04  1.0000E+00
I05:   3.6300E+30 -6.2700E+00  1.5413E+04  1.0000E+01
I06:   1.6000E+31 -6.4300E+00  1.6415E+04  2.5000E+01
I07:   2.4900E+31 -6.4500E+00  1.7076E+04  5.0000E+01
I08:   2.4100E+31 -6.4300E+00  1.7418E+04  7.5000E+01
I09:   2.0500E+31 -6.4000E+00  1.7640E+04  1.0000E+02
43. DICACOJ+NO(+M)=DICACDO+HNO(+M)           1.00E+00    0.0         0.0
I01:   1.1800E+16 -2.3000E+00  3.4670E+03  1.0000E-03
I02:   3.6900E+20 -3.5900E+00  6.2180E+03  1.0000E-02
I03:   2.5500E+25 -4.9600E+00  9.4000E+03  1.0000E-01
I04:   4.9100E+29 -6.1500E+00  1.2642E+04  1.0000E+00
I05:   2.1900E+32 -6.8500E+00  1.5472E+04  1.0000E+01
I06:   5.3000E+32 -6.9200E+00  1.6387E+04  2.5000E+01
I07:   5.1400E+32 -6.8800E+00  1.6976E+04  5.0000E+01
I08:   3.7500E+32 -6.8300E+00  1.7274E+04  7.5000E+01
I09:   2.6000E+32 -6.7600E+00  1.7465E+04  1.0000E+02
44. NG+H=NG2J+H2                             2.40E+08    1.5      4124.8
45. NG+O=NG2J+OH                             1.70E+08    1.5      1584.9
46. NG+OH=NG2J+H2O                           1.20E+06    2.0         0.0
47. NG+CH3=NG2J+CH4                          8.10E+05    1.9      7306.3
48. NG+NH2=NG2J+NH3                          9.20E+05    1.9      6105.0
49. NG+O2=NG2J+HO2                           1.29E+02    3.0     44425.0
50. NG+H=NG1J+H2                             9.60E+08    1.5      5918.8
51. NG+O=NG1J+OH                             6.80E+08    1.5      3654.9
52. NG+OH=NG1J+H2O                           4.80E+06    2.0        62.1
53. NG+CH3=NG1J+CH4                          3.24E+06    1.9      9100.3
54. NG+NH2=NG1J+NH3                          3.68E+06    1.9      6739.8
55. NG+O2=NG1J+HO2                           5.14E+02    3.0     47185.0
56. NG+H2O=CACACOH+HNO3                      8.64E+00    3.0     41090.0
57. CACACOH+HNO3=H2O+CACACDO+HONO            4.56E-02    3.9     56218.0
58. NG+H2O=DICACOH+HNO3                      7.93E+00    3.0     38752.0
59. DICACOH+HNO3=H2O+DICACDO+HONO            3.28E-02    3.9     57190.0
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60.	CACACOJ+H=CACACDO+H2	4.57E+12	0.0	449.7
61.	CACACOJ+HO2=CACACDO+H2O2	1.06E+17	-1.4	4563.8
62.	CACACOJ+O2=CACACDO+HO2	4.90E+17	-1.4	6320.4
63.	CACACOJ+O=CACACDO+OH	3.80E+14	-0.7	278.1
64.	CACACOJ+OH=CACACDO+H2O	3.37E+13	-0.2	473.3
65.	DICACOJ+H=DICACDO+H2	2.88E+12	0.1	-288.1
66.	DICACOJ+HO2=DICACDO+H2O2	3.45E+16	-1.1	3349.2
67.	DICACOJ+O2=DICACDO+HO2	2.23E+17	-1.4	6385.5
68.	DICACOJ+O=DICACDO+OH	4.73E+12	0.0	-546.7
69.	DICACOJ+OH=DICACDO+H2O	4.86E+11	0.1	-1072.8
70.	DICACDO=HCOCDOCA+HONO	7.63E+17	-1.0	41823.0
71.	DICACDO=CACDOCOJ+NO2	5.53E+17	-1.0	35980.0
72.	DICACDO=DICJACDO+H	1.43E+14	0.0	90970.0
73.	CACDOCOJ+H=HCOCDOCA+H2	1.73E+09	0.1	-300.6
74.	CACDOCOJ+HO2=HCOCDOCA+H2O2	1.86E+17	-1.3	4754.3
75.	CACDOCOJ+NO2=HCOCDOCA+HNO2	9.15E+15	-1.1	2130.8
76.	CACDOCOJ+NO2=HCOCDOCA+HONO	4.30E+17	-1.4	4832.3
77.	CACDOCOJ+O2=HCOCDOCA+HO2	1.70E+17	-1.5	4872.0
78.	CACDOCOJ+O=HCOCDOCA+OH	9.23E+15	-0.9	-54.4
79.	CACDOCOJ+OH=HCOCDOCA+H2O	1.26E+17	-1.2	1496.2
80.	CACDOCOJ+NO=HCOCDOCA+HNO	1.49E+17	-1.4	4953.7
81.	CACDOCOJ=CDJOCA+CH2O	3.61E+13	0.2	6106.2
82.	CACDOCOJ=CJACDOCOH	6.38E+18	-1.4	18401.0
83.	CJACDOCOH=ODCCDOCOH+NO2	2.69E+12	0.2	314.7
84.	DICACDO+H=DICJACDO+H2	9.60E+08	1.5	835.8
85.	DICACDO+O=DICJACDO+OH	6.80E+08	1.5	0.0
86.	DICACDO+OH=DICJACDO+H2O	4.80E+06	2.0	0.0
87.	DICACDO+CH3=DICJACDO+CH4	3.24E+06	1.9	4017.3
88.	DICACDO+NH2=DICJACDO+NH3	3.68E+06	1.9	4941.2
89.	DICACDO+NO2=DICJACDO+HONO	2.50E+07	1.3	16025.0
90.	DICACDO+NO2=DICJACDO+HNO2	2.84E-02	4.6	20739.0
91.	DICACDO+O2=DICJACDO+HO2	5.14E+02	3.0	39365.0
92.	DICJACDO=HCOCDOCA+NO2	2.04E+12	0.2	540.4
93.	CACACDO=DICDOCA+HONO	1.31E+18	-1.0	43066.0
94.	CACACDO=HCOCDOCA+HONO	1.11E+18	-1.1	38244.0
95.	CACACDO=HCOCOJCA+NO2	4.62E+15	-0.4	38424.0
96.	CACACDO=HCOCACOJ+NO2	5.62E+17	-0.9	38148.0
97.	CACACDO=CACACDJO+H	3.04E+15	0.0	89610.0
98.	CACACDO=CACJACDO+H	2.27E+14	0.0	89060.0
99.	CACACDO=CJACACDO+H	1.14E+17	0.0	98430.0
100.	HCOCOJCA+H=HCOCDOCA+H2	2.71E+14	-0.5	841.2
101.	HCOCOJCA+HO2=HCOCDOCA+H2O2	1.52E+16	-1.2	3297.0
102.	HCOCOJCA+NO2=HCOCDOCA+HNO2	4.34E+15	-0.3	2856.5
103.	HCOCOJCA+NO2=HCOCDOCA+HONO	8.82E+17	-1.3	7032.2
104.	HCOCOJCA+O2=HCOCDOCA+HO2	8.57E+17	-1.4	7563.3
105.	HCOCOJCA+O=HCOCDOCA+OH	5.60E+08	1.5	8107.5
106.	HCOCOJCA+OH=HCOCDOCA+H2O	3.72E+14	-0.6	31.4
107.	HCOCOJCA+NO=HCOCDOCA+HNO	5.69E+16	-1.2	4508.1
108.	HCOCOJCA=CHOCHO+CH2O+NO2	3.54E+12	0.4	13693.0
109.	HCOCOJCA=HCOCONO2+HCO	1.03E+13	0.3	6877.8
110.	HCOCACOJ+H=DICDOCA+H2	4.57E+12	0.0	449.7
111.	HCOCACOJ+HO2=DICDOCA+H2O2	1.06E+17	-1.4	4563.8
112.	HCOCACOJ+NO2=DICDOCA+HNO2	4.09E+16	-1.4	1916.5
113.	HCOCACOJ+NO2=DICDOCA+HONO	1.27E+18	-1.4	6517.4
114.	HCOCACOJ+O2=DICDOCA+HO2	4.90E+17	-1.4	6320.4
115.	HCOCACOJ+O=DICDOCA+OH	3.80E+14	-0.7	278.1
116.	HCOCACOJ+OH=DICDOCA+H2O	3.37E+13	-0.2	473.3

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117. HCOCACOJ+NO=DICDOCA+HNO                  1.66E+17   -1.4     3590.2
118. HCOCACOJ=HCOCJONO2+CH2O                  2.66E+12    0.3    10255.0
119. HCOCACOJ=ODCJCACOH                       2.18E+18   -1.5     9413.7
120. ODCJCACOH=CO+COHCDO+NO2                  2.10E+11    0.8    12539.0
121. CACACDO+H=CACACDJO+H2                    2.40E+08    1.5      341.8
122. CACACDO+O=CACACDJO+OH                    1.70E+08    1.5        0.0
123. CACACDO+OH=CACACDJO+H2O                  1.20E+06    2.0        0.0
124. CACACDO+CH3=CACACDJO+CH4                 8.10E+05    1.9     3523.3
125. CACACDO+NH2=CACACDJO+NH3                 9.20E+05    1.9     4766.4
126. CACACDO+O2=CACACDJO+HO2                  1.29E+02    3.0    38605.0
127. CACACDJO=ACCJA+CO                        8.16E+12    0.3    12051.0
128. CACACDO+NO2=CACACDJO+HONO                4.39E-03    4.4    11026.0
129. CACACDO+NO2=CACACDJO+HNO2                4.63E+01    3.3    17579.0
130. CACACDJO+NO2=HCOCONO2+NO2+CO2+NO         8.39E+15   -0.8     1930.0
131. OH+CACACDO=CACACDOOJ                     7.25E+03    0.9       47.0
132. CACACDOOJ=HOCHO+HCOCONO2+NO2             3.71E+13    0.2     5596.6
133. CACACDJO+OH(+M)=CACACDOOH(+M)            1.00E+00    0.0        0.0
I01:   1.6400+114 -3.5050E+01  2.2666E+04  1.0000E-03
I02:   5.9600+115 -3.4220E+01  2.5800E+04  1.0000E-02
I03:   3.2200+106 -3.0290E+01  2.6215E+04  1.0000E-01
I04:   4.0700E+86 -2.3440E+01  2.2228E+04  1.0000E+00
I05:   9.6800E+61 -1.5430E+01  1.5514E+04  1.0000E+01
I06:   1.9100E+52 -1.2340E+01  1.2612E+04  2.5000E+01
I07:   2.3000E+45 -1.0150E+01  1.0483E+04  5.0000E+01
I08:   4.0200E+41 -8.9600E+00  9.3090E+03  7.5000E+01
I09:   1.2700E+39 -8.1700E+00  8.5220E+03  1.0000E+02
134. CACACDJO+OH(+M)=CDCONO2+CO2+HNO3(+M)     1.00E+00    0.0        0.0
I01:   1.5700E+13 -6.0000E-02  7.3000E+01  1.0000E-03
I02:   6.9700E+14 -5.4000E-01  1.0280E+03  1.0000E-02
I03:   2.7000E+18 -1.5400E+00  3.6530E+03  1.0000E-01
I04:   8.6800E+17 -1.3000E+00  5.3250E+03  1.0000E+00
I05:   7.4500E+10  8.8000E-01  4.5300E+03  1.0000E+01
I06:   4.3700E+06  2.1500E+00  3.5920E+03  2.5000E+01
I07:   1.4300E+03  3.1900E+00  2.7260E+03  5.0000E+01
I08:   1.1600E+01  3.8000E+00  2.1780E+03  7.5000E+01
I09:   3.8200E-01  4.2400E+00  1.7790E+03  1.0000E+02
135. CACACDOOH(+M)=CDCONO2+CO2+HNO3(+M)      1.00E+00    0.0        0.0
I01:   6.6900E+62 -1.5120E+01  7.1823E+04  1.0000E-03
I02:   8.9700E+53 -1.2230E+01  6.9450E+04  1.0000E-02
I03:   1.9100E+44 -9.1300E+00  6.6621E+04  1.0000E-01
I04:   2.3100E+35 -6.3000E+00  6.3875E+04  1.0000E+00
I05:   3.4600E+27 -3.8400E+00  6.1375E+04  1.0000E+01
I06:   6.7400E+24 -3.0000E+00  6.0492E+04  2.5000E+01
I07:   8.7100E+22 -2.4100E+00  5.9874E+04  5.0000E+01
I08:   6.3200E+21 -2.0500E+00  5.9498E+04  7.5000E+01
I09:   8.8600E+20 -1.7800E+00  5.9217E+04  1.0000E+02
136. CACACDO+H=CACJACDO+H2                    2.40E+08    1.5      -15.7
137. CACACDO+O=CACJACDO+OH                    1.70E+08    1.5        0.0
138. CACACDO+OH=CACJACDO+H2O                  1.20E+06    2.0        0.0
139. CACACDO+CH3=CACJACDO+CH4                 8.10E+05    1.9     3165.8
140. CACACDO+NH2=CACJACDO+NH3                 9.20E+05    1.9     4639.9
141. CACACDO+NO2=CACJACDO+HONO                2.50E+07    1.3    14944.0
142. CACACDO+NO2=CACJACDO+HNO2                7.10E-03    4.6    19429.0
143. CACACDO+O2=CACJACDO+HO2                  1.29E+02    3.0    38055.0
144. CACJACDO=HCOCDOCA+NO2                    2.50E+12    0.2    -1073.6
145. CACACDO+H=CJACACDO+H2                    4.80E+08    1.5     6074.8
146. CACACDO+O=CJACACDO+OH                    3.40E+08    1.5     3834.9
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147.	CACACDO+OH=CJACACDO+H2O	2.40E+06	2.0	182.1
148.	CACACDO+CH3=CJACACDO+CH4	1.62E+06	1.9	9256.3
149.	CACACDO+NH2=CJACACDO+NH3	1.84E+06	1.9	6795.0
150.	CACACDO+NO2=CJACACDO+HONO	2.50E+07	1.3	22674.0
151.	CACACDO+NO2=CJACACDO+HNO2	1.42E-02	4.6	28799.0
152.	CACACDO+O2=CJACACDO+HO2	2.57E+02	3.0	47425.0
153.	CJACACDO=DICDOCA+NO2	2.00E+13	0.0	911.0
154.	HCOCDOCA=ODCICDO2+HONO	3.06E+17	-1.0	39201.0
155.	HCOCDOCA=ODCCDOCOJ+NO2	4.35E+17	-0.9	37832.0
156.	HCOCDOCA=HCOCDOCJA+H	1.03E+14	0.0	87800.0
157.	HCOCDOCA=CDJOCDOCA+H	7.89E+14	0.0	87230.0
158.	ODCCDOCOJ+H=ODCICDO2+H2	1.73E+09	0.1	-300.6
159.	ODCCDOCOJ+HO2=ODCICDO2+H2O2	1.86E+17	-1.3	4754.3
160.	ODCCDOCOJ+NO2=ODCICDO2+HNO2	9.15E+15	-1.1	2130.8
161.	ODCCDOCOJ+NO2=ODCICDO2+HONO	4.30E+17	-1.4	4832.3
162.	ODCCDOCOJ+O2=ODCICDO2+HO2	1.70E+17	-1.5	4872.0
163.	ODCCDOCOJ+O=ODCICDO2+OH	9.23E+15	-0.9	-54.4
164.	ODCCDOCOJ+OH=ODCICDO2+H2O	1.26E+17	-1.2	1496.2
165.	ODCCDOCOJ+NO=ODCICDO2+HNO	1.49E+17	-1.4	4953.7
166.	HCOCDOCA+H=HCOCDOCJA+H2	4.80E+08	1.5	-834.7
167.	HCOCDOCA+O=HCOCDOCJA+OH	3.40E+08	1.5	0.0
168.	HCOCDOCA+OH=HCOCDOCJA+H2O	2.40E+06	2.0	0.0
169.	HCOCDOCA+CH3=HCOCDOCJA+CH4	1.62E+06	1.9	2346.8
170.	HCOCDOCA+NH2=HCOCDOCJA+NH3	1.84E+06	1.9	4350.1
171.	HCOCDOCA+NO2=HCOCDOCJA+HONO	2.50E+07	1.3	13904.0
172.	HCOCDOCA+NO2=HCOCDOCJA+HNO2	1.42E-02	4.6	18169.0
173.	HCOCDOCA+O2=HCOCDOCJA+HO2	2.57E+02	3.0	36795.0
174.	HCOCDOCJA=ODCICDO2+NO2	7.47E+12	0.3	4456.7
175.	HCOCDOCA+H=CDJOCDOCA+H2	2.40E+08	1.5	0.0
176.	HCOCDOCA+O=CDJOCDOCA+OH	1.70E+08	1.5	0.0
177.	HCOCDOCA+OH=CDJOCDOCA+H2O	1.20E+06	2.0	0.0
178.	HCOCDOCA+CH3=CDJOCDOCA+CH4	8.10E+05	1.9	1976.3
179.	HCOCDOCA+NH2=CDJOCDOCA+NH3	9.20E+05	1.9	4219.0
180.	HCOCDOCA+O2=CDJOCDOCA+HO2	1.29E+02	3.0	36225.0
181.	CDJOCDOCA=CDJOCA+CO	1.30E+13	0.6	8400.6
182.	HCOCDOCA+NO2=CDJOCDOCA+HONO	4.39E-03	4.4	11026.0
183.	HCOCDOCA+NO2=CDJOCDOCA+HNO2	4.63E+01	3.3	17579.0
184.	CDJOCDOCA+NO2=CDJOCA+CO2+NO	8.39E+15	-0.8	1930.0
185.	DICDOCA=ODCICDO2+HONO	1.87E+18	-1.0	39070.0
186.	DICDOCA=DICDOCOJ+NO2	5.00E+16	-0.7	36847.0
187.	DICDOCA=DICDOCJA+H	5.92E+14	0.0	82280.0
188.	DICDOCA=DICDJOCA+H	7.22E+14	0.0	89740.0
189.	DICDOCOJ+H=ODCICDO2+H2	1.73E+09	0.1	-300.6
190.	DICDOCOJ+HO2=ODCICDO2+H2O2	1.86E+17	-1.3	4754.3
191.	DICDOCOJ+NO2=ODCICDO2+HNO2	9.15E+15	-1.1	2130.8
192.	DICDOCOJ+NO2=ODCICDO2+HONO	4.30E+17	-1.4	4832.3
193.	DICDOCOJ+O2=ODCICDO2+HO2	1.70E+17	-1.5	4872.0
194.	DICDOCOJ+O=ODCICDO2+OH	9.23E+15	-0.9	-54.4
195.	DICDOCOJ+OH=ODCICDO2+H2O	1.26E+17	-1.2	1496.2
196.	DICDOCOJ+NO=ODCICDO2+HNO	1.49E+17	-1.4	4953.7
197.	DICDOCOJ=CHOCHO+HCO	3.15E+12	0.4	4903.0
198.	DICDOCA+H=DICDOCJA+H2	2.40E+08	1.5	0.0
199.	DICDOCA+O=DICDOCJA+OH	1.70E+08	1.5	0.0
200.	DICDOCA+OH=DICDOCJA+H2O	1.20E+06	2.0	0.0
201.	DICDOCA+CH3=DICDOCJA+CH4	8.10E+05	1.9	0.0
202.	DICDOCA+NH2=DICDOCJA+NH3	9.20E+05	1.9	3080.5
203.	DICDOCA+NO2=DICDOCJA+HONO	2.50E+07	1.3	9350.5

204.	DICDOCA+NO2=DICDOCJA+HNO2	7.10E-03	4.6	12649.0
205.	DICDOCA+O2=DICDOCJA+HO2	1.29E+02	3.0	31275.0
206.	DICDOCJA=ODCICDO2+NO2	1.00E+13	0.2	1940.3
207.	DICDOCA+H=DICDJOCA+H2	4.80E+08	1.5	419.8
208.	DICDOCA+O=DICDJOCA+OH	3.40E+08	1.5	0.0
209.	DICDOCA+OH=DICDJOCA+H2O	2.40E+06	2.0	0.0
210.	DICDOCA+CH3=DICDJOCA+CH4	1.62E+06	1.9	3601.3
211.	DICDOCA+NH2=DICDJOCA+NH3	1.84E+06	1.9	4794.0
212.	DICDOCA+O2=DICDJOCA+HO2	2.57E+02	3.0	38725.0
213.	DICDJOCA=HCOCJONO2+CO	5.72E+11	0.7	10883.0
214.	DICDOCA+NO2=DICDJOCA+HONO	8.78E-03	4.4	11026.0
215.	DICDOCA+NO2=DICDJOCA+HNO2	9.26E+01	3.3	17579.0
216.	DICDJOCA+NO2=HCOCJONO2+CO2+NO	8.39E+15	-0.8	1930.0
217.	CDOCACOH=ODCCDOCOH+HONO	5.21E+17	-1.0	34889.0
218.	CDOCACOH=CDOCOJCOH+NO2	1.87E+18	-1.1	34725.0
219.	CDOCACOH=HCOCACOJ+H	7.35E+14	0.0	104000.0
220.	CDOCACOH=CDOCJACOH+H	8.71E+14	0.0	86900.0
221.	CDOCACOH=ODCJCACOH+H	3.14E+14	0.0	88150.0
222.	CDOCOJCOH+H=ODCCDOCOH+H2	4.02E+10	0.5	-120.1
223.	CDOCOJCOH+HO2=ODCCDOCOH+H2O2	3.24E+16	-1.1	4591.6
224.	CDOCOJCOH+NO2=ODCCDOCOH+HNO2	6.55E+15	-1.0	2213.5
225.	CDOCOJCOH+NO2=ODCCDOCOH+HONO	4.77E+17	-1.3	5113.0
226.	CDOCOJCOH+O2=ODCCDOCOH+HO2	1.78E+16	-1.4	5163.3
227.	CDOCOJCOH+O=ODCCDOCOH+OH	2.77E+12	0.3	259.1
228.	CDOCOJCOH+OH=ODCCDOCOH+H2O	3.72E+14	-0.6	31.4
229.	CDOCOJCOH+NO=ODCCDOCOH+HNO	8.22E+10	0.1	-406.6
230.	CDOCOJCOH=CHOCHO+CH2OH	1.28E+13	0.3	7525.8
231.	CDOCOJCOH=HCO+COHCDO	3.70E+13	0.3	7904.9
232.	CDOCACOH+H=HCOCACOJ+H2	2.40E+08	1.5	9675.8
233.	CDOCACOH+O=HCOCACOJ+OH	1.70E+08	1.5	7989.9
234.	CDOCACOH+OH=HCOCACOJ+H2O	1.20E+06	2.0	2952.1
235.	CDOCACOH+CH3=HCOCACOJ+CH4	8.10E+05	1.9	12857.0
236.	CDOCACOH+NH2=HCOCACOJ+NH3	9.20E+05	1.9	8069.2
237.	CDOCACOH+NO2=HCOCACOJ+HONO	2.50E+07	1.3	27244.0
238.	CDOCACOH+NO2=HCOCACOJ+HNO2	7.10E-03	4.6	34339.0
239.	CDOCACOH+O2=HCOCACOJ+HO2	1.29E+02	3.0	52965.0
240.	CDOCACOH+H=CDOCJACOH+H2	2.40E+08	1.5	0.0
241.	CDOCACOH+O=CDOCJACOH+OH	1.70E+08	1.5	0.0
242.	CDOCACOH+OH=CDOCJACOH+H2O	1.20E+06	2.0	0.0
243.	CDOCACOH+CH3=CDOCJACOH+CH4	8.10E+05	1.9	1761.8
244.	CDOCACOH+NH2=CDOCJACOH+NH3	9.20E+05	1.9	4143.1
245.	CDOCACOH+NO2=CDOCJACOH+HONO	2.50E+07	1.3	13162.0
246.	CDOCACOH+NO2=CDOCJACOH+HNO2	7.10E-03	4.6	17269.0
247.	CDOCACOH+O2=CDOCJACOH+HO2	1.29E+02	3.0	35895.0
248.	CDOCACOH+H=ODCJCACOH+H2	2.40E+08	1.5	-607.2
249.	CDOCACOH+O=ODCJCACOH+OH	1.70E+08	1.5	0.0
250.	CDOCACOH+OH=ODCJCACOH+H2O	1.20E+06	2.0	0.0
251.	CDOCACOH+CH3=ODCJCACOH+CH4	8.10E+05	1.9	2574.3
252.	CDOCACOH+NH2=ODCJCACOH+NH3	9.20E+05	1.9	4430.6
253.	CDOCACOH+O2=ODCJCACOH+HO2	1.29E+02	3.0	37145.0
254.	CDOCJACOH=ODCCDOCOH+NO2	1.04E+13	0.2	-548.8
255.	DICDOCA+H=HCOCACOJ	8.00E+12	0.0	6400.0
256.	CDOCACOH+NO2=ODCJCACOH+HONO	4.39E-03	4.4	11026.0
257.	CDOCACOH+NO2=ODCJCACOH+HNO2	4.63E+01	3.3	17579.0
258.	ODCJCACOH+NO2=COHCDO+NO2+CO2+NO	8.39E+15	-0.8	1930.0
259.	ODCCDOCOH+H=ODCCDOCOJ+H2	2.40E+08	1.5	12373.0
260.	ODCCDOCOH+O=ODCCDOCOJ+OH	1.70E+08	1.5	11102.0

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261. ODCCDOCOH+OH=ODCCDOCOJ+H2O              1.20E+06    2.0     5027.1
262. ODCCDOCOH+CH3=ODCCDOCOJ+CH4             8.10E+05    1.9    15555.0
263. ODCCDOCOH+NH2=ODCCDOCOJ+NH3             9.20E+05    1.9     9023.7
264. ODCCDOCOH+NO2=ODCCDOCOJ+HONO            2.50E+07    1.3    30668.0
265. ODCCDOCOH+NO2=ODCCDOCOJ+HNO2            7.10E-03    4.6    38489.0
266. ODCCDOCOH+O2=ODCCDOCOJ+HO2              1.29E+02    3.0    57115.0
267. ODCCDOCOJ=ODCCDJO+CH2O                  1.05E+13    0.2     7924.1
268. ODCCDOCOJ=OCJCDOCOH                     1.93E+18   -1.3     5978.9
269. ODCCDOCOH+H=OCJCDOCOH+H2                2.40E+08    1.5       10.3
270. ODCCDOCOH+O=OCJCDOCOH+OH                1.70E+08    1.5        0.0
271. ODCCDOCOH+OH=OCJCDOCOH+H2O              1.20E+06    2.0        0.0
272. ODCCDOCOH+CH3=OCJCDOCOH+CH4             8.10E+05    1.9     3191.8
273. ODCCDOCOH+NH2=OCJCDOCOH+NH3             9.20E+05    1.9     4649.1
274. ODCCDOCOH+O2=OCJCDOCOH+HO2              1.29E+02    3.0    38095.0
275. OCJCDOCOH=COHCDJO+CO                    6.16E+14    0.0     8743.2
276. ODCCDOCOH+NO2=OCJCDOCOH+HONO            4.39E-03    4.4    11026.0
277. ODCCDOCOH+NO2=OCJCDOCOH+HNO2            4.63E+01    3.3    17579.0
278. OCJCDOCOH+NO2=COHCDJO+CO2+NO            8.39E+15   -0.8     1930.0
279. ODCCDOCOH+H=ODCKCJOH+H2                 4.80E+08    1.5        0.0
280. ODCCDOCOH+O=ODCKCJOH+OH                 3.40E+08    1.5        0.0
281. ODCCDOCOH+OH=ODCKCJOH+H2O               2.40E+06    2.0        0.0
282. ODCCDOCOH+CH3=ODCKCJOH+CH4              1.62E+06    1.9        0.0
283. ODCCDOCOH+NH2=ODCKCJOH+NH3              1.84E+06    1.9     1364.7
284. ODCCDOCOH+NO2=ODCKCJOH+HONO             2.50E+07    1.3     3196.1
285. ODCCDOCOH+NO2=ODCKCJOH+HNO2             1.42E-02    4.6     5189.0
286. ODCCDOCOH+O2=ODCKCJOH+HO2               2.57E+02    3.0    23815.0
287. ODCICDO2+H=ODCKCJOH                     2.40E+13    0.0     4110.0
288. ODCKCJOH+NO2(+M)=COHONOKK(+M)           1.00E+00    0.0        0.0
I01:   1.1800E+60 -1.9450E+01  2.2934E+04  1.0000E-03
I02:   8.2800E+64 -2.0230E+01  2.3744E+04  1.0000E-02
I03:   9.5900E+69 -2.0960E+01  2.5010E+04  1.0000E-01
I04:   1.2600E+73 -2.1050E+01  2.7099E+04  1.0000E+00
I05:   1.8200E+70 -1.9410E+01  2.8357E+04  1.0000E+01
I06:   6.1800E+66 -1.8080E+01  2.8094E+04  2.5000E+01
I07:   2.0100E+63 -1.6840E+01  2.7551E+04  5.0000E+01
I08:   8.9500E+60 -1.6030E+01  2.7100E+04  7.5000E+01
I09:   1.4400E+59 -1.5420E+01  2.6724E+04  1.0000E+02
289. ODCKCJOH+NO2(+M)=COHOJKK+NO(+M)         1.00E+00    0.0        0.0
I01:   3.1000E+01  3.0000E+00  9.5490E+03  1.0000E-03
I02:   3.1100E+01  3.0000E+00  9.5490E+03  1.0000E-02
I03:   3.3600E+01  2.9900E+00  9.5690E+03  1.0000E-01
I04:   3.5900E+02  2.6900E+00  1.0183E+04  1.0000E+00
I05:   2.8700E+05  1.8800E+00  1.2318E+04  1.0000E+01
I06:   1.3900E+06  1.7100E+00  1.3214E+04  2.5000E+01
I07:   1.3300E+06  1.7400E+00  1.3740E+04  5.0000E+01
I08:   7.0400E+05  1.8400E+00  1.3959E+04  7.5000E+01
I09:   3.3300E+05  1.9500E+00  1.4069E+04  1.0000E+02
290. ODCKCJOH+NO2(+M)=HONO+ODCICDO2(+M)     1.00E+00    0.0        0.0
I01:   2.0600E+01  2.6100E+00  9.5490E+03  1.0000E-03
I02:   2.0600E+01  2.6100E+00  9.5490E+03  1.0000E-02
I03:   2.1900E+01  2.6000E+00  9.5640E+03  1.0000E-01
I04:   2.3100E+02  2.3100E+00  1.0173E+04  1.0000E+00
I05:   1.8500E+05  1.4900E+00  1.2310E+04  1.0000E+01
I06:   8.8000E+05  1.3200E+00  1.3204E+04  2.5000E+01
I07:   8.2200E+05  1.3600E+00  1.3726E+04  5.0000E+01
I08:   4.2800E+05  1.4600E+00  1.3943E+04  7.5000E+01
I09:   2.0000E+05  1.5700E+00  1.4052E+04  1.0000E+02
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291. COHONOKK(+M)=COHOJKK+NO(+M)              1.00E+00    0.0        0.0
I01:   3.1300E+59 -1.5110E+01  4.3652E+04  1.0000E-03
I02:   2.0500E+59 -1.4700E+01  4.4804E+04  1.0000E-02
I03:   5.0600E+54 -1.2970E+01  4.4424E+04  1.0000E-01
I04:   5.0600E+50 -1.1480E+01  4.4121E+04  1.0000E+00
I05:   2.4800E+44 -9.3200E+00  4.2827E+04  1.0000E+01
I06:   4.5000E+41 -8.4100E+00  4.2167E+04  2.5000E+01
I07:   2.2000E+39 -7.6600E+00  4.1560E+04  5.0000E+01
I08:   8.7100E+37 -7.2000E+00  4.1177E+04  7.5000E+01
I09:   9.0600E+36 -6.8800E+00  4.0905E+04  1.0000E+02
292. COHONOKK(+M)=HONO+ODCICDO2(+M)           1.00E+00    0.0        0.0
I01:   6.7500E+58 -1.5320E+01  4.3292E+04  1.0000E-03
I02:   3.0100E+58 -1.4880E+01  4.4367E+04  1.0000E-02
I03:   5.6300E+53 -1.3110E+01  4.3914E+04  1.0000E-01
I04:   5.0700E+49 -1.1610E+01  4.3565E+04  1.0000E+00
I05:   2.7200E+43 -9.4800E+00  4.2259E+04  1.0000E+01
I06:   5.3600E+40 -8.5800E+00  4.1602E+04  2.5000E+01
I07:   2.8200E+38 -7.8400E+00  4.1001E+04  5.0000E+01
I08:   1.1700E+37 -7.3900E+00  4.0622E+04  7.5000E+01
I09:   1.2600E+36 -7.0800E+00  4.0353E+04  1.0000E+02
293. COHOJKK=ODCCDJO+HOCHO                   5.24E+12    0.2     1938.9
294. COHOJKK=OH+ODCICDO2                     4.04E+12    0.5    29443.0
295. ODCICDO2+H=ODCJKIDO+H2                  4.80E+08    1.5        0.0
296. ODCICDO2+O=ODCJKIDO+OH                  3.40E+08    1.5        0.0
297. ODCICDO2+OH=ODCJKIDO+H2O                2.40E+06    2.0        0.0
298. ODCICDO2+CH3=ODCJKIDO+CH4               1.62E+06    1.9        0.0
299. ODCICDO2+NH2=ODCJKIDO+NH3               1.84E+06    1.9     1601.6
300. ODCICDO2+O2=ODCJKIDO+HO2                2.57E+02    3.0    24845.0
301. ODCJKIDO=ODCCDJO+CO                     1.30E+16   -0.5    11309.0
302. ODCICDO2+NO2=ODCJKIDO+HONO              8.78E-03    4.4    11026.0
303. ODCICDO2+NO2=ODCJKIDO+HNO2              9.26E+01    3.3    17579.0
304. ODCCDJO+HCO=ODCICDO2                    2.00E+13    0.0        0.0
305. ODCJKIDO+NO2=CO2+ODCCDJO+NO             8.39E+15   -0.8     1930.0
306. HCOCONO2=CHOCHO+HONO                    3.02E+17   -0.8    38624.0
307. HCOCONO2=CDOCOJ+NO2                     4.35E+17   -0.9    37832.0
308. HCOCONO2=HCOCJONO2+H                    2.32E+15    0.0    87920.0
309. HCOCONO2=CDJOCA+H                       3.38E+14    0.0    88350.0
310. HCOCONO2+H=HCOCJONO2+H2                 4.80E+08    1.5     -756.7
311. HCOCONO2+O=HCOCJONO2+OH                 3.40E+08    1.5        0.0
312. HCOCONO2+OH=HCOCJONO2+H2O               2.40E+06    2.0        0.0
313. HCOCONO2+CH3=HCOCJONO2+CH4              1.62E+06    1.9     2424.8
314. HCOCONO2+NH2=HCOCJONO2+NH3              1.84E+06    1.9     4377.7
315. HCOCONO2+NO2=HCOCJONO2+HONO             2.50E+07    1.3    14003.0
316. HCOCONO2+NO2=HCOCJONO2+HNO2             1.42E-02    4.6    18289.0
317. HCOCONO2+O2=HCOCJONO2+HO2               2.57E+02    3.0    36915.0
318. HCOCJONO2=CHOCHO+NO2                    7.78E+10    0.5     1690.6
319. HCOCONO2+H=CDJOCA+H2                    2.40E+08    1.5     -477.2
320. HCOCONO2+O=CDJOCA+OH                    1.70E+08    1.5        0.0
321. HCOCONO2+OH=CDJOCA+H2O                  1.20E+06    2.0        0.0
322. HCOCONO2+CH3=CDJOCA+CH4                 8.10E+05    1.9     2704.3
323. HCOCONO2+NH2=CDJOCA+NH3                 9.20E+05    1.9     4476.6
324. HCOCONO2+O2=CDJOCA+HO2                  1.29E+02    3.0    37345.0
325. CDJOCA=CO+CH2O+NO2                      1.74E+12    0.7    13726.0
326. HCOCONO2+NO2=CDJOCA+HONO                4.39E-03    4.4    11026.0
327. HCOCONO2+NO2=CDJOCA+HNO2                4.63E+01    3.3    17579.0
328. CDJOCA+NO2=CO2+CH2O+NO2+NO              8.39E+15   -0.8     1930.0
329. OH+HCOCONO2=CDOOJA                      5.71E+02    2.0      858.0
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330. CDOOJA=HOCHO+CH2O+NO2                      3.86E+12    0.4     9440.7
331. CDJOCA+OH(+M)=CDOOHA(+M)                  1.00E+00    0.0        0.0
I01:   1.3000E+63 -2.0240E+01  1.2182E+04  1.0000E-03
I02:   4.9000E+67 -2.0560E+01  1.2382E+04  1.0000E-02
I03:   3.8700E+71 -2.0520E+01  1.3375E+04  1.0000E-01
I04:   2.1900E+69 -1.8690E+01  1.4583E+04  1.0000E+00
I05:   1.7500E+56 -1.3910E+01  1.2533E+04  1.0000E+01
I06:   9.8600E+48 -1.1490E+01  1.0767E+04  2.5000E+01
I07:   2.1300E+43 -9.6400E+00  9.2530E+03  5.0000E+01
I08:   1.1500E+40 -8.5800E+00  8.3390E+03  7.5000E+01
I09:   6.2400E+37 -7.8500E+00  7.6900E+03  1.0000E+02
332. CDJOCA+OH(+M)=HONO+CH2O+CO2(+M)           1.00E+00    0.0        0.0
I01:   5.9800E+13 -2.4000E-01  2.5400E+02  1.0000E-03
I02:   5.9800E+13 -2.4000E-01  2.5400E+02  1.0000E-02
I03:   6.7500E+13 -2.6000E-01  2.8400E+02  1.0000E-01
I04:   2.1700E+15 -6.8000E-01  1.3010E+03  1.0000E+00
I05:   3.7200E+15 -6.8000E-01  2.8770E+03  1.0000E+01
I06:   4.6900E+13 -9.0000E-02  2.8720E+03  2.5000E+01
I07:   2.7800E+11  5.9000E-01  2.5570E+03  5.0000E+01
I08:   7.5300E+09  1.0700E+00  2.2610E+03  7.5000E+01
I09:   4.6700E+08  1.4300E+00  2.0060E+03  1.0000E+02
333. CDOOHA(+M)=HONO+CH2O+CO2(+M)              1.00E+00    0.0        0.0
I01:   3.1200E+56 -1.3280E+01  7.2651E+04  1.0000E-03
I02:   2.9900E+49 -1.0940E+01  7.1013E+04  1.0000E-02
I03:   5.0100E+41 -8.4100E+00  6.8907E+04  1.0000E-01
I04:   6.8200E+33 -5.9000E+00  6.6575E+04  1.0000E+00
I05:   7.6200E+26 -3.7000E+00  6.4402E+04  1.0000E+01
I06:   3.3300E+24 -2.9600E+00  6.3645E+04  2.5000E+01
I07:   8.9100E+22 -2.4700E+00  6.3137E+04  5.0000E+01
I08:   1.3200E+22 -2.2100E+00  6.2867E+04  7.5000E+01
I09:   3.7600E+21 -2.0400E+00  6.2689E+04  1.0000E+02
334. ACCJA=Y3COCA+NO2                          3.16E+12    0.5    18183.0
335. Y3COCA=Y3COCOJ+NO2                        4.56E+19   -1.5    29017.0
336. HOYCCO+H=Y3COCOJ+H2                       2.40E+08    1.5     5489.8
337. HOYCCO+O=Y3COCOJ+OH                       1.70E+08    1.5     3159.9
338. HOYCCO+OH=Y3COCOJ+H2O                     1.20E+06    2.0     -267.9
339. HOYCCO+CH3=Y3COCOJ+CH4                    8.10E+05    1.9     8671.3
340. HOYCCO+NH2=Y3COCOJ+NH3                    9.20E+05    1.9     6588.0
341. HOYCCO+NO2=Y3COCOJ+HONO                   2.50E+07    1.3    21932.0
342. HOYCCO+NO2=Y3COCOJ+HNO2                   7.10E-03    4.6    27899.0
343. HOYCCO+O2=Y3COCOJ+HO2                     1.29E+02    3.0    46525.0
344. Y3COCOJ=CJOCDO                            5.71E+12    0.1      -56.1
345. Y3COCOJ=CDOCOJ                            1.38E+13    0.0     1471.0
346. HOYCCO+H=HOYCJCO+H2                       2.40E+08    1.5     8031.3
347. HOYCCO+O=HOYCJCO+OH                       1.70E+08    1.5     6092.4
348. HOYCCO+OH=HOYCJCO+H2O                     1.20E+06    2.0     1687.1
349. HOYCCO+CH3=HOYCJCO+CH4                    8.10E+05    1.9    11213.0
350. HOYCCO+NH2=HOYCJCO+NH3                    9.20E+05    1.9     7487.3
351. HOYCCO+NO2=HOYCJCO+HONO                   2.50E+07    1.3    25157.0
352. HOYCCO+NO2=HOYCJCO+HNO2                   7.10E-03    4.6    31809.0
353. HOYCCO+O2=HOYCJCO+HO2                     1.29E+02    3.0    50435.0
354. HOYCJCO=CJCDOOH                           1.55E+11    0.7    11184.0
355. HOYCCO+H=HOYCCJO+H2                       4.80E+08    1.5     8115.8
356. HOYCCO+O=HOYCCJO+OH                       3.40E+08    1.5     6189.9
357. HOYCCO+OH=HOYCCJO+H2O                     2.40E+06    2.0     1752.1
358. HOYCCO+CH3=HOYCCJO+CH4                    1.62E+06    1.9    11297.0
359. HOYCCO+NH2=HOYCCJO+NH3                    1.84E+06    1.9     7517.2
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360. HOYCCO+NO2=HOYCCJO+HONO                    2.50E+07    1.3    25264.0
361. HOYCCO+NO2=HOYCCJO+HNO2                    1.42E-02    4.6    31939.0
362. HOYCCO+O2=HOYCCJO+HO2                      2.57E+02    3.0    50565.0
363. HOYCCJO=CJOHCDO                            5.42E+12    0.2     7300.6
364. COCDO+H=CJOCDO+H2                          7.20E+08    1.5     6113.8
365. COCDO+O=CJOCDO+OH                          5.10E+08    1.5     3879.9
366. COCDO+OH=CJOCDO+H2O                        3.60E+06    2.0      212.1
367. COCDO+CH3=CJOCDO+CH4                       2.43E+06    1.9     9295.3
368. COCDO+NH2=CJOCDO+NH3                       2.76E+06    1.9     6808.8
369. COCDO+NO2=CJOCDO+HONO                      2.50E+07    1.3    22724.0
370. COCDO+NO2=CJOCDO+HNO2                      2.13E-02    4.6    28859.0
371. COCDO+O2=CJOCDO+HO2                        3.86E+02    3.0    47485.0
372. CJOCDO(+M)<=>CH2O+HCO(+M)                  1.00E+00    0.0        0.0
I01:   8.2730E+36 -8.3800E+00  3.6590E+04  1.0000E-03
I02:   8.0190E+36 -8.1800E+00  3.7180E+04  4.0000E-03
I03:   1.5480E+36 -7.7700E+00  3.7560E+04  1.8000E-02
I04:   3.7440E+34 -7.1000E+00  3.7630E+04  7.5000E-02
I05:   9.9310E+31 -6.1600E+00  3.7330E+04  3.1600E-01
I06:   3.9990E+28 -4.9900E+00  3.6670E+04  1.3340E+00
I07:   5.0070E+24 -3.6900E+00  3.5740E+04  5.6230E+00
I08:   5.0070E+20 -2.3800E+00  3.4670E+04  2.3714E+01
I09:   1.1050E+17 -1.2100E+00  3.3610E+04  1.0000E+02
373. COCDO+H=COCDJO+H2                          2.40E+08    1.5     5983.8
374. COCDO+O=COCDJO+OH                          1.70E+08    1.5     3729.9
375. COCDO+OH=COCDJO+H2O                        1.20E+06    2.0      112.1
376. COCDO+CH3=COCDJO+CH4                       8.10E+05    1.9     9165.3
377. COCDO+NH2=COCDJO+NH3                       9.20E+05    1.9     6762.8
378. COCDO+O2=COCDJO+HO2                        1.29E+02    3.0    47285.0
379. CJOCDO=COCDJO                              2.28E+11    0.5    39358.0
380. COCDJO(+M)<=>CH3+CO2(+M)                   1.00E+00    0.0        0.0
I01:   9.7200E+12 -1.3100E+00  9.4167E+03  5.0000E-02
I02:   1.2500E+16 -1.8300E+00  1.1341E+04  1.0000E+00
I03:   1.0400E+18 -2.1000E+00  1.2827E+04  1.0000E+01
I04:   8.6900E+17 -1.8100E+00  1.3657E+04  1.0000E+02
381. COCDJO(+M)<=>CH3O+CO(+M)                   1.00E+00    0.0        0.0
I01:   1.0300E+03  1.2900E+00  2.5401E+04  5.0000E-02
I02:   4.0900E+05  8.1000E-01  2.1969E+04  1.0000E+00
I03:   9.0200E+14 -1.7200E+00  2.1768E+04  1.0000E+01
I04:   2.8250E+22 -3.4400E+00  2.3592E+04  1.0000E+02
382. COCDO+NO2=COCDJO+HONO                      4.39E-03    4.4    11026.0
383. COCDO+NO2=COCDJO+HNO2                      4.63E+01    3.3    17579.0
384. COCDJO+NO2=CH3O+CO2+NO                     8.39E+15   -0.8     1930.0
385. CCDOOH+H=CJCDOOH+H2                        2.40E+08    1.5     5255.8
386. CCDOOH+O=CJCDOOH+OH                        1.70E+08    1.5     2889.9
387. CCDOOH+OH=CJCDOOH+H2O                      1.20E+06    2.0     -447.9
388. CCDOOH+CH3=CJCDOOH+CH4                     8.10E+05    1.9     8437.3
389. CCDOOH+NH2=CJCDOOH+NH3                     9.20E+05    1.9     6505.2
390. CCDOOH+NO2=CJCDOOH+HONO                    2.50E+07    1.3    21635.0
391. CCDOOH+NO2=CJCDOOH+HNO2                    7.10E-03    4.6    27539.0
392. CCDOOH+O2=CJCDOOH+HO2                      1.29E+02    3.0    46165.0
393. CJCDOOH=CH3CO2                             4.40E+11    0.4    41948.0
394. CCDOOH+H=CH3CO2+H2                         2.40E+08    1.5    13706.0
395. CCDOOH+O=CH3CO2+OH                         1.70E+08    1.5    12640.0
396. CCDOOH+OH=CH3CO2+H2O                       1.20E+06    2.0     6052.1
397. CCDOOH+CH3=CH3CO2+CH4                      8.10E+05    1.9    16887.0
398. CCDOOH+NH2=CH3CO2+NH3                      9.20E+05    1.9     9495.2
399. CCDOOH+NO2=CH3CO2+HONO                     2.50E+07    1.3    32359.0
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400. CCDOOH+NO2=CH3CO2+HNO2                    7.10E-03    4.6    40539.0
401. CCDOOH+O2=CH3CO2+HO2                      1.29E+02    3.0    59165.0
402. COHCDO+H=CDOCOJ+H2                        2.40E+08    1.5    11873.0
403. COHCDO+O=CDOCOJ+OH                        1.70E+08    1.5    10525.0
404. COHCDO+OH=CDOCOJ+H2O                      1.20E+06    2.0     4642.1
405. COHCDO+CH3=CDOCOJ+CH4                     8.10E+05    1.9    15054.0
406. COHCDO+NH2=CDOCOJ+NH3                     9.20E+05    1.9     8846.6
407. COHCDO+NO2=CDOCOJ+HONO                    2.50E+07    1.3    30033.0
408. COHCDO+NO2=CDOCOJ+HNO2                    7.10E-03    4.6    37719.0
409. COHCDO+O2=CDOCOJ+HO2                      1.29E+02    3.0    56345.0
410. CDOCOJ=CHOCHO+H                           1.87E+10    1.1    22949.0
411. COHCDO+H=CJOHCDO+H2                       4.80E+08    1.5        0.0
412. COHCDO+O=CJOHCDO+OH                       3.40E+08    1.5        0.0
413. COHCDO+OH=CJOHCDO+H2O                     2.40E+06    2.0        0.0
414. COHCDO+CH3=CJOHCDO+CH4                    1.62E+06    1.9        0.0
415. COHCDO+NH2=CJOHCDO+NH3                    1.84E+06    1.9     2121.4
416. COHCDO+NO2=CJOHCDO+HONO                   2.50E+07    1.3     5910.3
417. COHCDO+NO2=CJOHCDO+HNO2                   1.42E-02    4.6     8479.0
418. COHCDO+O2=CJOHCDO+HO2                     2.57E+02    3.0    27105.0
419. CDOCOJ=CJOHCDO                            3.35E+11    0.5    25335.0
420. CDOCOJ=COHCDJO                            2.90E+11    0.5    29518.0
421. CJOHCDO+O<=>CHOCHO+OH                     1.46E-03    4.7     1727.0
422. CJOHCDO+OH<=>CHOCHO+H2O                   5.81E-03    4.3    -3560.0
423. CJOHCDO+H<=>CHOCHO+H2                     9.45E+02    3.1     8701.1
424. CJOHCDO+HO2<=>CHOCHO+H2O2                 6.47E-07    5.3    10533.1
425. CJOHCDO+CH3<=>CHOCHO+CH4                  2.04E+00    3.6     7721.0
426. CJOHCDO+CH3O2<=>CHOCHO+CH3O2H             3.24E-07    5.3    10533.1
427. CJOHCDO+NO2(+M)=COHONOK(+M)               1.00E+00    0.0        0.0
I01:   3.3300E+42 -1.4250E+01  2.0081E+04  1.0000E-03
I02:   6.1100E+45 -1.4670E+01  2.0462E+04  1.0000E-02
I03:   4.0300E+49 -1.5130E+01  2.0916E+04  1.0000E-01
I04:   4.2900E+53 -1.5500E+01  2.1623E+04  1.0000E+00
I05:   2.8700E+55 -1.5170E+01  2.2950E+04  1.0000E+01
I06:   3.7300E+54 -1.4580E+01  2.3375E+04  2.5000E+01
I07:   1.0300E+53 -1.3880E+01  2.3463E+04  5.0000E+01
I08:   5.1300E+51 -1.3360E+01  2.3387E+04  7.5000E+01
I09:   4.0800E+50 -1.2950E+01  2.3268E+04  1.0000E+02
428. CJOHCDO+NO2(+M)=COHOJK+NO(+M)             1.00E+00    0.0        0.0
I01:   2.7800E+01  3.0100E+00  9.5340E+03  1.0000E-03
I02:   2.7800E+01  3.0100E+00  9.5340E+03  1.0000E-02
I03:   2.7900E+01  3.0100E+00  9.5350E+03  1.0000E-01
I04:   2.8900E+01  3.0000E+00  9.5440E+03  1.0000E+00
I05:   1.6200E+02  2.7900E+00  1.0019E+04  1.0000E+01
I06:   1.1600E+03  2.5500E+00  1.0646E+04  2.5000E+01
I07:   4.9100E+03  2.3800E+00  1.1228E+04  5.0000E+01
I08:   8.7400E+03  2.3200E+00  1.1565E+04  7.5000E+01
I09:   1.0800E+04  2.3000E+00  1.1788E+04  1.0000E+02
429. CJOHCDO+NO2(+M)=CHOCHO+HONO(+M)           1.00E+00    0.0        0.0
I01:   2.1000E+01  2.7000E+00  9.6630E+03  1.0000E-03
I02:   2.1000E+01  2.7000E+00  9.6630E+03  1.0000E-02
I03:   2.0900E+01  2.7000E+00  9.6620E+03  1.0000E-01
I04:   2.0900E+01  2.7000E+00  9.6590E+03  1.0000E+00
I05:   1.1100E+02  2.4900E+00  1.0103E+04  1.0000E+01
I06:   8.3000E+02  2.2500E+00  1.0733E+04  2.5000E+01
I07:   3.5800E+03  2.0800E+00  1.1318E+04  5.0000E+01
I08:   6.3500E+03  2.0200E+00  1.1656E+04  7.5000E+01
I09:   7.7700E+03  2.0000E+00  1.1877E+04  1.0000E+02
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430. COHONOK(+M)=COHOJK+NO(+M)                1.00E+00    0.0        0.0
I01:   5.1500E+51 -1.2860E+01  4.0948E+04  1.0000E-03
I02:   2.5200E+53 -1.3020E+01  4.2486E+04  1.0000E-02
I03:   6.3000E+50 -1.1880E+01  4.2740E+04  1.0000E-01
I04:   1.1500E+48 -1.0730E+01  4.2937E+04  1.0000E+00
I05:   4.3100E+43 -9.1300E+00  4.2373E+04  1.0000E+01
I06:   1.6200E+41 -8.3100E+00  4.1852E+04  2.5000E+01
I07:   1.5100E+39 -7.6400E+00  4.1363E+04  5.0000E+01
I08:   9.1000E+37 -7.2400E+00  4.1054E+04  7.5000E+01
I09:   1.1100E+37 -6.9400E+00  4.0813E+04  1.0000E+02
431. COHONOK(+M)=CHOCHO+HONO(+M)              1.00E+00    0.0        0.0
I01:   2.4900E+50 -1.2600E+01  3.9626E+04  1.0000E-03
I02:   1.8400E+51 -1.2570E+01  4.0892E+04  1.0000E-02
I03:   8.1600E+47 -1.1250E+01  4.0772E+04  1.0000E-01
I04:   4.4700E+44 -1.0000E+01  4.0628E+04  1.0000E+00
I05:   1.2400E+40 -8.4000E+00  3.9873E+04  1.0000E+01
I06:   5.6500E+37 -7.6200E+00  3.9334E+04  2.5000E+01
I07:   6.7300E+35 -6.9900E+00  3.8850E+04  5.0000E+01
I08:   4.8400E+34 -6.6100E+00  3.8551E+04  7.5000E+01
I09:   6.8100E+33 -6.3300E+00  3.8321E+04  1.0000E+02
432. COHOJK=HCO+HOCHO                        4.84E+12    0.2      359.2
433. COHCDO+H=COHCDJO+H2                     2.40E+08    1.5     1446.8
434. COHCDO+O=COHCDJO+OH                     1.70E+08    1.5        0.0
435. COHCDO+OH=COHCDJO+H2O                   1.20E+06    2.0        0.0
436. COHCDO+CH3=COHCDJO+CH4                  8.10E+05    1.9     4628.3
437. COHCDO+NH2=COHCDJO+NH3                  9.20E+05    1.9     5157.4
438. COHCDO+O2=COHCDJO+HO2                   1.29E+02    3.0    40305.0
439. COHCDJO=CH2OH+CO                        6.81E+12    0.4    12330.0
440. COHCDO+NO2=COHCDJO+HONO                 4.39E-03    4.4    11026.0
441. COHCDO+NO2=COHCDJO+HNO2                 4.63E+01    3.3    17579.0
442. COHCDJO+NO2=CH2OH+CO2+NO                8.39E+15   -0.8     1930.0
443. C2H2+OH(+M)<=>C2H2OH(+M)                1.00E+00    0.0        0.0
I01:   3.9130E+32 -7.1260E+00  5.8240E+03  1.0000E-02
I02:   1.0670E+32 -6.8470E+00  5.5080E+03  2.5000E-02
I03:   1.6460E+32 -6.7170E+00  5.8220E+03  1.0000E-01
I04:   1.3870E+31 -6.0870E+00  6.3480E+03  1.0000E+00
I05:   2.8920E+29 -5.2880E+00  7.0550E+03  1.0000E+01
I06:   1.3670E+25 -3.7540E+00  6.5430E+03  1.0000E+02
444. SC2H2OH<=>C2H2OH                        2.65E+36   -8.9    51019.0
445. SC2H2OH<=>CH2CO+H                       5.69E+52  -13.4    45049.0
446. SC2H2OH<=>HCCOH+H                       5.40E+46  -11.6    44323.0
447. SC2H2OH+O2<=>CH2CO+HO2                  5.26E+17   -1.6      869.0
448. SC2H2OH+O2<=>HCCOH+HO2                  5.51E+03    2.5     -414.0
449. DIOHCH2=H2+HOCHO                        2.69E+17   -0.9    77653.0
450. CH2O+H2O+H2O=DIOHCH2+H2O                2.07E-08    4.9    12817.0
451. DIOHCH2+H2O=H2+H2O+HOCHO                8.21E+06    1.5    50373.0
452. DIOHCH2+H2O+CO=CH2O+H2O+HOCHO           8.37E-10    5.8    50381.0
453. DIOHCH2+HONO=HOCHO+H2O+HNO              2.64E+04    2.1    28776.0
454. DIOHCH2+HNO3=HONO+H2O+HOCHO             4.06E-02    4.2    46505.0
455. DIOHCH2+CH2O=HOCHO+CH3OH                2.43E+06    1.4    19011.0
456. NO+HOCHO=HNO+HOCO                       5.32E+04    2.8    51274.0
457. NO+HOCHO=HONJOCHO                       1.99E+08    0.8    41593.0
458. HONJOCHO=HONO+HCO                       1.37E+11    1.0    34663.0
459. NO+HOCHO=HCJOHONO                       8.24E+01    2.6    56534.0
460. HCJOHONO=H+ONOCHO                       4.04E+16   -0.5    29115.0
461. NO+HOCHO=OJNHCHO                        4.36E+07    0.9    39542.0
462. OJNHCHO=HCO+HNO2                        1.83E+11    0.9    40398.0
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463. NO2+HCO(+M)=O2NCHO(+M)                    1.00E+00    0.0         0.0
I01:   1.8500E+17 -6.2000E+00  3.7360E+03  1.0000E-03
I02:   4.7200E+19 -6.5200E+00  4.3080E+03  1.0000E-02
I03:   6.0800E+19 -6.0700E+00  4.3850E+03  1.0000E-01
I04:   7.9000E+19 -5.5100E+00  4.3990E+03  1.0000E+00
I05:   1.1300E+20 -4.7500E+00  4.3990E+03  1.0000E+01
I06:   4.7400E+20 -4.5500E+00  4.5420E+03  2.5000E+01
I07:   4.5800E+21 -4.5400E+00  4.7390E+03  5.0000E+01
I08:   2.5300E+22 -4.5900E+00  4.8560E+03  7.5000E+01
I09:   8.9600E+22 -4.6400E+00  4.9200E+03  1.0000E+02
464. NO2+HCO(+M)=HNO2+CO(+M)                   1.00E+00    0.0         0.0
I01:   1.1500E-06  5.3700E+00  2.5400E+02  1.0000E-03
I02:   1.1500E-06  5.3700E+00  2.5400E+02  1.0000E-02
I03:   1.1500E-06  5.3700E+00  2.5400E+02  1.0000E-01
I04:   1.1500E-06  5.3700E+00  2.5400E+02  1.0000E+00
I05:   1.1400E-06  5.3700E+00  2.5600E+02  1.0000E+01
I06:   1.1400E-06  5.3700E+00  2.5900E+02  2.5000E+01
I07:   1.1300E-06  5.3800E+00  2.6400E+02  5.0000E+01
I08:   1.1100E-06  5.3800E+00  2.6900E+02  7.5000E+01
I09:   1.1000E-06  5.3800E+00  2.7400E+02  1.0000E+02
465. NO2+HCO(+M)=HONO+CO(+M)                   1.00E+00    0.0         0.0
     Declared duplicate reaction...
I01:   6.7200E+09  7.2000E-01 -4.8500E+02  1.0000E-03
I02:   6.7200E+09  7.2000E-01 -4.8500E+02  1.0000E-02
I03:   6.7200E+09  7.2000E-01 -4.8500E+02  1.0000E-01
I04:   6.7200E+09  7.2000E-01 -4.8500E+02  1.0000E+00
I05:   6.7100E+09  7.2000E-01 -4.8500E+02  1.0000E+01
I06:   6.7100E+09  7.2000E-01 -4.8500E+02  2.5000E+01
I07:   6.7000E+09  7.2000E-01 -4.8500E+02  5.0000E+01
I08:   6.6900E+09  7.2000E-01 -4.8500E+02  7.5000E+01
I09:   6.6700E+09  7.2000E-01 -4.8600E+02  1.0000E+02
466. NO2+HCO(+M)=ONOCHO(+M)                    1.00E+00    0.0         0.0
     Declared duplicate reaction...
I01:   1.4700E+06 -4.9800E+00  3.5080E+03  1.0000E-03
I02:   2.0700E+09 -5.5200E+00  3.7010E+03  1.0000E-02
I03:   1.4000E+13 -6.1100E+00  3.8510E+03  1.0000E-01
I04:   1.2200E+17 -6.4000E+00  4.0720E+03  1.0000E+00
I05:   1.9200E+19 -5.7500E+00  4.3690E+03  1.0000E+01
I06:   2.8800E+19 -5.2400E+00  4.2780E+03  2.5000E+01
I07:   6.3000E+19 -4.9300E+00  4.1940E+03  5.0000E+01
I08:   1.4600E+20 -4.8100E+00  4.1640E+03  7.5000E+01
I09:   3.0900E+20 -4.7600E+00  4.1550E+03  1.0000E+02
467. NO2+HCO(+M)=OCHO+NO(+M)                   1.00E+00    0.0         0.0
I01:   7.3300E+00  3.1800E+00 -3.1200E+02  1.0000E-03
I02:   7.3300E+00  3.1800E+00 -3.1200E+02  1.0000E-02
I03:   7.3300E+00  3.1800E+00 -3.1200E+02  1.0000E-01
I04:   7.3300E+00  3.1800E+00 -3.1200E+02  1.0000E+00
I05:   7.3400E+00  3.1800E+00 -3.1200E+02  1.0000E+01
I06:   7.3600E+00  3.1800E+00 -3.1200E+02  2.5000E+01
I07:   7.3800E+00  3.1800E+00 -3.1200E+02  5.0000E+01
I08:   7.4100E+00  3.1800E+00 -3.1200E+02  7.5000E+01
I09:   7.4500E+00  3.1800E+00 -3.1200E+02  1.0000E+02
468. NO2+HCO(+M)=HNO+CO2(+M)                   1.00E+00    0.0         0.0
I01:   9.8100E+01  2.4600E+00  1.3400E+02  1.0000E-03
I02:   9.8100E+01  2.4600E+00  1.3400E+02  1.0000E-02
I03:   9.8100E+01  2.4600E+00  1.3400E+02  1.0000E-01
I04:   9.8200E+01  2.4600E+00  1.3400E+02  1.0000E+00
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I05:   9.8900E+01  2.4600E+00  1.3300E+02  1.0000E+01
I06:   1.0000E+02  2.4600E+00  1.3200E+02  2.5000E+01
I07:   1.0200E+02  2.4500E+00  1.2900E+02  5.0000E+01
I08:   1.0400E+02  2.4500E+00  1.2500E+02  7.5000E+01
I09:   1.0600E+02  2.4500E+00  1.2100E+02  1.0000E+02
469. NO2+HCO(+M)=HONO+CO(+M)                1.00E+00    0.0         0.0
     Declared duplicate reaction...
I01:   5.8900E+00  2.9500E+00 -5.5800E+02  1.0000E-03
I02:   5.8900E+00  2.9500E+00 -5.5800E+02  1.0000E-02
I03:   5.8900E+00  2.9500E+00 -5.5800E+02  1.0000E-01
I04:   5.8900E+00  2.9500E+00 -5.5800E+02  1.0000E+00
I05:   5.8900E+00  2.9500E+00 -5.5800E+02  1.0000E+01
I06:   5.8800E+00  2.9500E+00 -5.5600E+02  2.5000E+01
I07:   5.8800E+00  2.9500E+00 -5.5400E+02  5.0000E+01
I08:   5.8800E+00  2.9500E+00 -5.5100E+02  7.5000E+01
I09:   5.8800E+00  2.9500E+00 -5.4800E+02  1.0000E+02
470. O2NCHO(+M)=HNO2+CO(+M)                 1.00E+00    0.0         0.0
I01:   5.2900E+22 -6.1200E+00  5.3445E+04  1.0000E-03
I02:   5.1100E+23 -6.1200E+00  5.3441E+04  1.0000E-02
I03:   3.6700E+24 -6.0600E+00  5.3409E+04  1.0000E-01
I04:   3.0100E+24 -5.6700E+00  5.3186E+04  1.0000E+00
I05:   1.0100E+23 -4.6100E+00  5.2951E+04  1.0000E+01
I06:   2.4700E+23 -4.3800E+00  5.3198E+04  2.5000E+01
I07:   2.3700E+24 -4.4000E+00  5.3489E+04  5.0000E+01
I08:   1.7900E+25 -4.5000E+00  5.3689E+04  7.5000E+01
I09:   9.0400E+25 -4.6000E+00  5.3824E+04  1.0000E+02
471. O2NCHO(+M)=HONO+CO(+M)                 1.00E+00    0.0         0.0
I01:   2.4200E+37 -8.5500E+00  3.8574E+04  1.0000E-03
I02:   2.4300E+38 -8.5500E+00  3.8575E+04  1.0000E-02
I03:   2.5200E+39 -8.5500E+00  3.8577E+04  1.0000E-01
I04:   3.1500E+40 -8.5900E+00  3.8588E+04  1.0000E+00
I05:   1.9100E+41 -8.5800E+00  3.8461E+04  1.0000E+01
I06:   1.3000E+41 -8.4500E+00  3.8305E+04  2.5000E+01
I07:   5.4700E+40 -8.2800E+00  3.8159E+04  5.0000E+01
I08:   2.7400E+40 -8.1500E+00  3.8071E+04  7.5000E+01
I09:   1.5400E+40 -8.0500E+00  3.8006E+04  1.0000E+02
472. O2NCHO(+M)=ONOCHO(+M)                  1.00E+00    0.0         0.0
I01:   2.4200E+28 -5.9600E+00  3.8582E+04  1.0000E-03
I02:   2.4300E+29 -5.9600E+00  3.8583E+04  1.0000E-02
I03:   2.5600E+30 -5.9700E+00  3.8587E+04  1.0000E-01
I04:   3.6400E+31 -6.0300E+00  3.8612E+04  1.0000E+00
I05:   3.5400E+32 -6.0900E+00  3.8528E+04  1.0000E+01
I06:   3.0200E+32 -5.9900E+00  3.8386E+04  2.5000E+01
I07:   1.5000E+32 -5.8500E+00  3.8249E+04  5.0000E+01
I08:   8.2900E+31 -5.7400E+00  3.8166E+04  7.5000E+01
I09:   4.9700E+31 -5.6500E+00  3.8103E+04  1.0000E+02
473. ONOCHO(+M)=OCHO+NO(+M)                 1.00E+00    0.0         0.0
I01:   1.0900E+28 -7.0600E+00  3.6714E+04  1.0000E-03
I02:   2.5300E+30 -7.3700E+00  3.6680E+04  1.0000E-02
I03:   6.6000E+33 -7.8800E+00  3.6876E+04  1.0000E-01
I04:   5.2600E+36 -8.0600E+00  3.7824E+04  1.0000E+00
I05:   2.1000E+39 -8.2200E+00  4.0059E+04  1.0000E+01
I06:   3.3500E+38 -7.7900E+00  4.0382E+04  2.5000E+01
I07:   1.9800E+37 -7.3000E+00  4.0368E+04  5.0000E+01
I08:   2.6000E+36 -6.9700E+00  4.0283E+04  7.5000E+01
I09:   5.3300E+35 -6.7200E+00  4.0188E+04  1.0000E+02
474. ONOCHO(+M)=HNO+CO2(+M)                 1.00E+00    0.0         0.0
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I01:   6.0900E+32 -7.5300E+00  2.6622E+04  1.0000E-03
I02:   9.8000E+33 -7.5700E+00  2.7447E+04  1.0000E-02
I03:   1.9700E+34 -7.3300E+00  2.8379E+04  1.0000E-01
I04:   2.0000E+31 -6.1000E+00  2.8393E+04  1.0000E+00
I05:   8.7300E+28 -5.1500E+00  2.8478E+04  1.0000E+01
I06:   2.0500E+27 -4.5800E+00  2.8186E+04  2.5000E+01
I07:   8.5200E+25 -4.1200E+00  2.7877E+04  5.0000E+01
I08:   1.3100E+25 -3.8500E+00  2.7682E+04  7.5000E+01
I09:   3.5100E+24 -3.6600E+00  2.7537E+04  1.0000E+02
475. ONOCHO(+M)=HCO+NO2(+M)                  1.00E+00    0.0         0.0
     Declared duplicate reaction...
I01:   6.1300E+07 -5.2800E+00  7.5187E+04  1.0000E-03
I02:   1.3800E+10 -5.5900E+00  7.5117E+04  1.0000E-02
I03:   3.1000E+13 -6.0700E+00  7.5001E+04  1.0000E-01
I04:   1.3500E+17 -6.4300E+00  7.4692E+04  1.0000E+00
I05:   1.9400E+25 -7.9700E+00  7.5840E+04  1.0000E+01
I06:   3.1000E+28 -8.5100E+00  7.6203E+04  2.5000E+01
I07:   7.9600E+30 -8.8900E+00  7.6439E+04  5.0000E+01
I08:   2.4800E+32 -9.1200E+00  7.6606E+04  7.5000E+01
I09:   3.0800E+33 -9.2800E+00  7.6739E+04  1.0000E+02
476. ONOCHO(+M)=HONO+CO(+M)                  1.00E+00    0.0         0.0
I01:   2.9700E+27 -7.6400E+00  4.1143E+04  1.0000E-03
I02:   6.7400E+29 -7.9500E+00  4.1083E+04  1.0000E-02
I03:   1.6000E+33 -8.4500E+00  4.1062E+04  1.0000E-01
I04:   6.7100E+36 -8.8100E+00  4.1425E+04  1.0000E+00
I05:   2.3800E+42 -9.7000E+00  4.4123E+04  1.0000E+01
I06:   4.6000E+42 -9.5100E+00  4.4876E+04  2.5000E+01
I07:   1.1100E+42 -9.1500E+00  4.5172E+04  5.0000E+01
I08:   2.6900E+41 -8.8700E+00  4.5246E+04  7.5000E+01
I09:   7.6800E+40 -8.6500E+00  4.5251E+04  1.0000E+02
477. NO+HOCO(+M)=HOCDONO(+M)                 1.00E+00    0.0         0.0
I01:   5.7800E+30 -7.7900E+00  1.2430E+03  1.0000E-03
I02:   7.3100E+31 -7.8100E+00  1.4150E+03  1.0000E-02
I03:   9.4500E+32 -7.8300E+00  2.0160E+03  1.0000E-01
I04:   2.4900E+33 -7.6300E+00  2.8790E+03  1.0000E+00
I05:   1.1000E+32 -6.9100E+00  3.4010E+03  1.0000E+01
I06:   5.6300E+30 -6.4000E+00  3.3610E+03  2.5000E+01
I07:   2.8200E+29 -5.9300E+00  3.2090E+03  5.0000E+01
I08:   3.6500E+28 -5.6100E+00  3.0680E+03  7.5000E+01
I09:   7.5300E+27 -5.3700E+00  2.9450E+03  1.0000E+02
478. NO+HOCO(+M)=HNO+CO2(+M)                 1.00E+00    0.0         0.0
I01:   6.3800E+07  7.4000E-01 -3.7680E+03  1.0000E-03
I02:   1.0500E+08  6.8000E-01 -3.6370E+03  1.0000E-02
I03:   9.6500E+08  4.0000E-01 -3.0240E+03  1.0000E-01
I04:   9.8200E+10 -1.6000E-01 -1.6070E+03  1.0000E+00
I05:   1.2400E+13 -7.3000E-01  3.8500E+02  1.0000E+01
I06:   2.7200E+13 -8.0000E-01  1.1270E+03  2.5000E+01
I07:   2.0800E+13 -7.4000E-01  1.5850E+03  5.0000E+01
I08:   1.1600E+13 -6.6000E-01  1.7940E+03  7.5000E+01
I09:   6.2500E+12 -5.7000E-01  1.9110E+03  1.0000E+02
479. HOCDONO(+M)=HNO+CO2(+M)                 1.00E+00    0.0         0.0
I01:   7.1600E+43 -1.1080E+01  3.8696E+04  1.0000E-03
I02:   8.2600E+44 -1.1090E+01  3.8863E+04  1.0000E-02
I03:   8.4000E+45 -1.1080E+01  3.9442E+04  1.0000E-01
I04:   2.1300E+46 -1.0880E+01  4.0298E+04  1.0000E+00
I05:   7.0200E+44 -1.0130E+01  4.0768E+04  1.0000E+01
I06:   3.1700E+43 -9.6000E+00  4.0707E+04  2.5000E+01
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I07:   1.3600E+42 -9.1100E+00  4.0529E+04  5.0000E+01
I08:   1.7600E+41 -8.7900E+00  4.0387E+04  7.5000E+01
I09:   3.6200E+40 -8.5500E+00  4.0263E+04  1.0000E+02
480. HOCO+NO=HONO+CO                          3.30E+04    2.0    24505.0
481. HOCO+NO=HNO+CO2                          4.09E+08    1.2     9476.3
482. OCHO+NO2=HNO2+CO2                        2.28E+00    2.3     6366.6
483. OCHO+NO2=HONO+CO2                        4.41E+05    0.4    10448.0
     Declared duplicate reaction...
484. OCHO+NO2=HONO+CO2                        3.79E+00    2.1     3980.3
     Declared duplicate reaction...
485. NO2+HOCO=HNO2+CO2                        2.81E+06    1.6     4820.9
486. NO2+HOCO(+M)=HOCDOONO(+M)                1.00E+00    0.0        0.0
I01:   3.8100E-19  2.4900E+00  1.2152E+04  1.0000E-03
I02:   3.4500E-18  2.5100E+00  1.2127E+04  1.0000E-02
I03:   1.5900E-17  2.6000E+00  1.1926E+04  1.0000E-01
I04:   4.5500E-19  3.3300E+00  1.0281E+04  1.0000E+00
I05:   4.6100E-12  1.3800E+00  8.9700E+03  1.0000E+01
I06:   3.4200E+06 -3.7900E+00  1.3708E+04  2.5000E+01
I07:   1.5700E+21 -7.8600E+00  1.8070E+04  5.0000E+01
I08:   3.0500E+26 -9.1700E+00  1.9565E+04  7.5000E+01
I09:   1.8800E+28 -9.4700E+00  1.9960E+04  1.0000E+02
487. NO2+HOCO(+M)=HNO2+CO2(+M)                1.00E+00    0.0        0.0
I01:   1.2400E+00  3.4000E+00  1.0782E+04  1.0000E-03
I02:   1.2400E+00  3.4000E+00  1.0782E+04  1.0000E-02
I03:   1.2400E+00  3.4000E+00  1.0782E+04  1.0000E-01
I04:   1.2400E+00  3.4000E+00  1.0782E+04  1.0000E+00
I05:   1.2400E+00  3.4000E+00  1.0782E+04  1.0000E+01
I06:   1.2400E+00  3.4000E+00  1.0782E+04  2.5000E+01
I07:   1.2400E+00  3.4000E+00  1.0782E+04  5.0000E+01
I08:   1.2400E+00  3.4000E+00  1.0782E+04  7.5000E+01
I09:   1.2400E+00  3.4000E+00  1.0782E+04  1.0000E+02
488. NO2+HOCO(+M)=HONO+CO2(+M)                1.00E+00    0.0        0.0
     Declared duplicate reaction...
I01:   1.1400E+01  3.2100E+00  1.0953E+04  1.0000E-03
I02:   1.1400E+01  3.2100E+00  1.0953E+04  1.0000E-02
I03:   1.1400E+01  3.2100E+00  1.0953E+04  1.0000E-01
I04:   1.1400E+01  3.2100E+00  1.0953E+04  1.0000E+00
I05:   1.1400E+01  3.2100E+00  1.0953E+04  1.0000E+01
I06:   1.1400E+01  3.2100E+00  1.0953E+04  2.5000E+01
I07:   1.1400E+01  3.2100E+00  1.0953E+04  5.0000E+01
I08:   1.1400E+01  3.2100E+00  1.0953E+04  7.5000E+01
I09:   1.1400E+01  3.2100E+00  1.0953E+04  1.0000E+02
489. HOCDOONO(+M)=HNO2+CO2(+M)                1.00E+00    0.0        0.0
I01:   3.6300E+22 -5.4200E+00  2.1121E+04  1.0000E-03
I02:   1.1400E+24 -5.5200E+00  2.1256E+04  1.0000E-02
I03:   1.2700E+27 -6.0100E+00  2.1828E+04  1.0000E-01
I04:   1.2700E+30 -6.4500E+00  2.2559E+04  1.0000E+00
I05:   1.4200E+31 -6.3200E+00  2.3499E+04  1.0000E+01
I06:   3.4000E+31 -6.2800E+00  2.4059E+04  2.5000E+01
I07:   3.3400E+31 -6.1600E+00  2.4412E+04  5.0000E+01
I08:   1.7000E+31 -6.0100E+00  2.4522E+04  7.5000E+01
I09:   9.5700E+30 -5.8900E+00  2.4581E+04  1.0000E+02
490. HOCDOONO(+M)=HONO+CO2(+M)                1.00E+00    0.0        0.0
I01:   3.3200E+26 -5.8200E+00  1.6697E+04  1.0000E-03
I02:   4.8400E+27 -5.8800E+00  1.6866E+04  1.0000E-02
I03:   2.8200E+29 -6.1000E+00  1.7692E+04  1.0000E-01
I04:   5.2300E+30 -6.1700E+00  1.8803E+04  1.0000E+00
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I05:   1.1100E+30 -5.6600E+00  1.9487E+04  1.0000E+01
I06:   5.6600E+29 -5.4700E+00  1.9759E+04  2.5000E+01
I07:   2.0600E+29 -5.2600E+00  1.9880E+04  5.0000E+01
I08:   7.1700E+28 -5.0800E+00  1.9875E+04  7.5000E+01
I09:   3.2200E+28 -4.9500E+00  1.9856E+04  1.0000E+02
491. NO2+HOCO(+M)=HOCDONO2(+M)                1.00E+00    0.0        0.0
I01:   6.5900E-21  2.1400E+00 -6.8220E+03  1.0000E-03
I02:   6.7100E-20  2.1400E+00 -6.8210E+03  1.0000E-02
I03:   8.0000E-19  2.1100E+00 -6.8070E+03  1.0000E-01
I04:   4.0000E-17  1.9000E+00 -6.6810E+03  1.0000E+00
I05:   1.0700E-11  5.6000E-01 -5.7890E+03  1.0000E+01
I06:   1.0600E-06 -8.2000E-01 -4.7090E+03  2.5000E+01
I07:   6.4200E-01 -2.4500E+00 -3.2840E+03  5.0000E+01
I08:   1.7300E+04 -3.7100E+00 -2.1140E+03  7.5000E+01
I09:   7.9500E+07 -4.7500E+00 -1.1130E+03  1.0000E+02
492. NO2+HOCO(+M)=HONO+CO2(+M)               1.00E+00    0.0        0.0
     Declared duplicate reaction...
I01:   1.2000E+02  2.5200E+00 -2.5640E+03  1.0000E-03
I02:   1.2000E+02  2.5200E+00 -2.5640E+03  1.0000E-02
I03:   1.2000E+02  2.5200E+00 -2.5640E+03  1.0000E-01
I04:   1.2000E+02  2.5200E+00 -2.5640E+03  1.0000E+00
I05:   1.2000E+02  2.5200E+00 -2.5640E+03  1.0000E+01
I06:   1.2000E+02  2.5200E+00 -2.5640E+03  2.5000E+01
I07:   1.2000E+02  2.5200E+00 -2.5640E+03  5.0000E+01
I08:   1.2000E+02  2.5200E+00 -2.5640E+03  7.5000E+01
I09:   1.2000E+02  2.5200E+00 -2.5640E+03  1.0000E+02
493. HOCDONO2(+M)=HONO+CO2(+M)               1.00E+00    0.0        0.0
I01:   1.3600E+14 -2.2400E+00  6.5230E+03  1.0000E-03
I02:   1.3500E+15 -2.2400E+00  6.5230E+03  1.0000E-02
I03:   1.3900E+16 -2.2500E+00  6.5280E+03  1.0000E-01
I04:   1.1300E+17 -2.2200E+00  6.5290E+03  1.0000E+00
I05:   8.3200E+18 -2.4900E+00  7.0830E+03  1.0000E+01
I06:   4.2100E+19 -2.5900E+00  7.4020E+03  2.5000E+01
I07:   2.5700E+20 -2.7400E+00  7.7820E+03  5.0000E+01
I08:   4.1800E+20 -2.7500E+00  7.9450E+03  7.5000E+01
I09:   1.3200E+20 -2.5600E+00  7.8430E+03  1.0000E+02
494. HOCDONO+H2O=HONO+CO+H2O                 3.67E+06    1.8    53006.0
495. HOCHO+HONO=ONOCHO+H2O                   8.09E+03    2.2    10633.0
496. HOCO+HONO=CO2+H2O+NO                    6.32E+05    1.6    12582.0
497. OCHO+HONO=CO2+H2O+NO                    3.62E+06    1.7     1288.7
498. ONOCHO+H2O=CO2+HNO+H2O                  6.06E+08    1.6    46885.0
499. HOCHO+CO=CO2+CH2O                       5.96E+08    1.0    53415.0
500. HOCHO+CO+H2O=CO2+CH2O+H2O               4.24E-05    3.1    99880.0
501. CO+OCHO=CO2+HCO                         2.52E+08    1.7      758.6
502. C2H3+NO2=CH2CHO+NO                      7.73E+14   -0.6        0.0
503. C2H4+NO2=C2H3+HONO                      2.50E+07    1.3    30049.0
504. C2H4+NO2=C2H3+HNO2                      2.84E-02    4.6    37739.0
505. CH2O+NO2=HCO+HNO2                       3.48E+13    0.0    23720.0
506. CH2OH+NO2=CH2O+HONO                     1.17E+15   -0.5        0.0
507. CH2CO+NO2=HCCO+HONO                     2.50E+07    1.3    29200.0
508. CH2CO+NO2=HCCO+HNO2                     1.42E-02    4.6    36709.0
509. NO2+HCCO=CO+HCO+NO                      8.76E+12   -0.3        0.0
510. NO2+HCCO=CO2+HCNO                       5.84E+12   -0.3        0.0
511. CH4+CO=CH2CO+H2                         1.53E+01    3.9   117700.0
512. NH3+CO=HNCO+H2                          5.13E+01    3.2    87538.0
513. NH3+CO=H2NCHO                           2.01E+03    2.9    74466.0
514. H2NCHO=HNCO+H2                          2.02E+09    1.2    73165.0
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515. H2NCHO=NH2+HCO                          2.18E+16   -0.1    95526.0
516. HNCO+CO=HNCO+CO                         2.55E+02    2.6    80144.0
517. C3H3+NO2=CDCJCDO+NO                     6.49E+15   -1.1        0.0
518. HCO+H2CC=CDCJCDO                        1.00E+13    0.0        0.0
519. CDCJCDO=VCDJO                           1.75E+11    0.6    29830.0
520. VCDO+H=CDCJCDO+H2                       2.40E+08    1.5    12250.0
521. VCDO+O=CDCJCDO+OH                       1.70E+08    1.5    10960.0
522. VCDO+OH=CDCJCDO+H2O                     1.20E+06    2.0     4932.1
523. VCDO+CH3=CDCJCDO+CH4                    8.10E+05    1.9    15431.0
524. VCDO+NH2=CDCJCDO+NH3                    9.20E+05    1.9     8979.7
525. VCDO+HO2=CDCJCDO+H2O2                   1.40E+04    2.7    23657.0
526. VCDO+NO2=CDCJCDO+HONO                   2.50E+07    1.3    30511.0
527. VCDO+O2=CDCJCDO+HO2                     2.50E+07    1.3    54890.0
528. H2CC+NO2=CH2CO+NO                       5.00E+13    0.0        0.0
529. CHOCHO+CH3=ODCCDJO+CH4                  1.62E+06    1.9     1436.8
530. CHOCHO+HO2=ODCCDJO+H2O2                 1.40E+04    2.7    10736.0
531. CHOCHO+O2=ODCCDJO+HO2                   2.50E+07    1.3    37128.0
532. CHOCHO+NH2=ODCCDJO+NH3                  1.84E+06    1.9     4028.1
533. CHOCHO+NO2=ODCCDJO+HONO                 4.39E-03    4.4     8601.0
534. ODCCDJO=HCO+CO                          1.89E+13    0.0     9500.0
535. ODCCDJO+NO2=CO2+HCO+NO                  8.39E+15   -0.8     1930.0
536. ODCCDJO+HO2=CO2+HCO+OH                  3.01E+13    0.0        0.0
537. ODCCDJO+O=CO2+HCO                       9.64E+12    0.0        0.0
538. HCCOH+H=HCCO+H2                         2.40E+08    1.5        0.0
539. HCCOH+O=HCCO+OH                         1.70E+08    1.5        0.0
540. HCCOH+OH=HCCO+H2O                       1.20E+06    2.0        0.0
541. HCCOH+CH3=HCCO+CH4                      8.10E+05    1.9        0.0
542. HCCOH+HO2=HCCO+H2O2                     1.40E+04    2.7     1978.6
543. HCCOH+O2=HCCO+HO2                       2.50E+07    1.3    25091.0
544. HCCOH+NH2=HCCO+NH3                      9.20E+05    1.9      672.4
545. HCCOH+NO2=HCCO+HONO                     2.50E+07    1.3      717.0
546. HOCHO+M=CO+H2O+M                        9.04E+14    0.0    50300.0
547. HOCHO+M=CO2+H2+M                        2.02E+15    0.0    51350.0
548. HOCHO+OH+M=H2O+OCHO+M                   1.36E+10    0.0    -1560.0
549. HOCHO+H=HOCO+H2                         2.40E+08    1.5     5678.3
550. HOCHO+O=HOCO+OH                         1.70E+08    1.5     3369.9
551. HOCHO+OH=HOCO+H2O                       1.20E+06    2.0     -122.9
552. HOCHO+CH3=HOCO+CH4                      8.10E+05    1.9     8859.8
553. HOCHO+NH2=HOCO+NH3                      9.20E+05    1.9     6654.7
554. HOCHO+NO2=HOCO+HONO                     2.50E+07    1.3    22171.0
555. HOCHO+NO2=HOCO+HNO2                     7.10E-03    4.6    28189.0
556. HOCHO+O2=HOCO+HO2                       1.29E+02    3.0    46815.0
557. HOCHO+H=OCHO+H2                         2.40E+08    1.5    10904.0
558. HOCHO+O=OCHO+OH                         1.70E+08    1.5     9407.4
559. HOCHO+CH3=OCHO+CH4                      8.10E+05    1.9    14092.0
560. HOCHO+NH2=OCHO+NH3                      9.20E+05    1.9     8503.9
561. HOCHO+NO2=OCHO+HONO                     2.50E+07    1.3    28812.0
562. HOCHO+NO2=OCHO+HNO2                     7.10E-03    4.6    36239.0
563. CH2O+OCHO<=>HCO+HOCHO                   5.60E+12    0.0    13600.0
564. OCHO+HO2<=>HOCHO+O2                     3.50E+10    0.0    -3275.0
565. OCHO+H2O2<=>HOCHO+HO2                   2.40E+12    0.0    10000.0
566. CH3CHO+OH<=>CH3+HOCHO                   3.00E+15   -1.1        0.0
567. HOCO(+M)<=>CO+OH(+M)                    1.00E+00    0.0        0.0
I01:   1.5500E-08  2.9300E+00  8.7680E+03  1.0000E-03
I02:   1.7700E+03  3.4000E-01  1.8076E+04  3.0000E-03
I03:   2.0200E+13 -1.8700E+00  2.2755E+04  2.9600E-02
I04:   1.6800E+18 -3.0500E+00  2.4323E+04  9.8700E-02
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I05:   2.5000E+24 -4.6300E+00  2.7067E+04  2.9610E-01
I06:   4.5400E+26 -5.1200E+00  2.7572E+04  9.8690E-01
I07:   7.1200E+28 -5.6000E+00  2.8535E+04  2.9607E+00
I08:   5.4800E+29 -5.7000E+00  2.8899E+04  9.8690E+00
I09:   9.8900E+31 -6.1900E+00  3.0518E+04  2.9607E+01
     I10:   5.7400E+33 -6.5300E+00  3.2068E+04  9.8690E+01
     I11:   2.6100E+33 -6.2900E+00  3.2231E+04  2.9607E+02
     I12:   6.3000E+32 -5.9600E+00  3.2470E+04  9.8690E+02
568. HOCO(+M)<=>CO2+H(+M)                        1.00E+00    0.0        0.0
I01:   4.7580E+18 -3.8170E+00  1.7676E+04  1.0000E-03
I02:   2.2250E+20 -4.1490E+00  1.9037E+04  3.0000E-03
I03:   7.5640E+21 -4.4340E+00  2.0325E+04  9.9000E-03
I04:   9.1070E+24 -5.1890E+00  2.2419E+04  2.9600E-02
I05:   3.1440E+29 -6.3760E+00  2.5233E+04  9.8700E-02
I06:   1.1500E+32 -7.0370E+00  2.6662E+04  2.9610E-01
I07:   1.0690E+36 -8.1070E+00  2.9064E+04  9.8690E-01
I08:   2.4380E+36 -8.1530E+00  2.9336E+04  2.9607E+00
I09:   6.6630E+35 -7.9190E+00  2.9217E+04  9.8690E+00
     I10:   1.7230E+38 -8.5060E+00  3.1273E+04  2.9607E+01
     I11:   3.0070E+41 -9.2900E+00  3.3966E+04  9.8690E+01
     I12:   6.7670E+36 -7.8320E+00  3.1613E+04  2.9607E+02
     I13:   1.8970E+38 -8.0470E+00  3.4240E+04  9.8690E+02
569. HOCO+O=CO2+OH                               8.67E+12    0.0        0.0
570. HOCO+OH=CO2+H2O                             6.20E+12    0.0        0.0
571. HOCO+O2=CO2+HO2                             1.26E+12    0.0        0.0
572. CO+HOCO=CO2+HCO                             6.03E+09    0.0        0.0
573. C2H2+HOCO=CO2+C2H3                          1.81E+10    0.0        0.0
574. C2H4+HOCO=CO2+C2H5                          6.03E+09    0.0        0.0
575. HOCO=OCHO                                   2.84E+11    0.6    32065.0
576. HOCO+NO2=OH+CO2+NO                          1.00E+11    0.0        0.0
577. OCHO=H+CO2                                  1.34E+18   -1.3     2181.2
578. OCHO+H=CO2+H2                               1.73E+09    0.1     -300.6
579. OCHO+HO2=CO2+H2O2                           1.86E+17   -1.3     4754.3
580. OCHO+O2=CO2+HO2                             1.70E+17   -1.5     4872.0
581. OCHO+O=CO2+OH                               9.23E+15   -0.9      -54.4
582. OCHO+OH=CO2+H2O                             1.26E+17   -1.2     1496.2
583. OCHO+NO=CO2+HNO                             1.49E+17   -1.4     4953.7
584. O2+H=O+OH                                   3.52E+16   -0.7    17070.0
585. O+H2=H+OH                                   5.08E+04    2.7     6292.0
586. OH+H2=H+H2O                                 4.38E+13    0.0     6990.0
587. O+H2O=OH+OH                                 2.97E+06    2.0    13400.0
588. H2+M=H+H+M                                  4.58E+19   -1.4   104400.0
     H2              Enhanced by    2.500E+00
     H2O             Enhanced by    1.200E+01
     HE              Enhanced by    8.300E-01
     CO              Enhanced by    1.900E+00
     CO2             Enhanced by    3.800E+00
589. O+O+M=O2+M                                  6.16E+15   -0.5        0.0
     H2              Enhanced by    2.500E+00
     H2O             Enhanced by    1.200E+01
     AR              Enhanced by    8.300E-01
     HE              Enhanced by    8.300E-01
     CO              Enhanced by    1.900E+00
     CO2             Enhanced by    3.800E+00
590. O+H+M=OH+M                                  4.71E+18   -1.0        0.0
     H2              Enhanced by    2.500E+00
     H2O             Enhanced by    1.200E+01
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     AR              Enhanced by    7.500E-01
     HE              Enhanced by    7.500E-01
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
591. H+OH+M=H2O+M                           3.50E+22   -2.0        0.0
     H2              Enhanced by    7.300E-01
     H2O             Enhanced by    3.650E+00
     AR              Enhanced by    3.800E-01
     HE              Enhanced by    3.800E-01
     CO              Enhanced by    1.900E+00
     CO2             Enhanced by    3.800E+00
592. H+O2(+M)=HO2(+M)                       4.65E+12    0.4        0.0
     Low pressure limit:  0.17370E+20 -0.12300E+01  0.00000E+00
     H2              Enhanced by    1.300E+00
     H2O             Enhanced by    1.000E+01
     AR              Enhanced by    0.000E+00
     HE              Enhanced by    0.000E+00
     CO              Enhanced by    1.900E+00
     CO2             Enhanced by    3.800E+00
593. H+O2(+AR)=HO2(+AR)                     4.65E+12    0.4        0.0
     Low pressure limit:  0.68100E+19 -0.12000E+01  0.00000E+00
594. H+O2(+HE)=HO2(+HE)                     4.65E+12    0.4        0.0
     Low pressure limit:  0.91900E+19 -0.12000E+01  0.00000E+00
595. H2+O2=H+HO2                            5.18E+05    2.4    53500.0
596. HO2+H=OH+OH                            7.08E+13    0.0      295.0
597. HO2+O=OH+O2                            3.25E+13    0.0        0.0
598. HO2+OH=H2O+O2                          2.46E+13    0.0     -497.0
599. HO2+HO2=H2O2+O2                        1.30E+11    0.0    -1630.0
     Declared duplicate reaction...
600. HO2+HO2=H2O2+O2                        3.66E+14    0.0    12000.0
     Declared duplicate reaction...
601. H2O2(+M)=OH+OH(+M)                     2.00E+12    0.9    48750.0
     Low pressure limit:  0.24900E+25 -0.23000E+01  0.48750E+05
     H2              Enhanced by    3.700E+00
     N2              Enhanced by    1.500E+00
     O2              Enhanced by    1.200E+00
     HE              Enhanced by    6.500E-01
     H2O2            Enhanced by    7.700E+00
     H2O             Enhanced by    0.000E+00
     CO              Enhanced by    2.800E+00
     CO2             Enhanced by    1.600E+00
602. H2O2(+H2O)=OH+OH(+H2O)                 2.00E+12    0.9    48750.0
     Low pressure limit:  0.18650E+26 -0.23000E+01  0.48750E+05
603. H2O2+H=H2O+OH                          2.41E+13    0.0     3970.0
604. H2O2+H=H2+HO2                          2.15E+10    1.0     6000.0
605. H2O2+O=OH+HO2                          9.55E+06    2.0     3970.0
606. H2O2+OH=H2O+HO2                        1.74E+12    0.0      318.0
     Declared duplicate reaction...
607. H2O2+OH=H2O+HO2                        7.59E+13    0.0     7269.0
     Declared duplicate reaction...
608. CO+O(+M)=CO2(+M)                       1.36E+10    0.0     2384.0
     Low pressure limit:  0.11730E+25 -0.27900E+01  0.41910E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    1.200E+01
     HE              Enhanced by    7.000E-01
     AR              Enhanced by    7.000E-01
     CO              Enhanced by    1.750E+00
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     CO2             Enhanced by    3.600E+00
609. CO+O2=CO2+O                            1.12E+12    0.0    47700.0
610. CO+OH=CO2+H                            7.02E+04    2.0     -355.7
     Declared duplicate reaction...
611. CO+OH=CO2+H                            5.76E+12   -0.7      331.8
     Declared duplicate reaction...
612. CO+HO2=CO2+OH                          1.57E+05    2.2    17940.0
613. HCO+M=H+CO+M                           4.75E+11    0.7    14870.0
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    1.200E+01
     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
614. HCO+O2=CO+HO2                          7.58E+12    0.0      410.0
615. HCO+H=CO+H2                            7.34E+13    0.0        0.0
616. HCO+O=CO+OH                            3.02E+13    0.0        0.0
617. HCO+O=CO2+H                            3.00E+13    0.0        0.0
618. HCO+OH=CO+H2O                          1.02E+14    0.0        0.0
619. HCO+HO2=CO2+H+OH                       3.00E+13    0.0        0.0
620. HCO+HCO=H2+CO+CO                       3.00E+12    0.0        0.0
621. H+O+M=OH*+M                            1.50E+13    0.0     5975.0
     H2O             Enhanced by    6.500E+00
     O2              Enhanced by    4.000E-01
     N2              Enhanced by    4.000E-01
     AR              Enhanced by    3.500E-01
622. OH*+O2=OH+O2                           2.10E+12    0.5     -482.0
623. OH*+H2=OH+H2                           2.95E+12    0.5     -444.0
624. OH*+N2=OH+N2                           1.08E+11    0.5    -1242.0
625. OH*+AR=OH+AR                           1.69E+12    0.0     4135.0
626. OH*+H2O=OH+H2O                         5.93E+12    0.5     -861.0
627. OH*+CO2=OH+CO2                         2.75E+12    0.5     -968.0
628. OH*+CO=OH+CO                           3.23E+12    0.5     -787.0
629. OH*+OH=OH+OH                           6.01E+12    0.5     -764.0
630. OH*=OH+hv                              1.45E+06    0.0        0.0
631. NH2+OH=NH2OH                           2.98E+14   -0.3      -55.6
632. NH2+OH=NH+H2O                          2.84E+06    2.0    -2245.3
633. NH2+OH=NH3+O                           3.72E+00    3.5     -202.7
634. NH2OH+OH=HNOH+H2O                      1.54E+04    2.6    -3536.9
635. NH2OH+OH=NH2O+H2O                      1.53E+05    2.3    -1295.5
636. NH2OH+NH2=HNOH+NH3                     1.08E-01    4.0      -97.4
637. NH2OH+NH2=NH2O+NH3                     9.45E+00    3.4    -1013.4
638. NH2OH+NH=HNOH+NH2                      2.91E-03    4.4     1563.8
639. NH2OH+NH=NH2O+NH2                      1.46E-03    4.6     2424.1
640. NH+OH=H2O+N                            1.59E+07    1.7     -576.2
641. NH+OH=HNO+H                            3.24E+14   -0.4      -45.7
642. NH+NH=N2H2                             6.26E+13    0.0     -160.9
643. NH+NH=N+NH2                            5.66E-01    3.9      341.8
644. NH2+NH=N2H2+H                          4.26E+14   -0.3      -77.5
645. NH2+NH=N+NH3                           9.57E+03    2.5      107.3
646. NH2+NH2=N2H2+H2                        1.74E+08    1.0    11782.9
647. NH2+NH2=H2NN+H2                        7.16E+04    1.9     8802.4
648. NH2+NH2=NH+NH3                         5.63E+00    3.5      552.4
649. N2H4+H=NH2+NH3                         2.40E+09    0.0     3100.0
650. N2H4+O=N2H2+H2O                        4.40E+11    0.0    -1270.0
651. N2H4+N=N2H3+NH                         1.00E+10    1.0     2000.0
652. N2H4+NH=NH2+N2H3                       1.00E+09    1.5     2000.0
653. N2H4+NH2=NH3+N2H3                      4.82E+00    3.6      770.0
654. N2H3+N2H2=N2H4+NNH                     1.00E+13    0.0     6000.0
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655. N2H3+N2H3=N2H4+N2H2                    1.20E+13    0.0        0.0
656. N2H4+NO2=N2H3+HONO                     5.60E+04    2.5     7787.0
657. N2H3=N2H2+H                            3.60E+47  -10.4    68970.0
658. N2H3+H=NH+NH3                          1.00E+11    0.0        0.0
659. NH3+NH2=N2H3+H2                        1.00E+11    0.5    21600.0
660. N2H3+N=N2H2+NH                         1.00E+06    2.0        0.0
661. N2H3+NH=N2H2+NH2                       2.00E+13    0.0        0.0
662. N2H3+NNH=N2H2+N2H2                     1.00E+13    0.0     4000.0
663. N2H3+N2H3=NH3+NH3+N2                   3.00E+12    0.0        0.0
664. N2H3+O=NH2+NO+H                        3.00E+13    0.0     6800.0
665. N2H2+N=NNH+NH                          1.00E+06    2.0        0.0
666. NNH+NNH=N2H2+N2                        1.00E+13    0.0     4000.0
667. NH3+M=H2+NH+M                          6.31E+14    0.0    93400.0
668. NH3+HNO3=H2NONO+H2O                    2.32E+01    3.5    44930.0
669. NH3+HNO3=H2O+H2NNO2                    8.10E-01    3.5    43060.0
670. NH3+HOONO=H2NONO+H2O                   2.32E+01    3.5    29410.0
671. NH3+HONO=H2O+NH2NO                     2.20E+06    0.0        0.0
672. NH3+NH=N2H4                            6.50E+11    0.0    -1630.0
673. HO2+NH=HNO+OH                          1.52E+10    0.0        0.0
674. NH+NH=N2+H2                            1.00E+08    1.0        0.0
675. NH+NH=NNH+H                            5.10E+13    0.0        0.0
676. NH+OH=NO+H2                            2.00E+13    0.0        0.0
677. NH+N2O=N2+HNO                          2.00E+12    0.0     6000.0
678. NH+HONO=NH2+NO2                        1.00E+13    0.0        0.0
679. NH+O2=H+NO2                            2.30E+10    0.0     2482.0
680. NH2+M=NH+H+M                           3.16E+23   -2.0    91400.0
681. NH2+O=H2+NO                            5.00E+12    0.0        0.0
682. NH2+HO2=HNO+H2O                        5.68E+15   -1.1      707.0
683. NH2+HO2=NH2O+OH                        2.90E+17   -1.3     1250.0
684. NH2+O2(+M)=NH2QJ(+M)                   1.00E+00    0.0        0.0
I01:   5.9900E+16 -3.8600E+00  4.2690E+03  1.0000E-03
I02:   5.9900E+17 -3.8600E+00  4.2690E+03  1.0000E-02
I03:   6.0000E+18 -3.8600E+00  4.2700E+03  1.0000E-01
I04:   6.0700E+19 -3.8600E+00  4.2740E+03  1.0000E+00
I05:   6.7000E+20 -3.8700E+00  4.3160E+03  1.0000E+01
I06:   1.9000E+21 -3.8900E+00  4.3740E+03  2.5000E+01
I07:   4.3500E+21 -3.9000E+00  4.4490E+03  5.0000E+01
I08:   7.1400E+21 -3.9100E+00  4.5080E+03  7.5000E+01
I09:   1.0100E+22 -3.9200E+00  4.5570E+03  1.0000E+02
685. NH2+O2(+M)=NH2O+O(+M)                  1.00E+00    0.0        0.0
I01:   7.3700E+10  6.2000E-01  2.9871E+04  1.0000E-03
I02:   7.3700E+10  6.2000E-01  2.9871E+04  1.0000E-02
I03:   7.3700E+10  6.2000E-01  2.9871E+04  1.0000E-01
I04:   7.3700E+10  6.2000E-01  2.9871E+04  1.0000E+00
I05:   7.3700E+10  6.2000E-01  2.9871E+04  1.0000E+01
I06:   7.3700E+10  6.2000E-01  2.9871E+04  2.5000E+01
I07:   7.3700E+10  6.2000E-01  2.9871E+04  5.0000E+01
I08:   7.3700E+10  6.2000E-01  2.9871E+04  7.5000E+01
I09:   7.3700E+10  6.2000E-01  2.9871E+04  1.0000E+02
686. NH2+O2(+M)=NJH2Q(+M)                   1.00E+00    0.0        0.0
I01:   3.9200E-70  1.8370E+01  6.4850E+03  1.0000E-03
I02:   3.9200E-69  1.8370E+01  6.4850E+03  1.0000E-02
I03:   3.9100E-68  1.8370E+01  6.4850E+03  1.0000E-01
I04:   3.8400E-67  1.8380E+01  6.4870E+03  1.0000E+00
I05:   3.2700E-66  1.8410E+01  6.5080E+03  1.0000E+01
I06:   6.5000E-66  1.8460E+01  6.5480E+03  2.5000E+01
I07:   9.8100E-66  1.8520E+01  6.6300E+03  5.0000E+01
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I08:   1.2600E-65  1.8570E+01  6.7320E+03  7.5000E+01
I09:   1.6500E-65  1.8600E+01  6.8540E+03  1.0000E+02
687. NH2+O2(+M)=NH+HO2(+M)                   1.00E+00    0.0         0.0
I01:   6.3000E+07  1.0000E+00  4.0526E+04  1.0000E-03
I02:   6.3000E+07  1.0000E+00  4.0526E+04  1.0000E-02
I03:   6.3000E+07  1.0000E+00  4.0526E+04  1.0000E-01
I04:   6.3000E+07  1.0000E+00  4.0526E+04  1.0000E+00
I05:   6.3000E+07  1.0000E+00  4.0526E+04  1.0000E+01
I06:   6.3100E+07  1.0000E+00  4.0527E+04  2.5000E+01
I07:   6.3100E+07  1.0000E+00  4.0527E+04  5.0000E+01
I08:   6.3100E+07  1.0000E+00  4.0527E+04  7.5000E+01
I09:   6.3100E+07  1.0000E+00  4.0528E+04  1.0000E+02
688. NH2+O2(+M)=HNO+OH(+M)                   1.00E+00    0.0         0.0
I01:   8.5000E+05  1.5200E+00  2.2767E+04  1.0000E-03
I02:   8.5000E+05  1.5200E+00  2.2767E+04  1.0000E-02
I03:   8.5000E+05  1.5200E+00  2.2767E+04  1.0000E-01
I04:   8.5000E+05  1.5200E+00  2.2767E+04  1.0000E+00
I05:   8.5000E+05  1.5200E+00  2.2767E+04  1.0000E+01
I06:   8.5000E+05  1.5200E+00  2.2767E+04  2.5000E+01
I07:   8.5000E+05  1.5200E+00  2.2767E+04  5.0000E+01
I08:   8.5000E+05  1.5200E+00  2.2767E+04  7.5000E+01
I09:   8.5000E+05  1.5200E+00  2.2767E+04  1.0000E+02
689. NH2QJ(+M)=NH2O+O(+M)                    1.00E+00    0.0         0.0
I01:   3.5700E-17  5.3300E+00  6.7164E+04  1.0000E-03
I02:   3.5600E-16  5.3300E+00  6.7163E+04  1.0000E-02
I03:   3.4100E-15  5.3300E+00  6.7149E+04  1.0000E-01
I04:   2.2600E-14  5.3800E+00  6.7015E+04  1.0000E+00
I05:   5.5500E-15  5.8400E+00  6.5779E+04  1.0000E+01
I06:   9.5400E-17  6.4500E+00  6.4043E+04  2.5000E+01
I07:   3.4900E-19  7.2100E+00  6.1715E+04  5.0000E+01
I08:   4.8400E-21  7.7800E+00  5.9846E+04  7.5000E+01
I09:   1.4000E-22  8.2400E+00  5.8252E+04  1.0000E+02
690. NH2QJ(+M)=NJH2Q(+M)                     1.00E+00    0.0         0.0
I01:   4.5500E-14  4.1300E+00  5.2989E+04  1.0000E-03
I02:   4.5300E-13  4.1300E+00  5.2988E+04  1.0000E-02
I03:   4.3500E-12  4.1300E+00  5.2975E+04  1.0000E-01
I04:   2.9400E-11  4.1800E+00  5.2846E+04  1.0000E+00
I05:   8.6600E-12  4.6100E+00  5.1670E+04  1.0000E+01
I06:   2.0200E-13  5.1800E+00  5.0033E+04  2.5000E+01
I07:   1.2100E-15  5.8900E+00  4.7867E+04  5.0000E+01
I08:   2.7100E-17  6.3900E+00  4.6156E+04  7.5000E+01
I09:   1.2500E-18  6.7900E+00  4.4717E+04  1.0000E+02
691. NJH2Q(+M)=NH+HO2(+M)                    1.00E+00    0.0         0.0
I01:   4.9100E-08  2.8900E+00  1.1165E+05  1.0000E-03
I02:   2.4200E-25  8.4500E+00  1.0412E+05  1.0000E-02
I03:   5.4900E-29  9.7500E+00  1.0115E+05  1.0000E-01
I04:   1.3500E-33  1.1340E+01  9.7788E+04  1.0000E+00
I05:   2.6300E-32  1.1080E+01  9.5770E+04  1.0000E+01
I06:   3.3700E-45  1.5100E+01  8.9585E+04  2.5000E+01
I07:   8.6600E-50  1.6490E+01  8.5552E+04  5.0000E+01
I08:   1.4800E-51  1.6980E+01  8.2774E+04  7.5000E+01
I09:   1.9100E-45  1.5020E+01  8.2867E+04  1.0000E+02
692. NJH2Q(+M)=HNO+OH(+M)                    1.00E+00    0.0         0.0
I01:   7.4200E+10 -1.4300E+00  3.6320E+03  1.0000E-03
I02:   6.2500E+00  2.0100E+00 -7.2000E+01  1.0000E-02
I03:   2.4400E+04  1.2100E+00  7.9500E+02  1.0000E-01
I04:   1.0900E+07  6.9000E-01  1.3380E+03  1.0000E+00
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I05:   9.9700E+15 -1.7900E+00  4.0180E+03  1.0000E+01
I06:   3.0900E+07  9.9000E-01  1.0740E+03  2.5000E+01
I07:   2.7500E+07  1.1000E+00  9.8300E+02  5.0000E+01
I08:   4.9500E+08  7.6000E-01  1.3680E+03  7.5000E+01
I09:   1.6200E+17 -1.8500E+00  4.2120E+03  1.0000E+02
693. NH2+NO2=H2O+N2O                         2.59E+18   -2.2      455.0
694. NH2+NO2=NO+NH2O                         9.03E+11    0.0    -1512.1
695. NH2+NO2(+M)=H2NNO2(+M)                  1.00E+00    0.0        0.0
I01:   1.1700E+14 -2.6500E+00  1.3993E+04  1.0000E-03
I02:   1.6200E+15 -2.6500E+00  9.4670E+03  1.0000E-02
I03:   4.2800E+20 -3.8100E+00  4.6830E+03  1.0000E-01
I04:   4.3000E+27 -5.4400E+00  3.4900E+03  1.0000E+00
I05:   2.8900E+29 -5.6300E+00  3.5720E+03  1.0000E+01
I06:   1.5000E+29 -5.4400E+00  3.5050E+03  2.5000E+01
I07:   5.3800E+28 -5.2300E+00  3.4070E+03  5.0000E+01
I08:   2.4700E+28 -5.0800E+00  3.3390E+03  7.5000E+01
I09:   1.3100E+28 -4.9700E+00  3.2850E+03  1.0000E+02
696. NH2+NO2(+M)=HNNDOOH_Z(+M)               1.00E+00    0.0        0.0
I01:   3.5400E+16 -3.7100E+00  1.4136E+04  1.0000E-03
I02:   1.7000E+18 -3.8600E+00  9.8750E+03  1.0000E-02
I03:   2.2700E+24 -5.2300E+00  5.2450E+03  1.0000E-01
I04:   1.3900E+31 -6.8000E+00  3.9560E+03  1.0000E+00
I05:   1.4900E+32 -6.7500E+00  3.9010E+03  1.0000E+01
I06:   1.3900E+31 -6.3200E+00  3.7570E+03  2.5000E+01
I07:   7.7000E+29 -5.8600E+00  3.5990E+03  5.0000E+01
I08:   9.1400E+28 -5.5400E+00  3.4840E+03  7.5000E+01
I09:   1.6500E+28 -5.2900E+00  3.3890E+03  1.0000E+02
697. NH2+NO2(+M)=HNNO+OH(+M)                 1.00E+00    0.0        0.0
     Declared duplicate reaction...
I01:   1.3200E+20 -2.2700E+00  1.4568E+04  1.0000E-03
I02:   1.3200E+20 -2.2700E+00  1.4568E+04  1.0000E-02
I03:   1.3200E+20 -2.2700E+00  1.4568E+04  1.0000E-01
I04:   1.3200E+20 -2.2700E+00  1.4568E+04  1.0000E+00
I05:   1.3500E+20 -2.2700E+00  1.4573E+04  1.0000E+01
I06:   1.3700E+20 -2.2700E+00  1.4579E+04  2.5000E+01
I07:   1.3200E+20 -2.2600E+00  1.4596E+04  5.0000E+01
I08:   1.1900E+20 -2.2500E+00  1.4616E+04  7.5000E+01
I09:   1.0000E+20 -2.2200E+00  1.4634E+04  1.0000E+02
698. NH2+NO2(+M)=HNNDOOH(+M)                 1.00E+00    0.0        0.0
I01:   1.9000E+17 -3.8900E+00  1.4245E+04  1.0000E-03
I02:   7.4000E+18 -4.0100E+00  9.9680E+03  1.0000E-02
I03:   1.0000E+25 -5.4000E+00  5.3650E+03  1.0000E-01
I04:   6.3800E+31 -7.0100E+00  4.1140E+03  1.0000E+00
I05:   5.0800E+32 -6.9500E+00  4.1400E+03  1.0000E+01
I06:   2.9600E+31 -6.4700E+00  4.1940E+03  2.5000E+01
I07:   6.3100E+29 -5.9000E+00  4.1830E+03  5.0000E+01
I08:   3.1500E+28 -5.4700E+00  4.1240E+03  7.5000E+01
I09:   2.7000E+27 -5.1300E+00  4.0510E+03  1.0000E+02
699. NH2+NO2(+M)=HNNO+OH(+M)                 1.00E+00    0.0        0.0
     Declared duplicate reaction...
I01:   8.4500E+23 -3.6700E+00  1.5267E+04  1.0000E-03
I02:   8.4500E+23 -3.6700E+00  1.5267E+04  1.0000E-02
I03:   8.4500E+23 -3.6700E+00  1.5267E+04  1.0000E-01
I04:   8.4700E+23 -3.6700E+00  1.5266E+04  1.0000E+00
I05:   8.7400E+23 -3.6700E+00  1.5265E+04  1.0000E+01
I06:   9.0500E+23 -3.6700E+00  1.5271E+04  2.5000E+01
I07:   9.2700E+23 -3.6700E+00  1.5333E+04  5.0000E+01
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I08:   8.5900E+23 -3.6600E+00  1.5421E+04  7.5000E+01
I09:   7.0800E+23 -3.6300E+00  1.5505E+04  1.0000E+02
700. H2NNO2(+M)=HNNDOOH_Z(+M)                1.00E+00    0.0         0.0
I01:   1.3600E+31 -6.7100E+00  4.0260E+04  1.0000E-03
I02:   2.6500E+31 -6.5400E+00  4.0179E+04  1.0000E-02
I03:   1.5600E+31 -6.2100E+00  4.0392E+04  1.0000E-01
I04:   4.2100E+29 -5.5000E+00  4.0422E+04  1.0000E+00
I05:   1.1100E+27 -4.5700E+00  4.0016E+04  1.0000E+01
I06:   7.8700E+25 -4.1900E+00  3.9729E+04  2.5000E+01
I07:   9.0000E+24 -3.8900E+00  3.9470E+04  5.0000E+01
I08:   2.5600E+24 -3.7100E+00  3.9315E+04  7.5000E+01
I09:   1.0000E+24 -3.5800E+00  3.9198E+04  1.0000E+02
701. HNNDOOH_Z(+M)=HNNO+OH(+M)               1.00E+00    0.0         0.0
I01:   5.6400E+06 -4.1000E-01  8.1292E+04  1.0000E-03
I02:   2.5700E+07 -3.2000E-01  8.0827E+04  1.0000E-02
I03:   3.1600E+06  2.0000E-01  7.7500E+04  1.0000E-01
I04:   6.2700E+06  3.7000E-01  6.7474E+04  1.0000E+00
I05:   1.2400E+18 -2.4100E+00  5.7913E+04  1.0000E+01
I06:   9.0900E+23 -3.8200E+00  5.6798E+04  2.5000E+01
I07:   2.0600E+27 -4.5600E+00  5.6665E+04  5.0000E+01
I08:   4.2700E+28 -4.8100E+00  5.6710E+04  7.5000E+01
I09:   2.3600E+29 -4.9300E+00  5.6791E+04  1.0000E+02
702. HNNDOOH_Z(+M)=HNNDOOH(+M)               1.00E+00    0.0         0.0
I01:   2.2800E+30 -6.5900E+00  3.4948E+04  1.0000E-03
I02:   2.2200E+31 -6.5900E+00  3.4960E+04  1.0000E-02
I03:   1.6500E+32 -6.5600E+00  3.5039E+04  1.0000E-01
I04:   2.7000E+32 -6.3600E+00  3.5192E+04  1.0000E+00
I05:   2.5300E+31 -5.8400E+00  3.5224E+04  1.0000E+01
I06:   2.4300E+30 -5.4700E+00  3.5064E+04  2.5000E+01
I07:   2.1900E+29 -5.1100E+00  3.4841E+04  5.0000E+01
I08:   3.9800E+28 -4.8600E+00  3.4660E+04  7.5000E+01
I09:   1.1700E+28 -4.6800E+00  3.4524E+04  1.0000E+02
703. HNNDOOH(+M)=N2O+H2O(+M)                 1.00E+00    0.0         0.0
I01:   3.2500E+29 -6.4600E+00  3.4529E+04  1.0000E-03
I02:   3.2400E+30 -6.4600E+00  3.4553E+04  1.0000E-02
I03:   2.5800E+31 -6.4300E+00  3.4688E+04  1.0000E-01
I04:   3.4100E+31 -6.1800E+00  3.4933E+04  1.0000E+00
I05:   1.2400E+30 -5.4800E+00  3.5028E+04  1.0000E+01
I06:   5.9000E+28 -4.9900E+00  3.4853E+04  2.5000E+01
I07:   2.5500E+27 -4.5200E+00  3.4584E+04  5.0000E+01
I08:   3.0400E+26 -4.2100E+00  3.4374E+04  7.5000E+01
I09:   6.0000E+25 -3.9700E+00  3.4203E+04  1.0000E+02
704. HNNDOOH(+M)=HNNO+OH(+M)                 1.00E+00    0.0         0.0
I01:   4.0500E+08 -1.0200E+00  7.9357E+04  1.0000E-03
I02:   8.1700E+08 -8.3000E-01  7.8645E+04  1.0000E-02
I03:   1.3400E+06  2.1000E-01  7.3946E+04  1.0000E-01
I04:   1.2500E+04  9.9000E-01  6.2065E+04  1.0000E+00
I05:   6.1900E+17 -2.5400E+00  5.4166E+04  1.0000E+01
I06:   2.4600E+25 -4.4400E+00  5.4363E+04  2.5000E+01
I07:   4.9800E+29 -5.4400E+00  5.5039E+04  5.0000E+01
I08:   2.8200E+31 -5.8000E+00  5.5456E+04  7.5000E+01
I09:   2.1600E+32 -5.9600E+00  5.5724E+04  1.0000E+02
705. NH2+NO2(+M)=H2NONO(+M)                  1.00E+00    0.0         0.0
I01:   5.1000E-33  9.5700E+00  1.2610E+03  1.0000E-03
I02:   6.0500E-32  9.5400E+00  1.2890E+03  1.0000E-02
I03:   3.1600E-30  9.3300E+00  1.5640E+03  1.0000E-01
I04:   1.4400E-23  7.6900E+00  3.7130E+03  1.0000E+00
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I05:   3.2700E-01  1.4500E+00  1.0551E+04  1.0000E+01
I06:   4.9500E+01  9.1000E-01  7.9640E+03  2.5000E+01
I07:   1.1600E+03  6.0000E-01  5.2660E+03  5.0000E+01
I08:   2.4600E+04  2.8000E-01  3.8210E+03  7.5000E+01
I09:   3.9600E+05 -3.0000E-02  2.9210E+03  1.0000E+02
706. H2NONO(+M)=NH2O+NO(+M)                 1.00E+00    0.0        0.0
I01:   2.2600E+15 -2.6000E+00  1.2067E+04  1.0000E-03
I02:   2.2700E+16 -2.6000E+00  1.2069E+04  1.0000E-02
I03:   2.2900E+17 -2.6100E+00  1.2084E+04  1.0000E-01
I04:   2.2500E+18 -2.6000E+00  1.2180E+04  1.0000E+00
I05:   1.8400E+19 -2.5900E+00  1.2526E+04  1.0000E+01
I06:   3.1200E+19 -2.5400E+00  1.2738E+04  2.5000E+01
I07:   2.7600E+16 -1.5000E+00  1.1868E+04  5.0000E+01
I08:   8.9900E+16 -1.6000E+00  1.2142E+04  7.5000E+01
I09:   1.6700E+17 -1.6500E+00  1.2310E+04  1.0000E+02
707. H2NONO(+M)=H2NNO2(+M)                  1.00E+00    0.0        0.0
I01:   6.6200E-20  4.9500E+00  1.2084E+05  1.0000E-03
I02:   3.7600E-26  7.0600E+00  1.1699E+05  1.0000E-02
I03:   1.6900E-32  9.1900E+00  1.1293E+05  1.0000E-01
I04:   7.1700E-39  1.1310E+01  1.0771E+05  1.0000E+00
I05:   4.4100E-42  1.2470E+01  9.9915E+04  1.0000E+01
I06:   7.5500E-43  1.2770E+01  9.4754E+04  2.5000E+01
I07:   6.0900E-47  1.4100E+01  8.8299E+04  5.0000E+01
I08:   1.0800E-46  1.4060E+01  8.4755E+04  7.5000E+01
I09:   1.8400E-46  1.4020E+01  8.1972E+04  1.0000E+02
708. H2NNO2+HONO=NH3+N2O4                   6.67E+00    3.3    38263.0
709. H2NNO2+HNO3=NH3+N2O5                   1.55E+00    3.3    34266.0
710. H2NNO2+HONO=H2O+NO2+HNNO               9.79E-02    3.8    17650.0
711. H2NNO2+HNO3=H2O+HNNO+NO3               1.54E-02    3.8    45280.0
712. H2NNO2+OH=HNJNO2+H2O                   2.04E+06    2.0      566.0
713. H2NNO2+H=HNJNO2+H2                     5.42E+05    2.4     9917.0
714. H2NNO2+O=HNJNO2+OH                     9.40E+06    1.9     6460.0
715. H2NNO2+NO=HNJNO2+HNO                   1.04E+07    1.7    56640.0
716. H2NNO2+NO2=HNJNO2+HONO                 7.32E+00    3.3    22260.0
717. H2NNO2+NH=HNJNO2+NH2                   3.16E+14    0.0    26830.0
718. H2NNO2+NH2=HNJNO2+NH3                  4.82E+00    3.6      770.0
719. NH+NO2=HNJNO2                          1.00E+13    0.0        0.0
720. HNJNO2+NO2=HNOJNO2+NO                  8.45E+08    1.2     -675.0
721. HNOJNO2=HNO+NO2                        3.76E+13    0.3    12343.0
722. H2NNO2+H2O=HNNDOOH_Z+H2O               1.59E+01    2.9    10625.0
723. HNNDOOH_Z+H2O=HNNDOOH+H2O              1.57E+00    2.9     1709.1
724. HNNDOOH+H2O=N2O+H2O+H2O                1.02E+00    3.2     9501.4
725. H2NNO2+NH3=HNNDOOH_Z+NH3               5.51E+02    2.5     6344.6
726. HNNDOOH_Z+NH3=HNNDOOH+NH3              3.10E+01    2.6    -3334.0
727. HNNDOOH+NH3=N2O+H2O+NH3                2.66E+00    3.3     5351.9
728. H2NNO2+HNO3=HNNDOOH_Z+HNO3             1.66E-01    3.7    19776.0
729. HNNDOOH_Z+HNO3=HNNDOOH+HNO3            7.50E-01    3.1      569.7
730. HNNDOOH+HNO3=N2O+H2O+HNO3              1.28E+00    2.9     3121.5
731. H2NNO2+H2NNO2=HNNDOOH_Z+H2NNO2         1.66E-01    3.4    15365.0
732. HNNDOOH_Z+H2NNO2=HNNDOOH+H2NNO2        1.44E-02    3.5     7153.4
733. HNNDOOH+H2NNO2=N2O+H2O+H2NNO2          9.31E-04    4.2    14686.0
734. H2NNO2+HONO=HNNDOOH_Z+HONO             7.29E-02    3.6    14151.0
735. HNNDOOH_Z+HONO=HNNDOOH+HONO            5.91E-02    3.3     7202.0
736. HNNDOOH+HONO=N2O+H2O+HONO              9.57E-03    3.9    13828.0
737. NH2OH+NO2=NH2O+HNO2                    4.63E+01    3.3     4369.0
738. NH2OH+NO2=NH2O+HONO                    4.39E-03    4.4      556.0
739. NH2OH(+M)=NH2+OH(+M)                   1.40E+20   -1.3    64080.0
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     Low pressure limit:  0.54000E+38 -0.59600E+01  0.66783E+05
     TROE centering:      0.31000E+00  0.10000E-29  0.10000E+31  0.10000E+31
740. NH2OH+H=HNOH+H2                          4.80E+08    1.5     6246.0
741. NH2OH+H=NH2O+H2                          2.40E+08    1.5     5064.0
742. NH2OH+O=HNOH+OH                          3.30E+08    1.5     3863.0
743. NH2OH+O=NH2O+OH                          1.70E+08    1.5     3009.0
744. NH2O+HO2=O2+NH2OH                        2.90E+04    2.7    -1599.0
745. HNOH+HO2=NH2OH+O2                        2.90E+04    2.7    -1599.0
746. NH2OH+HO2=HNOH+H2O2                      2.90E+04    2.7     9552.0
747. NH2OH+HO2=NH2O+H2O2                      1.40E+04    2.7     6414.0
748. N2H4+O=NH2OH+NH                          2.90E+11    0.0    -1270.0
749. NH2O+M=HNO+H+M                           2.80E+24   -2.8    64915.0
     H2O             Enhanced by    1.000E+01
750. NH2O+M=HNOH+M                            1.10E+29   -4.0    44000.0
     H2O             Enhanced by    1.000E+01
751. NH2O+NO=HNO+HNO                          3.02E+03    2.1    16082.0
752. NH2O+HO2=HNO+H2O2                        2.90E+04    2.7    -1599.0
753. NH2O+NO2=HNO+HONO                        5.60E+04    2.5        0.0
754. NH2O+NH=NH2+HNO                          3.88E+04    2.4     8598.5
     Declared duplicate reaction...
755. NH2O+NH<=>NH2+HNO                        4.14E+12   -0.7      228.0
     Declared duplicate reaction...
756. NH2O+NH<=>NH3+NO                         5.83E+03    1.2     -149.0
757. NH2O+NH<=>NH2+HNO                        2.35E+14   -0.5      333.0
     Declared duplicate reaction...
758. HNO+HONO=H2O+NO+NO                       1.74E-01    3.6    19676.0
759. HNO2+HONO=H2O+N2O3                       1.38E-02    4.0    11811.0
760. N2O4+H2O=HONO+HNO3                       4.58E-02    4.5    29826.9
761. HNO3+HONO=H2O+ONONO2                     2.00E+06    2.1     6463.7
762. NO2+NO2=ONONO2                           1.44E+01    2.9     6332.9
763. HNO3+HNO2=H2O+NO2+NO2                    1.64E-03    4.2    31165.0
764. HNO3+HNO3=H2O+NO2+NO3                    6.04E-03    3.8    31310.0
765. N2O5+H2O=HNO3+HNO3                       2.84E-01    3.4    15697.0
766. HNO3+O=HONO+O2                           2.00E+13    0.0     8000.0
767. HNO3+OH=HONO+HO2                         2.00E+13    0.0     8000.0
768. OH+HNO3=H2O2+NO2                         4.82E+08    0.0        0.0
769. HO2+NO=HOONO                             2.62E+13   -0.2     -200.0
770. OH+NO2=HOONO                             2.47E+13    0.0        0.0
771. HOONO+NO=HONO+NO2                        5.00E+12    0.0     2000.0
772. HOONO=HNO3                               5.00E+10    0.0    18000.0
773. HOONO+OH=H2O+NO3                         9.03E+10    0.0        0.0
774. HNO2(+M)=HONO(+M)                        2.50E+14    0.0    32300.0
     Low pressure limit:  0.31000E+19  0.00000E+00  0.31500E+05
     TROE centering:      0.11490E+01  0.10000E-29  0.31250E+04  0.10000E+31
775. NO2+HO2=HNO2+O2                          1.90E+01    3.3     4983.0
776. NO3=NO+O2                                2.50E+06    0.0    12122.0
777. HNNO+NO2=NNH+NO3                         1.00E+13    0.0    12270.0
778. N2O3(+M)=NO+NO2(+M)                      4.80E+14    0.4     9700.0
     Low pressure limit:  0.38600E+39 -0.87000E+01  0.97000E+04
779. N2O5(+M)=NO3+NO2(+M)                     5.49E+14    0.1    22060.0
     Low pressure limit:  0.27500E+30 -0.35000E+01  0.21860E+05
780. HNOH+M=H+HNO+M                           2.00E+24   -2.8    58901.0
781. HNOH+HO2=HNO+H2O2                        2.90E+04    2.7    -1599.0
782. HNOH+NH2=HNO+NH3                         1.80E+06    1.9    -1152.0
783. HNNO+NO=N2O+HNO                          1.00E+12    0.0        0.0
784. NNH+OH=HONNH                             5.00E+13    0.0        0.0
785. HONNH=H2O+N2                             2.55E+11    0.7     9923.7
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786. NH2NO=N2+H2O                                 3.10E+34   -7.1    36262.0
787. NH2NO+H=HNNO+H2                              4.80E+08    1.5     7407.0
788. N2H3+O=NH2NO+H                               3.00E+13    0.0        0.0
789. H2NN+OH=NH2NO+H                              2.00E+12    0.0        0.0
790. NH2NO+O=HNNO+OH                              3.30E+08    1.5     4697.0
791. NH2NO+OH=HNNO+H2O                            2.40E+06    2.0      -70.0
792. H2NN+HO2=NH2NO+OH                            6.60E+05    1.9     7050.0
793. NH2NO+HO2=HNNO+H2O2                          2.90E+04    2.7    12620.0
794. NH2NO+NH2=HNNO+NH3                           1.80E+06    1.9     4538.0
795. NH2NO+NO2=HNNO+HNO2                          4.63E+01    3.3    14369.0
796. NH2NO+NO2=HNNO+HONO                          4.39E-03    4.4    10556.0
797. NH2NO+O2=HNNO+HO2                            3.01E+13    0.0    39390.0
798. N2O+NH2=N2+NH2O                              9.55E+04    2.3    32570.0
799. NH2+NO=H2+N2O                                1.00E+13    0.0    33700.0
800. NNH+O2=N2O+OH                                2.90E+11   -0.3      149.0
801. N2H2+NO=N2O+NH2                              4.00E+12    0.0    11915.0
802. HNNO+NO2=N2O+HONO                            1.00E+12    0.0        0.0
803. N2O+O2=N2+O3                                 6.46E+08    2.5    66569.0
804. N2O+NH3=N2+NH2OH                             2.47E+06    2.5    49182.0
805. N2O+N2H4=N2+H2O+N2H2                         7.86E+04    2.7    46467.0
806. N2O+NO2=N2+NO3                               1.03E+03    2.8    48602.0
807. N2O+NH2NO=N2+NH2O+NO                         3.17E+06    1.9    57986.0
808. N2O+H2NNO2=N2+HNO+HONO                       1.72E+05    2.8    53322.0
809. HO2+H2O2=OH+H2O+O2                           6.03E+10    0.0        0.0
810. O+OH+M=HO2+M                                 5.00E+16    0.0        0.0
811. H+HO2+M=H2O2+M                               3.61E+17   -0.7        0.0
812. H2O+O=H2+O2                                  1.07E+10    1.0    68700.0
813. NNH+O2=N2+H+O2                               5.00E+13    0.0        0.0
814. NNH+HO2=N2+H2O2                              1.40E+04    2.7    -1599.0
815. NNH+N=NH+N2                                  3.00E+13    0.0     2000.0
816. O2+O(+M)=O3(+M)                              1.69E+12    0.0        0.0
     Low pressure limit:  0.20000E+20  0.20000E+01  0.00000E+00
817. O3+O=O2+O2                                   5.66E+12    0.0     4200.0
818. O3+H=OH+O2                                   8.43E+13    0.0      930.0
819. O3+H=HO2+O                                   4.52E+11    0.0        0.0
820. O3+OH=O2+HO2                                 1.54E+12    0.0     2100.0
821. O3+NO=O2+NO2                                 1.25E+12    0.0        2.8
822. O3+NO2=O2+NO3                                9.74E+10    0.0     5000.0
823. NO2(+M)=NO+O(+M)                             7.60E+18   -1.3    73290.0
     Low pressure limit:  0.24700E+29 -0.33700E+01  0.74800E+05
     T&H values:       0.95000E+00 -0.10000E-03
     N2O             Enhanced by    1.500E+00
     H2O             Enhanced by    4.400E+00
     N2              Enhanced by    1.000E+00
     CO2             Enhanced by    2.300E+00
824. N2O(+M)=N2+O(+M)                             1.26E+12    0.0    62620.0
     Low pressure limit:  0.59700E+15  0.00000E+00  0.56640E+05
     N2O             Enhanced by    5.000E+00
     H2O             Enhanced by    9.000E+00
     N2              Enhanced by    1.000E+00
     CO2             Enhanced by    3.200E+00
     O2              Enhanced by    8.200E-01
825. H+NO(+M)=HNO(+M)                             1.52E+15   -0.4        0.0
     Low pressure limit:  0.40000E+21 -0.17500E+01  0.00000E+00
     N2O             Enhanced by    5.000E+00
     H2O             Enhanced by    5.000E+00
     N2              Enhanced by    1.000E+00
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     CO2             Enhanced by    1.300E+00
826. NO+OH(+M)=HONO(+M)                      1.99E+12   -0.1     -721.0
     Low pressure limit:  0.50800E+24 -0.25100E+01 -0.67600E+02
     T&H values:       0.62000E+00  0.00000E+00
     N2O             Enhanced by    5.000E+00
     H2O             Enhanced by    8.300E+00
     N2              Enhanced by    1.000E+00
     CO2             Enhanced by    1.500E+00
827. HCN(+M)=H+CN(+M)                        8.30E+17   -0.9   123800.0
     Low pressure limit:  0.35700E+27 -0.26000E+01  0.12490E+06
     T&H values:       0.95000E+00 -0.10000E-03
     N2O             Enhanced by    5.000E+00
     H2O             Enhanced by    5.000E+00
     N2              Enhanced by    1.000E+00
     CO2             Enhanced by    1.600E+00
828. CN+CN(+M)=C2N2(+M)                      5.66E+12    0.0        0.0
     Low pressure limit:  0.34300E+26 -0.26100E+01  0.00000E+00
     T&H values:       0.50000E+00  0.00000E+00
     N2O             Enhanced by    5.000E+00
     H2O             Enhanced by    5.000E+00
     N2              Enhanced by    1.000E+00
     CO2             Enhanced by    1.600E+00
829. HNCO(+M)=NH+CO(+M)                      6.00E+13    0.0    99800.0
     Low pressure limit:  0.21700E+29 -0.31000E+01  0.10190E+06
     T&H values:       0.90000E+00 -0.20000E-03
     N2O             Enhanced by    5.000E+00
     H2O             Enhanced by    5.000E+00
     N2              Enhanced by    1.000E+00
     CO2             Enhanced by    1.600E+00
830. HCN+H(+M)=H2CN(+M)                      3.31E+13    0.0     4844.0
     Low pressure limit:  0.16000E+25 -0.27300E+01  0.76600E+04
     T&H values:       0.95000E+00 -0.10000E-03
     N2O             Enhanced by    5.000E+00
     H2O             Enhanced by    5.000E+00
     N2              Enhanced by    1.000E+00
     CO2             Enhanced by    2.000E+00
831. CN+NO(+M)=NCNO(+M)                      3.98E+13    0.0        0.0
     Low pressure limit:  0.15600E+37 -0.62000E+01  0.48780E+04
     T&H values:       0.65000E+00  0.00000E+00
     N2O             Enhanced by    5.000E+00
     H2O             Enhanced by    5.000E+00
     N2              Enhanced by    1.000E+00
     CO2             Enhanced by    2.000E+00
832. CN+M=C+N+M                              2.50E+14    0.0   141100.0
     N2              Enhanced by    1.500E+00
     CO2             Enhanced by    2.400E+00
833. NO+M=N+O+M                              1.40E+15    0.0   148430.0
     N2              Enhanced by    1.000E+00
     H2              Enhanced by    2.200E+00
     H2O             Enhanced by    6.700E+00
     CO2             Enhanced by    3.000E+00
     N2O             Enhanced by    2.200E+00
834. N2+M=N+N+M                              3.71E+21   -1.6   225000.0
835. NO2+N=N2O+O                             3.49E+12    0.0     -437.0
836. NO2+NO2=NO+NO3                          9.64E+09    0.7    20920.0
837. NO2+NO2=NO+NO+O2                        4.51E+12    0.0    27600.0
838. NO2+NO3=NO+NO2+O2                       2.71E+10    0.0     2500.0
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839.	HNO+NO=N2O+OH	1.70E+13	0.0	29590.0
840.	HNO+O2=HO2+NO	1.00E+13	0.0	25000.0
841.	HNO+NO2=HONO+NO	4.42E+04	2.6	4042.0
842.	HONO+O=OH+NO2	1.20E+13	0.0	5961.0
843.	HONO+OH=H2O+NO2	1.27E+10	1.0	135.0
844.	HONO+NH2=NO2+NH3	9.20E+05	1.9	1920.0
845.	HNO+O=OH+NO	3.61E+13	0.0	0.0
846.	NH+O=NO+H	5.50E+13	0.0	0.0
847.	NH+O=N+OH	3.72E+13	0.0	0.0
848.	NH+NH=N2+H+H	5.10E+13	0.0	0.0
849.	NH+M=N+H+M	2.65E+14	0.0	75510.0
850.	CH+O2=HCO+O	3.30E+13	0.0	0.0
851.	CH+O=CO+H	5.70E+13	0.0	0.0
852.	CH+OH=HCO+H	3.00E+13	0.0	0.0
853.	CH+CO2=HCO+CO	3.40E+12	0.0	690.0
854.	CH+H=C+H2	1.50E+14	0.0	0.0
855.	C+O2=CO+O	2.00E+13	0.0	0.0
856.	C+OH=CO+H	5.00E+13	0.0	0.0
857.	O+HCCO=H+2CO	1.00E+14	0.0	0.0
858.	HCCO+O2=2CO+OH	1.60E+12	0.0	854.0
859.	H+HO2=O+H2O	3.01E+13	0.0	1721.0
860.	2H+H2=2H2	9.20E+16	-0.6	0.0
861.	2H+H2O=H2+H2O	6.00E+19	-1.2	0.0
862.	2H+CO2=H2+CO2	5.49E+20	-2.0	0.0
863.	CH+N2=NCN+H	2.22E+07	1.5	23367.0
864.	H+NCN=HCN+N	1.89E+14	0.0	8425.0
865.	NCN+N=CN+N2	2.00E+13	0.0	0.0
866.	CN+N=C+N2	1.04E+15	-0.5	0.0
867.	C+NO=CN+O	6.60E+13	0.0	0.0
868.	HCCO+NO=HCNO+CO	2.00E+13	0.0	0.0
869.	CH+N=CN+H	1.30E+13	0.0	0.0
870.	HCCO+N=HCN+CO	5.00E+13	0.0	0.0
871.	HCN+OH=CN+H2O	3.90E+06	1.8	10290.0
872.	OH+HCN=HNCO+H	1.98E-03	4.0	1000.0
873.	OH+HCN=NH2+CO	7.83E-04	4.0	4000.0
874.	HCN+O=NCO+H	1.38E+04	2.6	4980.0
875.	HCN+O=NH+CO	3.45E+03	2.6	4980.0
876.	HCN+O=CN+OH	2.70E+09	1.6	26600.0
877.	CN+H2=HCN+H	3.61E+08	1.6	3000.0
878.	CN+O=CO+N	2.05E+13	0.0	417.0
879.	CN+O2=NCO+O	2.60E+14	-0.5	0.0
880.	CN+OH=NCO+H	4.00E+13	0.0	0.0
881.	CN+HCN=C2N2+H	1.51E+07	1.7	1530.0
882.	CN+NO2=NCO+NO	6.16E+15	-0.8	344.0
883.	CN+CO2=NCO+CO	3.67E+06	2.2	26900.0
884.	CN+N2O=NCN+NO	6.00E+13	0.0	15360.0
885.	C2N2+O=NCO+CN	4.57E+12	0.0	8880.0
886.	NO+HO2=NO2+OH	2.11E+12	0.0	-479.0
887.	NO2+H=NO+OH	1.30E+14	0.0	361.0
888.	NO2+O=NO+O2	3.90E+12	0.0	-238.0
889.	NCO+H=NH+CO	5.40E+13	0.0	0.0
890.	NCO+O=NO+CO	4.52E+13	0.0	0.0
891.	NCO+O2=NO+CO2	2.00E+12	0.0	20000.0
892.	NCO+N=N2+CO	2.00E+13	0.0	0.0
893.	NCO+OH=NO+CO+H	2.00E+13	0.0	7500.0
894.	NCO+M=N+CO+M	1.14E+23	-1.9	59930.0
	N2O Enhanced by 5.000E+00			

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     H2O             Enhanced by    5.000E+00
     N2              Enhanced by    1.000E+00
     CO2             Enhanced by    1.500E+00
895. NCO+NO=N2O+CO                          3.98E+19   -2.2     1743.0
896. NCO+NO=CO2+N2                          1.46E+21   -2.7     1824.0
897. NCO+H2=HNCO+H                          2.07E+06    2.0     6020.0
898. NCO+NO2=CO2+N2O                        1.95E+13   -0.3     -620.0
899. NCO+NO2=CO+NO+NO                       1.77E+12   -0.3     -620.0
900. NH+O2=HNO+O                            4.61E+05    2.0     6500.0
901. NH+O2=NO+OH                            1.28E+06    1.5      100.0
902. NH+NO=N2O+H                            3.50E+14   -0.5       16.1
903. NH+NO=N2+OH                            2.16E+13   -0.2        0.0
904. N2O+OH=N2+HO2                          1.29E-02    4.7    36561.0
905. N2O+H=N2+OH                            1.30E+11    0.9    15210.0
906. NNH+O=N2O+H                            1.40E+14   -0.4      477.0
907. NNH+O=NO+NH                            3.30E+14   -0.2    -1013.0
908. N2O+O=N2+O2                            3.69E+12    0.0    15940.0
909. N2O+O=NO+NO                            9.16E+13    0.0    27680.0
910. NH+N=N2+H                              3.00E+13    0.0        0.0
911. N+H2=NH+H                              2.33E+14    0.0    30830.0
912. NH2+O=HNO+H                            4.60E+13    0.0        0.0
913. NH2+O=NH+OH                            7.00E+12    0.0        0.0
     Declared duplicate reaction...
914. NH2+O=NH+OH                            3.33E+08    1.5     5077.0
     Declared duplicate reaction...
915. NH2+H=NH+H2                            4.00E+13    0.0     3650.0
916. NH2+N=N2+H+H                           7.20E+13    0.0        0.0
917. NH2+O2=HNO+OH                          4.50E+12    0.0    25000.0
918. NH2+NH2=N2H3+H                         1.79E+13   -0.3    11320.0
919. NH2+NH2(+M)=N2H4(+M)                   1.00E+00    0.0        0.0
I01:   1.5000E+28 -5.7600E+00  3.3330E+03  1.0000E-03
I02:   1.5400E+29 -5.7700E+00  3.4380E+03  1.0000E-02
I03:   8.0800E+29 -5.7000E+00  3.7430E+03  1.0000E-01
I04:   3.0400E+29 -5.3200E+00  4.0750E+03  1.0000E+00
I05:   6.4400E+26 -4.3000E+00  3.7910E+03  1.0000E+01
I06:   1.2300E+25 -3.7200E+00  3.4140E+03  2.5000E+01
I07:   4.3300E+23 -3.2300E+00  3.0500E+03  5.0000E+01
I08:   5.7100E+22 -2.9500E+00  2.8160E+03  7.5000E+01
I09:   1.3400E+22 -2.7400E+00  2.6440E+03  1.0000E+02
920. NH+NO2=N2O+OH                           4.00E+12    0.0        0.0
921. NH+NO2=NO+HNO                           5.70E+12    0.0        0.0
922. N2H4+H=N2H3+H2                          5.50E+12    0.0     2268.0
923. N2H4+O=N2H3+OH                          6.70E+08    1.5     2851.0
924. N2H4+OH=N2H3+H2O                        4.80E+06    2.0     -646.0
925. N2H3+H=N2H2+H2                          2.40E+08    1.5      -10.0
926. N2H3+O=NH2+HNO                          3.00E+13    0.0        0.0
927. N2H3+O=N2H2+OH                          1.70E+08    1.5     -646.0
928. N2H3+OH=N2H2+H2O                        1.20E+06    2.0    -1192.0
929. N2H3+NH2=N2H2+NH3                       9.20E+05    1.9    -1152.0
930. N2H3+HO2=N2H2+H2O2                      2.90E+04    2.7    -1600.0
931. N2H3+HO2=N2H4+O2                        9.20E+05    1.9     2126.0
932. N2H2+M=NNH+H+M                          5.00E+16    0.0    50000.0
     H2O             Enhanced by    1.500E+01
     O2              Enhanced by    2.000E+00
     N2              Enhanced by    2.000E+00
     H2              Enhanced by    2.000E+00
933. N2H2+H=NNH+H2                           5.00E+13    0.0     1000.0
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934. N2H2+O=NH2+NO                          1.00E+13    0.0        0.0
935. N2H2+O=NNH+OH                          2.00E+13    0.0     1000.0
936. N2H2+OH=NNH+H2O                        1.00E+13    0.0     1000.0
937. N2H2+NH=NNH+NH2                        1.00E+13    0.0     1000.0
938. N2H2+NH2=NH3+NNH                       1.00E+13    0.0     1000.0
939. NH2+NO=NNH+OH                          2.29E+10    0.4     -815.0
940. NH2+NO=N2+H2O                          2.77E+20   -2.6     1258.0
941. NH3+OH=NH2+H2O                         2.04E+06    2.0      566.0
942. NH3+H=NH2+H2                           5.42E+05    2.4     9917.0
943. NH3(+M)=NH2+H(+M)                      5.50E+15    0.0   107792.0
     Low pressure limit:  0.22000E+17  0.00000E+00  0.93470E+05
944. NNH+NO=N2+HNO                          2.00E+13    0.0        0.0
945. NNH+H=N2+H2                            1.00E+14    0.0        0.0
946. NNH+OH=N2+H2O                          5.00E+13    0.0        0.0
947. NNH+NH2=N2+NH3                         5.00E+13    0.0        0.0
948. NNH+NH=N2+NH2                          5.00E+13    0.0        0.0
949. HNO+OH=NO+H2O                          1.30E+07    1.9     -958.0
950. H+HNO=H2+NO                            4.46E+11    0.7      655.0
951. HNO+NH2=NH3+NO                         2.00E+13    0.0     1000.0
952. N+NO=N2+O                              3.27E+12    0.3        0.0
953. O+NO=N+O2                              3.80E+09    1.0    41375.0
954. NO+H=N+OH                              1.70E+14    0.0    48800.0
955. HNO+HNO=N2O+H2O                        3.63E-03    4.0     1190.0
956. HNC+O=NH+CO                            5.44E+12    0.0        0.0
957. HNC+O=H+NCO                            1.60E+01    3.1     -224.0
958. HNC+OH=HNCO+H                          2.80E+13    0.0     3696.0
959. N2O+NO=N2+NO2                          4.29E+13    0.0    47130.0
960. NO+NO+NO=N2O+NO2                       1.07E+10    0.0    26800.0
961. HNC+OH=CN+H2O                          1.50E+12    0.0     7680.0
962. HNC+NO2=HNCO+NO                        1.00E+12    0.0    32000.0
963. HNCO+O=CO2+NH                          1.95E+14   -0.3    13020.0
964. HNCO+O=NCO+OH                          6.67E-04    4.5    -1770.0
965. HNCO+O=HNO+CO                          1.49E+08    1.6    44010.0
966. HNCO+OH=H2O+NCO                        4.79E+05    2.0     2560.0
967. HNCO+OH=NH2+CO2                        1.60E+05    2.0     2560.0
968. HNCO+HO2=NCO+H2O2                      3.00E+11    0.0    23700.0
969. HNCO+NH=NH2+NCO                        2.00E+13    0.0    19300.0
970. HNCO+H=NH2+CO                          2.25E+07    1.7     3800.0
971. HNCO+NO2=HNNO+CO2                      2.50E+12    0.0    26000.0
972. CH+NO=HCN+O                            1.10E+14    0.0        0.0
973. CN+NO=NCO+N                            5.50E+12    0.0    30620.0
974. CN+NO=N2+CO                            3.90E+11    0.0    27820.0
975. CN+NO=NCN+O                            1.80E+13    0.0    38190.0
976. CO+NO2=NO+CO2                          9.04E+13    0.0    33780.0
977. CH+NO2=HCO+NO                          1.01E+14    0.0        0.0
978. H2+NO2=HONO+H                          1.30E+04    2.8    29770.0
979. HONO+H=HNO+OH                          5.63E+10    0.9     4969.0
980. HONO+H=H2O+NO                          8.13E+06    1.9     3847.0
981. 2HONO=NO+NO2+H2O                       3.49E-01    3.6    12140.0
982. NNH(+M)=N2+H(+M)                       4.10E+09    1.1     5186.0
     Low pressure limit:  0.10000E+14  0.50000E+00  0.30600E+04
     N2O             Enhanced by    5.000E+00
     H2O             Enhanced by    9.000E+00
     N2              Enhanced by    1.000E+00
     O2              Enhanced by    8.200E-01
     HNO3            Enhanced by    5.000E+00
     NH3             Enhanced by    5.000E+00
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     NO3             Enhanced by    5.000E+00
983. NNH=N2+H                                  3.00E+08    0.0        0.0
984. HCN+M=HNC+M                               4.36E+26   -3.3    50194.0
985. HNO+NO+NO=HNNO+NO2                        1.70E+11    0.0     2100.0
986. HNNO+NO=NNH+NO2                           3.20E+12    0.0      270.0
987. HNNO+NO=N2+HONO                           2.60E+11    0.0      810.0
988. HNNO+M=H+N2O+M                            2.20E+15    0.0    21600.0
989. HNNO+M=N2+OH+M                            1.00E+15    0.0    25600.0
990. HNNO+OH=H2O+N2O                           2.00E+13    0.0        0.0
991. HNNO+H=H2+N2O                             2.00E+13    0.0        0.0
992. HCO+NO=HNO+CO                             7.23E+12    0.0        0.0
993. O+CH2<=>H+HCO                             8.00E+13    0.0        0.0
994. O+CH2(S)<=>H2+CO                          1.50E+13    0.0        0.0
995. O+CH2(S)<=>H+HCO                          1.50E+13    0.0        0.0
996. O+CH3<=>H+CH2O                            5.06E+13    0.0        0.0
997. O+CH4<=>OH+CH3                            1.02E+09    1.5     8600.0
998. O+CH2O<=>OH+HCO                           3.90E+13    0.0     3540.0
999. O+CH2OH<=>OH+CH2O                         1.00E+13    0.0        0.0
1000. O+CH3O<=>OH+CH2O                         1.00E+13    0.0        0.0
1001. O+CH3OH<=>OH+CH2OH                       3.88E+05    2.5     3100.0
1002. O+CH3OH<=>OH+CH3O                        1.30E+05    2.5     5000.0
1003. O+C2H<=>CH+CO                            5.00E+13    0.0        0.0
1004. O+C2H2<=>H+HCCO                          1.35E+07    2.0     1900.0
1005. O+C2H2<=>OH+C2H                          4.60E+19   -1.4    28950.0
1006. O+C2H2<=>CO+CH2                          6.94E+06    2.0     1900.0
1007. O+C2H3<=>H+CH2CO                         3.00E+13    0.0        0.0
1008. O+C2H4<=>CH3+HCO                         1.25E+07    1.8      220.0
1009. O+C2H5<=>CH3+CH2O                        2.24E+13    0.0        0.0
1010. O+C2H6<=>OH+C2H5                         8.98E+07    1.9     5690.0
1011. O+CH2CO<=>OH+HCCO                        1.00E+13    0.0     8000.0
1012. O+CH2CO<=>CH2+CO2                        1.75E+12    0.0     1350.0
1013. O2+CH2O<=>HO2+HCO                        1.00E+14    0.0    40000.0
1014. H+CH2(+M)<=>CH3(+M)                      6.00E+14    0.0        0.0
      Low pressure limit:  0.10400E+27 -0.27600E+01  0.16000E+04
      TROE centering:      0.56200E+00  0.91000E+02  0.58360E+04  0.85520E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
1015. H+CH2(S)<=>CH+H2                         3.00E+13    0.0        0.0
1016. H+CH3(+M)<=>CH4(+M)                      1.39E+16   -0.5      536.0
      Low pressure limit:  0.26200E+34 -0.47600E+01  0.24400E+04
      TROE centering:      0.78300E+00  0.74000E+02  0.29410E+04  0.69640E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    3.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
1017. H+CH4<=>CH3+H2                           6.60E+08    1.6    10840.0
1018. H+HCO(+M)<=>CH2O(+M)                     1.09E+12    0.5     -260.0
      Low pressure limit:  0.24700E+25 -0.25700E+01  0.42500E+03
      TROE centering:      0.78240E+00  0.27100E+03  0.27550E+04  0.65700E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
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      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
1019. H+CH2O(+M)<=>CH2OH(+M)                 5.40E+11    0.5     3600.0
      Low pressure limit:  0.12700E+33 -0.48200E+01  0.65300E+04
      TROE centering:      0.71870E+00  0.10300E+03  0.12910E+04  0.41600E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
1020. H+CH2O<=>HCO+H2                       5.74E+07    1.9     2742.0
1021. H+CH2OH(+M)<=>CH3OH(+M)               1.06E+12    0.5       86.0
      Low pressure limit:  0.43600E+32 -0.46500E+01  0.50800E+04
      TROE centering:      0.60000E+00  0.10000E+03  0.90000E+05  0.10000E+05
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
1022. H+CH2OH<=>H2+CH2O                     2.00E+13    0.0        0.0
1023. H+CH2OH<=>OH+CH3                      1.65E+11    0.7     -284.0
1024. H+CH2OH<=>CH2(S)+H2O                  3.28E+13   -0.1      610.0
1025. H+CH3O(+M)<=>CH3OH(+M)                2.43E+12    0.5       50.0
      Low pressure limit:  0.46600E+42 -0.74400E+01  0.14080E+05
      TROE centering:      0.70000E+00  0.10000E+03  0.90000E+05  0.10000E+05
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
1026. H+CH3O<=>H+CH2OH                      4.15E+07    1.6     1924.0
1027. H+CH3O<=>H2+CH2O                      2.00E+13    0.0        0.0
1028. H+CH3O<=>OH+CH3                       1.50E+12    0.5     -110.0
1029. H+CH3O<=>CH2(S)+H2O                   2.62E+14   -0.2     1070.0
1030. H+CH3OH<=>CH2OH+H2                    1.70E+07    2.1     4870.0
1031. H+CH3OH<=>CH3O+H2                     4.20E+06    2.1     4870.0
1032. H+C2H(+M)<=>C2H2(+M)                  1.00E+17   -1.0        0.0
      Low pressure limit:  0.37500E+34 -0.48000E+01  0.19000E+04
      TROE centering:      0.64640E+00  0.13200E+03  0.13150E+04  0.55660E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
1033. H+C2H2(+M)<=>C2H3(+M)                 5.60E+12    0.0     2400.0
      Low pressure limit:  0.38000E+41 -0.72700E+01  0.72200E+04
      TROE centering:      0.75070E+00  0.98500E+02  0.13020E+04  0.41670E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
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      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
1034. H+C2H3(+M)<=>C2H4(+M)                  6.08E+12    0.3      280.0
      Low pressure limit:  0.14000E+31 -0.38600E+01  0.33200E+04
      TROE centering:      0.78200E+00  0.20750E+03  0.26630E+04  0.60950E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
1035. H+C2H3<=>H2+C2H2                       3.00E+13    0.0        0.0
1036. H+C2H4(+M)<=>C2H5(+M)                  5.40E+11    0.5     1820.0
      Low pressure limit:  0.60000E+42 -0.76200E+01  0.69700E+04
      TROE centering:      0.97530E+00  0.21000E+03  0.98400E+03  0.43740E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
1037. H+C2H4<=>C2H3+H2                       1.32E+06    2.5    12240.0
1038. H+C2H5(+M)<=>C2H6(+M)                  5.21E+17   -1.0     1580.0
      Low pressure limit:  0.19900E+42 -0.70800E+01  0.66850E+04
      TROE centering:      0.84220E+00  0.12500E+03  0.22190E+04  0.68820E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
1039. H+C2H5<=>H2+C2H4                       2.00E+12    0.0        0.0
1040. H+C2H6<=>C2H5+H2                       1.15E+08    1.9     7530.0
1041. H+HCCO<=>CH2(S)+CO                     1.00E+14    0.0        0.0
1042. H+HCCOH<=>H+CH2CO                      1.00E+13    0.0        0.0
1043. H2+CO(+M)<=>CH2O(+M)                   4.30E+07    1.5    79600.0
      Low pressure limit:  0.50700E+28 -0.34200E+01  0.84350E+05
      TROE centering:      0.93200E+00  0.19700E+03  0.15400E+04  0.10300E+05
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
1044. OH+CH2<=>H+CH2O                        2.00E+13    0.0        0.0
1045. OH+CH2<=>CH+H2O                        1.13E+07    2.0     3000.0
1046. OH+CH2(S)<=>H+CH2O                     3.00E+13    0.0        0.0
1047. OH+CH3(+M)<=>CH3OH(+M)                 2.79E+18   -1.4     1330.0
      Low pressure limit:  0.40000E+37 -0.59200E+01  0.31400E+04
      TROE centering:      0.41200E+00  0.19500E+03  0.59000E+04  0.63940E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
1048. OH+CH3<=>CH2+H2O                       5.60E+07    1.6     5420.0
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1049. OH+CH3<=>CH2(S)+H2O                    6.44E+17   -1.3     1417.0
1050. OH+CH4<=>CH3+H2O                       1.00E+08    1.6     3120.0
1051. OH+CH2O<=>HCO+H2O                      3.43E+09    1.2     -447.0
1052. OH+CH2OH<=>H2O+CH2O                    5.00E+12    0.0        0.0
1053. OH+CH3O<=>H2O+CH2O                     5.00E+12    0.0        0.0
1054. OH+CH3OH<=>CH2OH+H2O                   1.44E+06    2.0     -840.0
1055. OH+CH3OH<=>CH3O+H2O                    6.30E+06    2.0     1500.0
1056. OH+C2H<=>H+HCCO                        2.00E+13    0.0        0.0
1057. OH+C2H2<=>H+CH2CO                      2.18E-04    4.5    -1000.0
1058. OH+C2H2<=>H+HCCOH                      5.04E+05    2.3    13500.0
1059. OH+C2H2<=>C2H+H2O                      3.37E+07    2.0    14000.0
1060. OH+C2H2<=>CH3+CO                       4.83E-04    4.0    -2000.0
1061. OH+C2H3<=>H2O+C2H2                     5.00E+12    0.0        0.0
1062. OH+C2H4<=>C2H3+H2O                     3.60E+06    2.0     2500.0
1063. OH+C2H6<=>C2H5+H2O                     3.54E+06    2.1      870.0
1064. OH+CH2CO<=>HCCO+H2O                    7.50E+12    0.0     2000.0
1065. HO2+CH2<=>OH+CH2O                      2.00E+13    0.0        0.0
1066. HO2+CH3<=>O2+CH4                       1.00E+12    0.0        0.0
1067. HO2+CH3<=>OH+CH3O                      2.00E+13    0.0        0.0
1068. HO2+CH2O<=>HCO+H2O2                    5.60E+06    2.0    12000.0
1069. C+CH2<=>H+C2H                          5.00E+13    0.0        0.0
1070. C+CH3<=>H+C2H2                         5.00E+13    0.0        0.0
1071. CH+H2<=>H+CH2                          1.08E+14    0.0     3110.0
1072. CH+H2O<=>H+CH2O                        5.71E+12    0.0     -755.0
1073. CH+CH2<=>H+C2H2                        4.00E+13    0.0        0.0
1074. CH+CH3<=>H+C2H3                        3.00E+13    0.0        0.0
1075. CH+CH4<=>H+C2H4                        6.00E+13    0.0        0.0
1076. CH+CO(+M)<=>HCCO(+M)                   5.00E+13    0.0        0.0
      Low pressure limit:  0.26900E+29 -0.37400E+01  0.19360E+04
      TROE centering:      0.57570E+00  0.23700E+03  0.16520E+04  0.50690E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
1077. CH+CH2O<=>H+CH2CO                      9.46E+13    0.0     -515.0
1078. CH+HCCO<=>CO+C2H2                      5.00E+13    0.0        0.0
1079. CH2+O2=>OH+H+CO                        5.00E+12    0.0     1500.0
1080. CH2+H2<=>H+CH3                         5.00E+05    2.0     7230.0
1081. 2CH2<=>H2+C2H2                         1.60E+15    0.0    11944.0
1082. CH2+CH3<=>H+C2H4                       4.00E+13    0.0        0.0
1083. CH2+CH4<=>2CH3                         2.46E+06    2.0     8270.0
1084. CH2+HCCO<=>C2H3+CO                     3.00E+13    0.0        0.0
1085. CH2(S)+N2<=>CH2+N2                     1.50E+13    0.0      600.0
1086. CH2(S)+O2<=>H+OH+CO                    2.80E+13    0.0        0.0
1087. CH2(S)+O2<=>CO+H2O                     1.20E+13    0.0        0.0
1088. CH2(S)+H2<=>CH3+H                      7.00E+13    0.0        0.0
1089. CH2(S)+H2O(+M)<=>CH3OH(+M)             4.82E+17   -1.2     1145.0
      Low pressure limit:  0.18800E+39 -0.63600E+01  0.50400E+04
      TROE centering:      0.60270E+00  0.20800E+03  0.39220E+04  0.10180E+05
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
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1090. CH2(S)+H2O<=>CH2+H2O                    3.00E+13    0.0        0.0
1091. CH2(S)+CH3<=>H+C2H4                     1.20E+13    0.0     -570.0
1092. CH2(S)+CH4<=>2CH3                       1.60E+13    0.0     -570.0
1093. CH2(S)+CO<=>CH2+CO                      9.00E+12    0.0        0.0
1094. CH2(S)+CO2<=>CH2+CO2                    7.00E+12    0.0        0.0
1095. CH2(S)+CO2<=>CO+CH2O                    1.40E+13    0.0        0.0
1096. CH2(S)+C2H6<=>CH3+C2H5                  4.00E+13    0.0     -550.0
1097. CH3+O2<=>O+CH3O                         3.56E+13    0.0    30480.0
1098. CH3+O2<=>OH+CH2O                        2.31E+12    0.0    20315.0
1099. CH3+H2O2<=>HO2+CH4                      2.45E+04    2.5     5180.0
1100. 2CH3(+M)<=>C2H6(+M)                     6.77E+16   -1.2      654.0
      Low pressure limit:  0.34000E+42 -0.70300E+01  0.27620E+04
      TROE centering:      0.61900E+00  0.73200E+02  0.11800E+04  0.99990E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
1101. 2CH3<=>H+C2H5                           6.84E+12    0.1    10600.0
1102. CH3+HCO<=>CH4+CO                        2.65E+13    0.0        0.0
1103. CH3+CH2O<=>HCO+CH4                      3.32E+03    2.8     5860.0
1104. CH3+CH3OH<=>CH2OH+CH4                   3.00E+07    1.5     9940.0
1105. CH3+CH3OH<=>CH3O+CH4                    1.00E+07    1.5     9940.0
1106. CH3+C2H4<=>C2H3+CH4                     2.27E+05    2.0     9200.0
1107. CH3+C2H6<=>C2H5+CH4                     6.14E+06    1.7    10450.0
1108. CH2OH+O2<=>HO2+CH2O                     1.80E+13    0.0      900.0
1109. CH3O+O2<=>HO2+CH2O                      4.28E-13    7.6    -3530.0
1110. C2H+O2<=>HCO+CO                         1.00E+13    0.0     -755.0
1111. C2H+H2<=>H+C2H2                         5.68E+10    0.9     1993.0
1112. C2H3+O2<=>HCO+CH2O                      4.58E+16   -1.4     1015.0
1113. C2H4(+M)<=>H2+C2H2(+M)                  8.00E+12    0.4    86770.0
      Low pressure limit:  0.15800E+52 -0.93000E+01  0.97800E+05
      TROE centering:      0.73450E+00  0.18000E+03  0.10350E+04  0.54170E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
1114. C2H5+O2<=>HO2+C2H4                      8.40E+11    0.0     3875.0
1115. 2HCCO<=>2CO+C2H2                        1.00E+13    0.0        0.0
1116. NNH+CH3<=>CH4+N2                        2.50E+13    0.0        0.0
1117. NNH+O2<=>HO2+N2                         5.00E+12    0.0        0.0
1118. NNH+O<=>OH+N2                           2.50E+13    0.0        0.0
1119. H2CN+N<=>N2+CH2                         6.00E+13    0.0      400.0
1120. CH2+N2<=>HCN+NH                         1.00E+13    0.0    74000.0
1121. CH2(S)+N2<=>NH+HCN                      1.00E+11    0.0    65000.0
1122. C+NO<=>CO+N                             2.90E+13    0.0        0.0
1123. CH+NO<=>H+NCO                           1.62E+13    0.0        0.0
1124. CH+NO<=>N+HCO                           2.46E+13    0.0        0.0
1125. CH2+NO<=>H+HNCO                         3.10E+17   -1.4     1270.0
1126. CH2+NO<=>OH+HCN                         2.90E+14   -0.7      760.0
1127. CH2+NO<=>H+HCNO                         3.80E+13   -0.4      580.0
1128. CH2(S)+NO<=>H+HNCO                      3.10E+17   -1.4     1270.0
1129. CH2(S)+NO<=>OH+HCN                      2.90E+14   -0.7      760.0
1130. CH2(S)+NO<=>H+HCNO                      3.80E+13   -0.4      580.0
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1131. CH3+NO<=>HCN+H2O                        9.60E+13    0.0    28800.0
1132. CH3+NO<=>H2CN+OH                        1.00E+12    0.0    21750.0
1133. HCNO+H<=>H+HNCO                         2.10E+15   -0.7     2850.0
1134. HCNO+H<=>OH+HCN                         2.70E+11    0.2     2120.0
1135. HCNO+H<=>NH2+CO                         1.70E+14   -0.8     2890.0
1136. CH3+N<=>H2CN+H                          6.10E+14   -0.3      290.0
1137. CH3+N<=>HCN+H2                          3.70E+12    0.1      -90.0
1138. OH+NO2(+M)=HNO3(+M)                     2.41E+13    0.0        0.0
      Low pressure limit:  0.64200E+33 -0.54900E+01  0.23500E+04
      T&H values:       0.72500E+00 -0.25000E-03
      N2O             Enhanced by    5.000E+00
      H2O             Enhanced by    9.000E+00
      N2              Enhanced by    1.000E+00
      HNO3            Enhanced by    5.000E+00
      NH3             Enhanced by    5.000E+00
      NO3             Enhanced by    5.000E+00
1139. HNO3+H=NO3+H2                           2.40E+08    1.5    11600.0
1140. HNO3+H=NO2+H2O                          6.00E+13    0.0     9800.0
1141. HNO3+H=HNO2+OH                          6.00E+13    0.0     7000.0
1142. HNO3+H=HONO+OH                          2.00E+13    0.0     8000.0
1143. HNO3+O=NO3+OH                           2.00E+13    0.0    12000.0
1144. HNO3+OH=H2O+NO3                         4.34E+09    0.0    -1560.0
1145. HNO3+OH(+M)=H2O+NO3(+M)                 2.47E+08    0.0    -2860.0
      Low pressure limit:  0.68900E+15  0.00000E+00 -0.14400E+04
      N2O             Enhanced by    5.000E+00
      H2O             Enhanced by    9.000E+00
      N2              Enhanced by    1.000E+00
      HNO3            Enhanced by    5.000E+00
      NH3             Enhanced by    5.000E+00
      NO3             Enhanced by    5.000E+00
1146. NO3+H2O2=HNO3+HO2                       1.00E+12    0.0     8500.0
1147. HNO3+NH=HNOH+NO2                        1.50E+13    0.0     6000.0
1148. HNO3+NH2=NO3+NH3                        9.00E+05    2.0     7300.0
1149. HNO3+NH2=NH2O+HNO2                      3.00E+12    0.0     9000.0
1150. HNO3+NH3=NH2O+H2O+NO                    2.32E+01    3.5    44930.0
1151. HNO3+NO=HONO+NO2                        8.00E+06    2.0    11000.0
1152. HONO+NO3=HNO3+NO2                       1.00E+12    0.0     6000.0
1153. HNO2+NO3=HNO3+NO2                       1.00E+12    0.0     5000.0
1154. O+NO2(+M)=NO3(+M)                       1.33E+13    0.0        0.0
      Low pressure limit:  0.14900E+29 -0.40800E+01  0.24700E+04
      T&H values:       0.79000E+00 -0.18000E-03
      N2O             Enhanced by    5.000E+00
      H2O             Enhanced by    9.000E+00
      N2              Enhanced by    1.000E+00
      HNO3            Enhanced by    5.000E+00
      NH3             Enhanced by    5.000E+00
      NO3             Enhanced by    5.000E+00
1155. NO3+H=NO2+OH                            6.00E+13    0.0        0.0
1156. NO3+O=NO2+O2                            1.00E+13    0.0        0.0
1157. NO3+OH=HO2+NO2                          1.20E+13    0.0        0.0
1158. NO3+HO2=NO2+O2+OH                       2.50E+12    0.0        0.0
1159. NO3+NH=HNO+NO2                          1.50E+13    0.0        0.0
1160. NO3+NH=HNO3+N                           1.00E+12    0.0     5000.0
1161. NO3+NH2=HNO3+NH                         1.00E+12    0.0    10000.0
1162. NO3+NH2=NH2O+NO2                        9.00E+05    0.0      100.0
1163. NO3+NO3=2NO2+O2                         5.12E+11    0.0     4870.0
1164. NO2+HO2=HONO+O2                         1.00E+12    0.0     5000.0
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1165. HNOH+NO2=HONO+HNO                      6.00E+11    0.0     2000.0
1166. HNOH+H=NH2+OH                          4.00E+13    0.0        0.0
1167. HNOH+H=HNO+H2                          4.80E+08    1.5      378.0
1168. HNOH+O=HNO+OH                          7.00E+13    0.0        0.0
      Declared duplicate reaction...
1169. HNOH+O=HNO+OH                          3.30E+08    1.5     -358.0
      Declared duplicate reaction...
1170. HNOH+OH=HNO+H2O                        2.40E+06    2.0    -1192.0
1171. NH2O+H=NH2+OH                          4.00E+13    0.0        0.0
1172. NH2O+H=HNO+H2                          4.80E+08    1.5     1560.0
1173. NH2O+O=HNO+OH                          3.30E+08    1.5      487.0
1174. NH2O+OH=HNO+H2O                        2.40E+06    2.0    -1192.0
1175. NH2O+NH2=HNO+NH3                       1.80E+06    1.9    -1152.0
1176. HNO2+H=H2+NO2                          2.40E+08    1.5     4163.0
1177. HNO2+O=OH+NO2                          1.70E+08    1.5     2365.0
1178. HNO2+OH=H2O+NO2                        1.20E+06    2.0     -795.0
1179. HNO2+NH2=NO2+NH3                       9.20E+05    1.9      874.0
1180. NO3+CH2O=HNO3+HCO                      1.70E+12    0.0     5000.0
1181. NO3+HCO=H+CO2+NO2                      2.00E+13    0.0        0.0
1182. NO3+C2H4=C2H4O+NO2                     2.00E+12    0.0     5720.0
1183. C2H4O=CH4+CO                           1.21E+13    0.0    57200.0
1184. C2H4O=CH3CHO                           7.26E+13    0.0    57200.0
1185. C2H4O=CH3+HCO                          3.63E+13    0.0    57200.0
1186. C2H4O+CH3=CH4+CH2CHO                   1.10E+12    0.0    11800.0
1187. C2H4O+OH=H2O+CH2CHO                    1.40E+13    0.0     3360.0
1188. C2H4O+H=H2+CH2CHO                      3.80E+13    0.0     9197.0
1189. C2H4O+NO2=HONO+CH2CHO                  1.30E+12    0.0     3700.0
1190. C2H4O+NO3=HNO3+CH2CHO                  1.00E+12    0.0     6000.0
1191. H+CH2CHO<=>CH3+HCO                     2.20E+13    0.0        0.0
1192. H+CH2CHO<=>CH2CO+H2                    1.10E+13    0.0        0.0
1193. OH+CH2CHO<=>HCO+CH2OH                  3.01E+13    0.0        0.0
1194. OH+CH2CHO<=>H2O+CH2CO                  1.20E+13    0.0        0.0
1195. CH2CHO+NO=HNO+CH2CO                    1.00E+12    0.0     8600.0
1196. CH2CHO+NO2=HONO+CH2CO                  8.90E+12    0.0     -160.0
1197. CH2CHO+NO3=HNO3+CH2CO                  1.00E+12    0.0        0.0
1198. CH3+NO3=CH3O+NO2                       2.00E+13    0.0        0.0
1199. O+C2H5<=>H+CH3CHO                      1.10E+14    0.0        0.0
1200. O+CH3CHO<=>OH+CH2CHO                   2.92E+12    0.0     1808.0
1201. O+CH3CHO=>OH+CH3+CO                    2.92E+12    0.0     1808.0
1202. O2+CH3CHO=>HO2+CH3+CO                  3.01E+13    0.0    39150.0
1203. H+CH3CHO<=>CH2CHO+H2                   2.05E+09    1.2     2405.0
1204. H+CH3CHO=>CH3+H2+CO                    2.05E+09    1.2     2405.0
1205. OH+CH3CHO=>CH3+H2O+CO                  2.34E+10    0.7    -1113.0
1206. HO2+CH3CHO=>CH3+H2O2+CO                3.01E+12    0.0    11923.0
1207. CH3+CH3CHO=>CH3+CH4+CO                 2.72E+06    1.8     5920.0
1208. O+C2H4<=>H+CH2CHO                      6.70E+06    1.8      220.0
1209. C2H3+O2<=>O+CH2CHO                     3.03E+11    0.3       11.0
1210. C2H3+O2<=>HO2+C2H2                     1.34E+06    1.6     -384.0
1211. H+CH2CO(+M)<=>CH2CHO(+M)               4.86E+11    0.4    -1755.0
      Low pressure limit:  0.10120E+43 -0.76300E+01  0.38540E+04
      TROE centering:      0.46500E+00  0.20100E+03  0.17730E+04  0.53330E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
1212. O+CH2CHO=>H+CH2+CO2                    1.50E+14    0.0        0.0
1213. O2+CH2CHO=>OH+CO+CH2O                  1.81E+10    0.0        0.0
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1214.	CH3+NH=H2CN+H2	3.50E+13	0.0	290.0
1215.	HCO+HNO=CH2O+NO	6.00E+11	0.0	2000.0
1216.	CH2O+NO2=HCO+HONO	8.35E-11	6.7	8310.0
1217.	HCO+NO2=CO+HONO	1.24E+23	-3.3	2355.0
1218.	HCO+NO2=H+CO2+NO	8.39E+15	-0.8	1930.0
1219.	HCO+HCO=CH2O+CO	3.00E+13	0.0	0.0
1220.	CH4+NO2=CH3+HONO	1.20E+13	0.0	30000.0
1221.	CH3+NO2=CH3O+NO	1.40E+13	0.0	0.0
1222.	CH2+NO2=CH2O+NO	5.00E+13	0.0	0.0
1223.	H2CN+N=HCN+NH	7.20E+13	0.0	400.0
1224.	H2CN+H=HCN+H2	4.00E+13	0.0	0.0
1225.	OH+HCN=HOCN+H	1.10E+06	2.0	13373.0
1226.	HOCN+H<=>H+HNCO	2.00E+07	2.0	2000.0
1227.	HOCN+H=NH2+CO	1.20E+08	0.6	2076.0
1228.	HOCN+H=H2+NCO	2.40E+08	1.5	6617.0
1229.	CH3NHNH2+M=CH3NH+NH2+M	2.50E+14	0.0	40940.0
1230.	CH3NHNH2+H=CH3NNH2+H2	1.30E+13	0.0	2500.0
1231.	CH3NHNH2+H=CH3NH+NH3	4.46E+09	0.0	3100.0
1232.	CH3NHNH2+CH3=CH4+CH3NNH2	1.00E+13	0.0	6990.0
1233.	CH3NHNH2+NH2=NH3+CH3NNH2	1.00E+11	0.5	1990.0
1234.	CH3NNH2+M=CH3NNH+H+M	1.00E+17	0.0	35770.0
1235.	CH3NH+M=CH2NH+H+M	1.00E+16	0.0	23800.0
1236.	CH3NH+H=CH2NH+H2	1.00E+08	2.0	0.0
1237.	CH3NH+H=CH3+NH2	6.00E+13	0.0	0.0
1238.	CH3NNH+CH3=CH4+CH3NN	4.60E+13	0.0	4850.0
1239.	CH3NNH+NH2=NH3+CH3NN	4.60E+13	0.0	4850.0
1240.	CH3NN=CH3+N2	3.00E+06	0.0	0.0
1241.	CH3NNCH3=CH3NN+CH3	6.90E+15	0.0	50880.0
1242.	CH3NNCH3=C2H6+N2	2.00E+11	0.0	33000.0
1243.	CH2NH+M=HCN+H2+M	1.00E+14	0.0	10000.0
1244.	CH3NHNH2=CH3NNH+H2	3.16E+13	0.0	57000.0
1245.	CH3NHNH2=CH2NH+NH3	1.58E+13	0.0	54000.0
1246.	CH3NNH2+HO2=CH3NHNH2+O2	1.00E+06	2.0	0.0
1247.	CH3NN+HO2=CH3NNH+O2	1.00E+06	2.0	0.0
1248.	CH3NHNH2+O=CH3NNH+H2O	9.60E+12	0.0	0.0
1249.	CH3NNH2+OH=CH3NNH+H2O	1.00E+08	2.0	0.0
1250.	CH3NNH2+O=CH3NNH+OH	1.00E+08	2.0	0.0
1251.	CH3NNH2+HO2=CH3NNH+H2O2	1.00E+08	2.0	0.0
1252.	CH3NNH2+O2=CH3NNH+HO2	4.00E+12	0.0	0.0
1253.	CH3NHNH2+HO2=CH3NNH2+H2O2	2.70E+11	0.0	1987.0
1254.	CH3NNH+HO2=CH3NN+H2O2	1.00E+11	0.0	1987.0
1255.	CH3NHNH2+OH=CH3NNH2+H2O	3.92E+13	0.0	0.0
1256.	CH3NNH+OH=CH3NN+H2O	3.92E+13	0.0	0.0
1257.	CH3NHNH2+O=CH3NNH2+OH	9.60E+12	0.0	0.0
1258.	CH3NNH+O=CH3NN+OH	9.60E+12	0.0	0.0
1259.	CH3NH+OH=CH2NH+H2O	1.00E+08	2.0	0.0
1260.	CH3NH+O=CH2NH+OH	1.00E+08	2.0	0.0
1261.	CH3NH+O2=CH2NH+HO2	1.00E+07	2.0	6300.0
1262.	CH3NH+O=CH3O+NH	6.00E+13	0.0	0.0
1263.	CH3NH+OH=CH4+HNO	6.00E+12	0.0	0.0
1264.	CH3NH+O2=CH3O+HNO	6.00E+12	0.0	4000.0
1265.	CH2NH+O=CH2O+NH	1.00E+07	2.0	2800.0
1266.	CH2NH+OH=CH2O+NH2	1.80E+05	2.0	14800.0
1267.	CH2NH+O=H2CN+OH	3.16E+08	2.0	6100.0
1268.	H2CN+HO2=CH2NH+O2	7.87E+04	2.0	21700.0
1269.	CH2NH+OH=H2CN+H2O	1.00E+07	2.0	4000.0
1270.	H2CN+O=HCN+OH	1.00E+07	2.0	6100.0

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1271. H2CN+OH=HCN+H2O                          1.00E+07    2.0     3700.0
1272. H2CN+O2=HCN+HO2                          2.70E+04    2.0    17300.0
1273. H2CN+NO=HCN+HNO                          1.00E+07    2.0     4400.0
1274. CH3NNH2+NO2(+M)=CH3N(NH2)NO2(+M)         1.00E+13    0.0        0.0
      Low pressure limit:  0.10000E+18  0.00000E+00  0.00000E+00
1275. CH3NNH2+NO2(+M)=CH3N(NH2)ONO(+M)         1.00E+13    0.0        0.0
      Low pressure limit:  0.10000E+18  0.00000E+00  0.00000E+00
1276. CH3NHNH2+NO2=CH3NNH2+HONO                2.20E+11    0.0     5900.0
1277. CH3NNH+NO2=CH3NN+HONO                    2.20E+11    0.0     5900.0
1278. CH3NNH2+NO2=CH3NNH+HONO                  1.00E+08    2.0        0.0
1279. NH2+HO2=NH3+O2                           2.00E+13    0.0        0.0
1280. N2O4(+M)=NO2+NO2(+M)                     4.05E+18   -1.1    12840.0
      Low pressure limit:  0.19600E+29 -0.38000E+01  0.12800E+05
1281. CH3NHNH2+HNO3=NAMMH                      2.00E+13    0.0        0.0
1282. CH3NO2(+M)=CH3+NO2(+M)                   1.80E+16    0.0    58500.0
      Low pressure limit:  0.13000E+18  0.00000E+00  0.42000E+05
      T&H values:       0.18300E+00  0.00000E+00
1283. CH3NO2+H=CH3+HONO                        3.30E+12    0.0     3730.0
1284. CH3NO2+H=CH3NO+OH                        1.40E+12    0.0     3730.0
1285. CH3NO2+H=H2CNO2+H2                       5.40E+02    3.5     5200.0
1286. CH3NO2+O=H2CNO2+OH                       1.50E+13    0.0     5350.0
1287. CH3NO2+OH=H2CNO2+H2O                     5.00E+05    2.0     1000.0
1288. CH3NO2+OH=CH3OH+NO2                      2.00E+10    0.0    -1000.0
1289. CH3NO2+CH3=H2CNO2+CH4                    5.50E-01    4.0     8300.0
1290. CH3NO2+CH2(S)=H2CNO2+CH3                 1.20E+14    0.0        0.0
1291. CH3NO2+CH2=H2CNO2+CH3                    6.50E+12    0.0     7900.0
1292. H2CNO2=CH2O+NO                           1.00E+13    0.0    36000.0
1293. CH3+NO(+M)=CH3NO(+M)                     9.00E+12    0.0      119.0
      Low pressure limit:  0.32000E+24 -0.18700E+01  0.00000E+00
1294. CH3O+NO=CH2O+HNO                         1.30E+14   -0.7        0.0
1295. CH3O+NO(+M)=CH3ONO(+M)                   6.60E+14   -0.6        0.0
      Low pressure limit:  0.27000E+28 -0.35000E+01  0.00000E+00
1296. CH3O+NO2=CH2O+HONO                       6.00E+12    0.0     2285.0
1297. CHOCHO(+M)=HCO+HCO(+M)                   2.94E+14    0.0    67900.0
      Low pressure limit:  0.91900E+50 -0.94300E+01  0.74016E+05
      H2O             Enhanced by    1.200E+01
      N2              Enhanced by    1.500E+00
      NO              Enhanced by    1.500E+00
      CO2             Enhanced by    5.000E+00
      CH2O            Enhanced by    2.000E+00
      NO2             Enhanced by    5.000E+00
      CO              Enhanced by    5.000E+00
      CHOCHO          Enhanced by    5.000E+00
      H2              Enhanced by    1.500E+00
1298. CHOCHO+OH=H2O+CO+HCO                     3.40E+09    1.2      447.0
1299. CHOCHO+H=H2+CO+HCO                       4.58E+10    1.1     3280.0
1300. CHOCHO+O=OH+CO+HCO                       4.13E+11    0.6     2762.0
1301. CHOCHO+NO2=HONO+CO+HCO                   7.94E+11    0.0    19800.0
1302. CHOCHO+NO=HNO+HCO+CO                     1.00E+13    0.0    41000.0
1303. HCO+CHOCHO=CH2O+CO+HCO                   1.00E+13    0.0    11000.0
1304. CH2CO+O=CH2O+CO                          7.63E+11    0.0     1351.0
1305. CH2CO+O=HCO+H+CO                         7.63E+11    0.0     1351.0
1306. CH2CO+O=HCO+HCO                          7.63E+11    0.0     1351.0
1307. CH2CO+OH=CH2O+HCO                        3.33E+12    0.0        0.0
1308. CH2CO+OH=CH2OH+CO                        3.33E+12    0.0        0.0
1309. CH2CO+OH=CH3+CO2                         3.33E+12    0.0        0.0
1310. H+2O2<=>HO2+O2                           2.08E+19   -1.2        0.0
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1311. H+CH2O(+M)<=>CH3O(+M)                 5.40E+11    0.5     2600.0
      Low pressure limit:  0.22000E+31 -0.48000E+01  0.55600E+04
      TROE centering:      0.75800E+00  0.94000E+02  0.15550E+04  0.42000E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
1312. H+CH2CO<=>HCCO+H2                     5.00E+13    0.0     8000.0
1313. H+CH2CO<=>CH3+CO                      1.13E+13    0.0     3428.0
1314. CH2+CO(+M)<=>CH2CO(+M)                8.10E+11    0.5     4510.0
      Low pressure limit:  0.26900E+34 -0.51100E+01  0.70950E+04
      TROE centering:      0.59070E+00  0.27500E+03  0.12260E+04  0.51850E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
1315. O+CH3<=>H+H2+CO                       3.37E+13    0.0        0.0
1316. OH+CH3<=>H2+CH2O                      5.88E-14    6.7    -3020.0
1317. CH+H2(+M)<=>CH3(+M)                   1.97E+12    0.4     -370.0
      Low pressure limit:  0.48200E+26 -0.28000E+01  0.59000E+03
      TROE centering:      0.57800E+00  0.12200E+03  0.25350E+04  0.93650E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
1318. CH2+O2=>2H+CO2                        5.80E+12    0.0     1500.0
1319. CH2+O2<=>O+CH2O                       2.40E+12    0.0     1500.0
1320. CH2+CH2=>2H+C2H2                      2.00E+14    0.0    10989.0
1321. CH2(S)+H2O=>H2+CH2O                   6.82E+10    0.2     -935.0
1322. CH3+C2H5(+M)<=>C3H8(+M)               9.43E+12    0.0        0.0
      Low pressure limit:  0.27100E+75 -0.16820E+02  0.13065E+05
      TROE centering:      0.15270E+00  0.29100E+03  0.27420E+04  0.77480E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
1323. O+C3H8<=>OH+C3H7                      1.93E+05    2.7     3716.0
1324. H+C3H8<=>C3H7+H2                      1.32E+06    2.5     6756.0
1325. OH+C3H8<=>C3H7+H2O                    3.16E+07    1.8      934.0
1326. C3H7+H2O2<=>HO2+C3H8                  3.78E+02    2.7     1500.0
1327. CH3+C3H8<=>C3H7+CH4                   9.03E-01    3.6     7154.0
1328. CH3+C2H4(+M)<=>C3H7(+M)               2.55E+06    1.6     5700.0
      Low pressure limit:  0.30000E+64 -0.14600E+02  0.18170E+05
      TROE centering:      0.18940E+00  0.27700E+03  0.87480E+04  0.78910E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
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      C2H6            Enhanced by    3.000E+00
1329. O+C3H7<=>C2H5+CH2O                    9.64E+13    0.0        0.0
1330. H+C3H7(+M)<=>C3H8(+M)                 3.61E+13    0.0        0.0
      Low pressure limit:  0.44200E+62 -0.13545E+02  0.11357E+05
      TROE centering:      0.31500E+00  0.36900E+03  0.32850E+04  0.66670E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    6.000E+00
      CH4             Enhanced by    2.000E+00
      CO              Enhanced by    1.500E+00
      CO2             Enhanced by    2.000E+00
      C2H6            Enhanced by    3.000E+00
1331. H+C3H7<=>CH3+C2H5                     4.06E+06    2.2      890.0
1332. OH+C3H7<=>C2H5+CH2OH                  2.41E+13    0.0        0.0
1333. O2+C3H8<=>HO2+C3H7                    4.33E+12    0.3    47504.0
1334. HO2+C3H7=>OH+C2H5+CH2O                2.41E+13    0.0        0.0
1335. CH3+C3H7<=>2C2H5                      1.93E+13   -0.3        0.0
1336. CH3ONO2+O2=CH2O+NO2+HO2               2.77E+05    3.1    48118.0
1337. CH3ONO2+NO2=CH2O+NO2+HNO2             1.42E+00    4.1    28245.0
1338. CH3ONO2+NO2=CH2O+NO2+HONO             7.50E-10    7.1    22640.0
1339. CH3ONO2(+M)=CH3O+NO2(+M)              1.00E+00    0.0        0.0
I01:   9.4900E+41 -9.7000E+00  4.5990E+04  1.0000E-03
I02:   3.2000E+42 -9.5800E+00  4.6041E+04  1.0000E-02
I03:   4.2400E+42 -9.3300E+00  4.6334E+04  1.0000E-01
I04:   1.9300E+42 -8.9500E+00  4.6868E+04  1.0000E+00
I05:   3.9700E+39 -7.8600E+00  4.6774E+04  1.0000E+01
I06:   4.7300E+37 -7.1800E+00  4.6437E+04  2.5000E+01
I07:   1.5500E+36 -6.6700E+00  4.6153E+04  5.0000E+01
I08:   2.0300E+35 -6.3600E+00  4.5972E+04  7.5000E+01
I09:   4.5300E+34 -6.1400E+00  4.5831E+04  1.0000E+02
1340. CH3ONO2(+M)=CH2O+HONO(+M)             1.00E+00    0.0        0.0
I01:   2.5900E+28 -6.5400E+00  4.8507E+04  1.0000E-03
I02:   8.1300E+29 -6.6700E+00  4.7813E+04  1.0000E-02
I03:   6.4100E+30 -6.6300E+00  4.7470E+04  1.0000E-01
I04:   1.4800E+31 -6.4200E+00  4.7944E+04  1.0000E+00
I05:   1.7100E+29 -5.5200E+00  4.8084E+04  1.0000E+01
I06:   3.3400E+27 -4.9000E+00  4.7844E+04  2.5000E+01
I07:   1.4300E+26 -4.4100E+00  4.7620E+04  5.0000E+01
I08:   2.0800E+25 -4.1100E+00  4.7469E+04  7.5000E+01
I09:   4.8800E+24 -3.9000E+00  4.7345E+04  1.0000E+02
1341. CH3ONO2(+M)=CH3+NO3(+M)               1.00E+00    0.0        0.0
I01:   2.0500E-12  3.4500E+00  1.2726E+05  1.0000E-03
I02:   4.2400E-10  3.1200E+00  1.2597E+05  1.0000E-02
I03:   2.3800E-06  2.4000E+00  1.2322E+05  1.0000E-01
I04:   3.3100E+00  1.0600E+00  1.1871E+05  1.0000E+00
I05:   7.8900E+07 -5.1000E-01  1.1072E+05  1.0000E+01
I06:   2.3300E+11 -1.2600E+00  1.0647E+05  2.5000E+01
I07:   3.0200E+14 -1.9500E+00  1.0297E+05  5.0000E+01
I08:   2.7500E+16 -2.4000E+00  1.0085E+05  7.5000E+01
I09:   6.6300E+17 -2.7200E+00  9.9312E+04  1.0000E+02
1342. CH3ONO2(+M)=CH3OONO(+M)               1.00E+00    0.0        0.0
I01:   1.4300E+16 -3.5200E+00  6.9220E+04  1.0000E-03
I02:   2.8900E+18 -3.8500E+00  6.7944E+04  1.0000E-02
I03:   1.2600E+22 -4.5400E+00  6.5284E+04  1.0000E-01
I04:   1.5600E+27 -5.6000E+00  6.1549E+04  1.0000E+00
I05:   9.2700E+29 -5.9500E+00  5.8206E+04  1.0000E+01
I06:   1.5500E+30 -5.8200E+00  5.7665E+04  2.5000E+01
I07:   1.8600E+30 -5.7100E+00  5.7550E+04  5.0000E+01
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I08:   1.6600E+30 -5.6100E+00  5.7544E+04  7.5000E+01
I09:   1.2800E+30 -5.5200E+00  5.7545E+04  1.0000E+02
1343. CH3OONO(+M)=CH2O+HNO2(+M)              1.00E+00    0.0         0.0
I01:   1.9000E+42 -1.0580E+01  4.3560E+04  1.0000E-03
I02:   1.9000E+43 -1.0580E+01  4.3561E+04  1.0000E-02
I03:   1.9300E+44 -1.0580E+01  4.3572E+04  1.0000E-01
I04:   2.0100E+45 -1.0600E+01  4.3646E+04  1.0000E+00
I05:   1.3000E+46 -1.0630E+01  4.3830E+04  1.0000E+01
I06:   1.9900E+46 -1.0640E+01  4.3897E+04  2.5000E+01
I07:   2.4300E+46 -1.0650E+01  4.3934E+04  5.0000E+01
I08:   2.4400E+46 -1.0640E+01  4.3934E+04  7.5000E+01
I09:   2.8700E+46 -1.0660E+01  4.3959E+04  1.0000E+02
1344. CH3OONO(+M)=CH3OONOI(+M)               1.00E+00    0.0         0.0
I01:   2.6200E+46 -1.1100E+01  4.3538E+04  1.0000E-03
I02:   2.6300E+47 -1.1100E+01  4.3540E+04  1.0000E-02
I03:   2.6700E+48 -1.1100E+01  4.3551E+04  1.0000E-01
I04:   2.8000E+49 -1.1120E+01  4.3629E+04  1.0000E+00
I05:   1.8100E+50 -1.1140E+01  4.3820E+04  1.0000E+01
I06:   2.7600E+50 -1.1160E+01  4.3887E+04  2.5000E+01
I07:   3.3600E+50 -1.1160E+01  4.3925E+04  5.0000E+01
I08:   3.3800E+50 -1.1160E+01  4.3924E+04  7.5000E+01
I09:   3.9800E+50 -1.1180E+01  4.3950E+04  1.0000E+02
1345. CH3OONOI(+M)=CH3O+NO2(+M)              1.00E+00    0.0         0.0
I01:   4.5700E+43 -1.0300E+01  4.2142E+04  1.0000E-03
I02:   4.5700E+44 -1.0300E+01  4.2142E+04  1.0000E-02
I03:   4.5700E+45 -1.0300E+01  4.2142E+04  1.0000E-01
I04:   4.5700E+46 -1.0300E+01  4.2142E+04  1.0000E+00
I05:   4.5000E+47 -1.0300E+01  4.2142E+04  1.0000E+01
I06:   1.1000E+48 -1.0300E+01  4.2141E+04  2.5000E+01
I07:   2.1100E+48 -1.0290E+01  4.2140E+04  5.0000E+01
I08:   3.0400E+48 -1.0290E+01  4.2138E+04  7.5000E+01
I09:   3.9000E+48 -1.0290E+01  4.2137E+04  1.0000E+02
1346. CH3OONOI(+M)=CH3O2+NO(+M)              1.00E+00    0.0         0.0
I01:   2.6900E+37 -9.4900E+00  4.1771E+04  1.0000E-03
I02:   2.6900E+38 -9.4900E+00  4.1771E+04  1.0000E-02
I03:   2.6800E+39 -9.4900E+00  4.1770E+04  1.0000E-01
I04:   2.6700E+40 -9.4900E+00  4.1770E+04  1.0000E+00
I05:   2.5200E+41 -9.4800E+00  4.1765E+04  1.0000E+01
I06:   5.7100E+41 -9.4700E+00  4.1756E+04  2.5000E+01
I07:   9.7800E+41 -9.4500E+00  4.1742E+04  5.0000E+01
I08:   1.2600E+42 -9.4300E+00  4.1728E+04  7.5000E+01
I09:   1.4500E+42 -9.4100E+00  4.1715E+04  1.0000E+02
1347. CH3OONOI(+M)=CH2O+HONO(+M)             1.00E+00    0.0         0.0
      Declared duplicate reaction...
I01:   6.0300E+28 -7.1500E+00  4.1652E+04  1.0000E-03
I02:   6.0300E+29 -7.1500E+00  4.1652E+04  1.0000E-02
I03:   6.0300E+30 -7.1500E+00  4.1652E+04  1.0000E-01
I04:   5.9900E+31 -7.1500E+00  4.1652E+04  1.0000E+00
I05:   5.5800E+32 -7.1400E+00  4.1645E+04  1.0000E+01
I06:   1.2400E+33 -7.1200E+00  4.1635E+04  2.5000E+01
I07:   2.0600E+33 -7.1000E+00  4.1617E+04  5.0000E+01
I08:   2.5800E+33 -7.0700E+00  4.1601E+04  7.5000E+01
I09:   2.8800E+33 -7.0500E+00  4.1584E+04  1.0000E+02
1348. CH3OONOI(+M)=CH2O+HONO(+M)             1.00E+00    0.0         0.0
      Declared duplicate reaction...
I01:   2.8900E+13 -3.8200E+00  4.7775E+04  1.0000E-03
I02:   2.8900E+14 -3.8200E+00  4.7775E+04  1.0000E-02
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I03:   2.8800E+15 -3.8200E+00  4.7775E+04  1.0000E-01
I04:   2.8600E+16 -3.8200E+00  4.7768E+04  1.0000E+00
I05:   2.6300E+17 -3.8100E+00  4.7699E+04  1.0000E+01
I06:   5.7100E+17 -3.7800E+00  4.7590E+04  2.5000E+01
I07:   9.1800E+17 -3.7500E+00  4.7420E+04  5.0000E+01
I08:   1.1200E+18 -3.7100E+00  4.7263E+04  7.5000E+01
I09:   1.2300E+18 -3.6700E+00  4.7117E+04  1.0000E+02
1349. CH3O+NO2(+M)=CH3O2+NO(+M)              1.00E+00    0.0        0.0
I01:   3.8600E+11  6.0000E-02  1.7230E+04  1.0000E-03
I02:   3.8600E+11  6.0000E-02  1.7230E+04  1.0000E-02
I03:   3.8600E+11  6.0000E-02  1.7230E+04  1.0000E-01
I04:   3.8700E+11  6.0000E-02  1.7230E+04  1.0000E+00
I05:   3.9600E+11  6.0000E-02  1.7235E+04  1.0000E+01
I06:   3.9900E+11  6.0000E-02  1.7245E+04  2.5000E+01
I07:   3.6200E+11  7.0000E-02  1.7239E+04  5.0000E+01
I08:   3.1500E+11  9.0000E-02  1.7223E+04  7.5000E+01
I09:   2.7500E+11  1.1000E-01  1.7204E+04  1.0000E+02
1350. CH3O+NO2(+M)=CH2O+HONO(+M)             1.00E+00    0.0        0.0
I01:   2.2900E+04  2.0900E+00  1.8871E+04  1.0000E-03
I02:   2.2900E+04  2.0900E+00  1.8871E+04  1.0000E-02
I03:   2.2900E+04  2.0900E+00  1.8871E+04  1.0000E-01
I04:   2.2900E+04  2.0900E+00  1.8871E+04  1.0000E+00
I05:   2.3200E+04  2.0900E+00  1.8874E+04  1.0000E+01
I06:   2.3600E+04  2.0900E+00  1.8883E+04  2.5000E+01
I07:   2.2100E+04  2.1000E+00  1.8882E+04  5.0000E+01
I08:   1.9600E+04  2.1100E+00  1.8869E+04  7.5000E+01
I09:   1.7300E+04  2.1300E+00  1.8853E+04  1.0000E+02
1351. CH3O+NO2(+M)=CH2O+HNO2(+M)             1.00E+00    0.0        0.0
I01:   5.1800E+05  1.7700E+00  1.3434E+04  1.0000E-03
I02:   5.1800E+05  1.7700E+00  1.3433E+04  1.0000E-02
I03:   5.1700E+05  1.7700E+00  1.3432E+04  1.0000E-01
I04:   5.1200E+05  1.7700E+00  1.3423E+04  1.0000E+00
I05:   2.2600E+06  1.5900E+00  1.3805E+04  1.0000E+01
I06:   1.2200E+07  1.3900E+00  1.4414E+04  2.5000E+01
I07:   2.0400E+07  1.3400E+00  1.4889E+04  5.0000E+01
I08:   1.3700E+07  1.4100E+00  1.5093E+04  7.5000E+01
I09:   6.9500E+06  1.5100E+00  1.5186E+04  1.0000E+02
1352. CH3O+CH3O=CH2O+CH3OH                   6.03E+13    0.0        0.0
1353. CH3O+CH2O=CH3OH+HCO                    1.02E+11    0.0     2980.0
1354. CH3O2+M=CH3+O2+M                       4.34E+27   -3.4    30470.0
      Reverse Arrhenius coefficients:        5.44E+25   -3.3        0.0
1355. CH3O2H=CH3O+OH                         6.31E+14    0.0    42300.0
1356. CH3O2+CH2O=CH3O2H+HCO                  1.99E+12    0.0    11670.0
1357. C2H4+CH3O2=C2H3+CH3O2H                 1.13E+13    0.0    30430.0
1358. CH4+CH3O2=CH3+CH3O2H                   1.81E+11    0.0    18480.0
1359. CH3OH+CH3O2=CH2OH+CH3O2H               1.81E+12    0.0    13710.0
1360. CH3O2+CH3=CH3O+CH3O                    7.00E+12    0.0    -1000.0
1361. CH3O2+C2H5=CH3O+C2H5O                  7.00E+12    0.0    -1000.0
1362. CH3O2+HO2=CH3O2H+O2                    1.75E+10    0.0    -3275.0
1363. CH3O2+CH3O2=>CH2O+CH3OH+O2             3.11E+14   -1.6    -1051.0
1364. CH3O2+CH3O2=>O2+CH3O+CH3O              1.40E+16   -1.6     1860.0
1365. C2H6+CH3O2=C2H5+CH3O2H                 1.70E+13    0.0    20460.0
1366. CH3O2+CH3CHO=CH3O2H+CH3CO              3.01E+12    0.0    11930.0
1367. ETONO2+OH=CJCONO2+H2O                  5.50E+12    0.0     2400.0
1368. ETONO2+H=CJCONO2+H2                    3.18E+13    0.0     8700.0
1369. ETONO2+O=CJCONO2+OH                    6.70E+05    2.4     4700.0
1370. ETONO2+O2=CJCONO2+HO2                  1.97E+11    0.6    50090.0
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1371. ETONO2+NO2=CJCONO2+HNO2                 8.00E+13    0.0    33800.0
1372. ETONO2+NO2=CJCONO2+HONO                 1.10E+13    0.0    31100.0
1373. CJCONO2=C2H4+NO3                        3.19E+11    0.7    22353.0
1374. CJCONO2=CDCONO2+H                       6.55E+08    1.4    37642.0
1375. CJCONO2=C2H4O+NO2                       3.36E+08    1.3    18998.0
1376. C2H4O+NO2=YC2JO+HNO2                    1.89E+00    4.1    28245.0
1377. C2H4O+NO2=YC2JO+HONO                    9.07E-08    6.5    23232.0
1378. C2H4O+O2=YC2JO+HO2                      3.69E+05    3.1    48118.0
1379. C2H4O+H=YC2JO+H2                        9.60E+08    1.5     9071.3
1380. C2H4O+O=YC2JO+OH                        6.80E+08    1.5     7382.4
1381. C2H4O+OH=YC2JO+H2O                      4.80E+06    2.0        0.0
1382. C2H4O+CH3=YC2JO+CH4                     3.24E+06    1.9    12272.3
1383. YC2JO=CH2CHO                            2.20E+12    0.4    14334.0
1384. CJCONO2+OH=CDCONO2+H2O                  2.41E+13    0.0        0.0
1385. CJCONO2+H=CDCONO2+H2                    1.81E+12    0.0        0.0
1386. CJCONO2+O=CDCONO2+OH                    3.17E+12    0.0     -390.0
1387. CJCONO2+O2=CDCONO2+HO2                  8.43E+11    0.0     3880.0
1388. CJCONO2+NO2(+M)=COJCONO2+NO(+M)         1.00E+00    0.0        0.0
I01:   2.0300E+13  0.0000E+00  0.0000E+00  1.0000E-03
I02:   2.0300E+13  0.0000E+00  0.0000E+00  1.0000E-02
I03:   3.2500E+13 -6.0000E-02  1.1200E+02  1.0000E-01
I04:   6.9500E+15 -7.3000E-01  1.4900E+03  1.0000E+00
I05:   1.9600E+19 -1.6900E+00  4.1100E+03  1.0000E+01
I06:   4.4900E+19 -1.7700E+00  4.9210E+03  2.5000E+01
I07:   1.3000E+19 -1.5800E+00  5.2430E+03  5.0000E+01
I08:   2.5500E+18 -1.3600E+00  5.2780E+03  7.5000E+01
I09:   5.2500E+17 -1.1500E+00  5.2280E+03  1.0000E+02
1389. COJCONO2=CH2O+CH2O+NO2                  2.81E+09    1.3    13866.0
1390. CJCONO2+O2=CQJCONO2                     6.00E+12    0.0        0.0
1391. CQJCONO2=CDCONO2+HO2                    5.07E+05    1.5    29254.0
1392. CQJCONO2=CDOCQ+NO2                      1.35E+03    2.5    21510.0
1393. CH2CHO+HO2=CDOCQ                        1.00E+11    0.0        0.0
1394. CDOCOJ+OH=CDOCQ                         1.00E+13    0.0        0.0
1395. CDOCQ+NO2=CDJOCQ+HNO2                   4.63E+01    3.3    17499.0
1396. CDOCQ+NO2=CDJOCQ+HONO                   4.39E-03    4.4    10946.0
1397. CDOCQ+O2=CDJOCQ+HO2                     3.01E+13    0.0    39070.0
1398. CDOCQ+H=CDJOCQ+H2                       2.40E+08    1.5     -555.2
1399. CDOCQ+O=CDJOCQ+OH                       1.70E+08    1.5        0.0
1400. CDOCQ+OH=CDJOCQ+H2O                     1.20E+06    2.0        0.0
1401. CDOCQ+CH3=CDJOCQ+CH4                    8.10E+05    1.9     2645.8
1402. CDJOCQ=CH2O+OH+CO                       3.06E+18   -1.1    13072.0
1403. CDOCQ+NO2=CHOCHO+OH+HNO2                7.10E-03    4.6    15319.0
1404. CDOCQ+NO2=CHOCHO+OH+HONO                1.11E-06    5.9    10436.0
1405. CDOCQ+O2=CHOCHO+OH+HO2                  1.29E+02    3.0    35205.0
1406. CDOCQ+H=CHOCHO+OH+H2                    4.80E+08    1.5    -1874.7
1407. CDOCQ+O=CHOCHO+OH+OH                    3.40E+08    1.5    -5247.6
1408. CDOCQ+OH=CHOCHO+OH+H2O                  2.40E+06    2.0        0.0
1409. CDOCQ+CH3=CHOCHO+OH+CH4                 1.62E+06    1.9     1326.3
1410. CNO2CDO=CH2CHO+NO2                      1.27E+17   -0.7    50945.0
1411. CONOCDO=CDOCOJ+NO                       5.78E+16   -0.6    39377.0
1412. CDCONO2=CH2CHO+NO2                      2.73E+13    0.2    22572.0
1413. CNO2CDO=HONO+CH2CO                      1.06E+07    1.3    63478.0
1414. CDCONO2=CONOCDO                         1.31E+11    0.3    24547.0
1415. CDCONO2+H=CDCJONO2+H2                   2.40E+08    1.5    13420.0
1416. CDCONO2+O=CDCJONO2+OH                   1.70E+08    1.5    12310.0
1417. CDCONO2+OH=CDCJONO2+H2O                 1.20E+06    2.0     5832.1
1418. CDCONO2+CH3=CDCJONO2+CH4                8.10E+05    1.9    16601.0
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1419. CDCONO2+NH2=CDCJONO2+NH3              9.20E+05    1.9     9394.0
1420. CDCONO2+NO2=CDCJONO2+HONO             2.50E+07    1.3    31996.0
1421. CDCONO2+NO2=CDCJONO2+HNO2             7.10E-03    4.6    40099.0
1422. CDCONO2+O2=CDCJONO2+HO2               1.29E+02    3.0    58725.0
1423. CDCJONO2=CH2CO+NO2                    6.09E+11    0.5     1781.6
1424. CONOCDO+H=CJONOCDO+H2                 4.80E+08    1.5        0.0
1425. CONOCDO+O=CJONOCDO+OH                 3.40E+08    1.5        0.0
1426. CONOCDO+OH=CJONOCDO+H2O               2.40E+06    2.0        0.0
1427. CONOCDO+CH3=CJONOCDO+CH4              1.62E+06    1.9      871.3
1428. CONOCDO+NH2=CJONOCDO+NH3              1.84E+06    1.9     3828.0
1429. CONOCDO+NO2=CJONOCDO+HONO             2.50E+07    1.3    12032.0
1430. CONOCDO+NO2=CJONOCDO+HNO2             1.42E-02    4.6    15899.0
1431. CONOCDO+O2=CJONOCDO+HO2               2.57E+02    3.0    34525.0
1432. CJONOCDO=NO+CHOCHO                    7.01E+11    0.5     1870.4
1433. CONOCDO+H=CONOCDJO+H2                 2.40E+08    1.5     -139.2
1434. CONOCDO+O=CONOCDJO+OH                 1.70E+08    1.5        0.0
1435. CONOCDO+OH=CONOCDJO+H2O               1.20E+06    2.0        0.0
1436. CONOCDO+CH3=CONOCDJO+CH4              8.10E+05    1.9     3042.3
1437. CONOCDO+NH2=CONOCDJO+NH3              9.20E+05    1.9     4596.2
1438. CONOCDO+NO2=CONOCDJO+HONO             2.50E+07    1.3    14787.0
1439. CONOCDO+NO2=CONOCDJO+HNO2             7.10E-03    4.6    19239.0
1440. CONOCDO+O2=CONOCDJO+HO2               1.29E+02    3.0    37865.0
1441. CONOCDJO=NO2+CH2CO                    5.14E+11    0.6    15547.0
1442. CONOCDJO=CO+CH2O+NO                   8.49E+11    0.7    12467.0
1443. CNO2CDO+H=CJNO2CDO+H2                 4.80E+08    1.5     3026.3
1444. CNO2CDO+O=CJNO2CDO+OH                 3.40E+08    1.5      317.4
1445. CNO2CDO+OH=CJNO2CDO+H2O               2.40E+06    2.0        0.0
1446. CNO2CDO+CH3=CJNO2CDO+CH4              1.62E+06    1.9     6207.8
1447. CNO2CDO+NH2=CJNO2CDO+NH3              1.84E+06    1.9     5716.3
1448. CNO2CDO+NO2=CJNO2CDO+HONO             2.50E+07    1.3    18805.0
1449. CNO2CDO+NO2=CJNO2CDO+HNO2             1.42E-02    4.6    24109.0
1450. CNO2CDO+O2=CJNO2CDO+HO2               2.57E+02    3.0    42735.0
1451. CJNO2CDO=KDCNOHOJ                     1.87E+10    0.6    19166.0
1452. KDCNOHOJ=HCCO+HONO                    7.46E+06    2.7    16962.0
1453. CNO2CDO+H=CNO2CDJO+H2                 2.40E+08    1.5      484.8
1454. CNO2CDO+O=CNO2CDJO+OH                 1.70E+08    1.5        0.0
1455. CNO2CDO+OH=CNO2CDJO+H2O               1.20E+06    2.0        0.0
1456. CNO2CDO+CH3=CNO2CDJO+CH4              8.10E+05    1.9     3666.3
1457. CNO2CDO+NH2=CNO2CDJO+NH3              9.20E+05    1.9     4817.0
1458. CNO2CDO+NO2=CNO2CDJO+HONO             2.50E+07    1.3    15579.0
1459. CNO2CDO+NO2=CNO2CDJO+HNO2             7.10E-03    4.6    20199.0
1460. CNO2CDO+O2=CNO2CDJO+HO2               1.29E+02    3.0    38825.0
1461. CNO2CDJO=H2CNO2+CO                    7.39E+11    0.7    10567.0
1462. ETONO2+H=CH3CHO+NO2+H2                4.80E+08    1.5     5151.8
1463. ETONO2+O=CH3CHO+NO2+OH                3.40E+08    1.5     2859.9
1464. ETONO2+OH=CH3CHO+NO2+H2O              2.40E+06    2.0     -557.9
1465. ETONO2+CH3=CH3CHO+NO2+CH4             1.62E+06    1.9     8352.8
1466. ETONO2+O2=CH3CHO+NO2+HO2              1.29E+02    3.0    46015.0
1467. ETONO2+NO2=CH3CHO+NO2+HNO2            7.10E-03    4.6    26129.0
1468. ETONO2+NO2=CH3CHO+NO2+HONO            3.72E-07    6.1    21099.0
1469. ETONO2(+M)=C2H5O+NO2(+M)              1.00E+00    0.0        0.0
I01:   9.9500E+50 -1.2420E+01  4.5970E+04  1.0000E-03
I02:   1.2700E+52 -1.2440E+01  4.7228E+04  1.0000E-02
I03:   1.4000E+48 -1.0900E+01  4.6975E+04  1.0000E-01
I04:   6.0900E+43 -9.2800E+00  4.6541E+04  1.0000E+00
I05:   4.0500E+39 -7.7800E+00  4.5975E+04  1.0000E+01
I06:   1.8200E+37 -6.9900E+00  4.5451E+04  2.5000E+01
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I07:   2.1500E+35 -6.3600E+00  4.4974E+04  5.0000E+01
I08:   1.3200E+34 -5.9600E+00  4.4658E+04  7.5000E+01
I09:   1.8500E+33 -5.6800E+00  4.4429E+04  1.0000E+02
1470. ETONO2(+M)=CH3CHO+HONO(+M)             1.00E+00    0.0         0.0
I01:   1.5300E+40 -1.0390E+01  4.7797E+04  1.0000E-03
I02:   5.6400E+43 -1.1060E+01  4.9359E+04  1.0000E-02
I03:   1.8600E+41 -9.8900E+00  4.9569E+04  1.0000E-01
I04:   7.2700E+37 -8.4900E+00  4.9655E+04  1.0000E+00
I05:   1.4700E+34 -7.0700E+00  4.9476E+04  1.0000E+01
I06:   6.1000E+31 -6.2500E+00  4.9013E+04  2.5000E+01
I07:   5.6700E+29 -5.5700E+00  4.8551E+04  5.0000E+01
I08:   2.8400E+28 -5.1400E+00  4.8230E+04  7.5000E+01
I09:   3.3900E+27 -4.8400E+00  4.7994E+04  1.0000E+02
1471. ETONO2(+M)=C2H4+HNO3(+M)               1.00E+00    0.0         0.0
I01:   1.0300E+35 -9.0300E+00  4.9675E+04  1.0000E-03
I02:   6.2800E+40 -1.0320E+01  5.0841E+04  1.0000E-02
I03:   8.6000E+39 -9.5700E+00  5.1279E+04  1.0000E-01
I04:   3.8400E+37 -8.4200E+00  5.1785E+04  1.0000E+00
I05:   3.5300E+34 -7.1600E+00  5.2001E+04  1.0000E+01
I06:   1.7000E+32 -6.3400E+00  5.1624E+04  2.5000E+01
I07:   1.4900E+30 -5.6400E+00  5.1196E+04  5.0000E+01
I08:   6.7900E+28 -5.1900E+00  5.0882E+04  7.5000E+01
I09:   7.4100E+27 -4.8700E+00  5.0648E+04  1.0000E+02
1472. ETONO2(+M)=C2H5+NO3(+M)                1.00E+00    0.0         0.0
I01:   4.3700E-07  1.5200E+00  1.2716E+05  1.0000E-03
I02:   1.9000E-01  2.0000E-01  1.2245E+05  1.0000E-02
I03:   7.3200E+01 -1.3000E-01  1.1382E+05  1.0000E-01
I04:   9.2000E+07 -1.4600E+00  1.0234E+05  1.0000E+00
I05:   4.3900E+22 -5.1700E+00  9.1430E+04  1.0000E+01
I06:   3.2100E+30 -7.1400E+00  8.9347E+04  2.5000E+01
I07:   1.7100E+36 -8.5300E+00  8.8923E+04  5.0000E+01
I08:   1.2500E+39 -9.1800E+00  8.9002E+04  7.5000E+01
I09:   1.0900E+41 -9.6200E+00  8.9219E+04  1.0000E+02
1473. ETONO2(+M)=CCOONO(+M)                  1.00E+00    0.0         0.0
I01:   3.6900E+24 -6.3700E+00  6.2830E+04  1.0000E-03
I02:   1.3200E+31 -7.9400E+00  5.9422E+04  1.0000E-02
I03:   2.1100E+36 -8.9300E+00  5.7178E+04  1.0000E-01
I04:   2.8100E+40 -9.5400E+00  5.8208E+04  1.0000E+00
I05:   3.2800E+41 -9.3000E+00  5.9931E+04  1.0000E+01
I06:   1.4000E+40 -8.6900E+00  6.0090E+04  2.5000E+01
I07:   3.1200E+38 -8.0600E+00  5.9967E+04  5.0000E+01
I08:   1.7500E+37 -7.6200E+00  5.9781E+04  7.5000E+01
I09:   2.0100E+36 -7.2900E+00  5.9618E+04  1.0000E+02
1474. CCOONO(+M)=CH3CHO+HNO2(+M)             1.00E+00    0.0         0.0
I01:   7.3100E+45 -1.2520E+01  4.1677E+04  1.0000E-03
I02:   7.3200E+46 -1.2520E+01  4.1678E+04  1.0000E-02
I03:   7.4100E+47 -1.2520E+01  4.1683E+04  1.0000E-01
I04:   8.0500E+48 -1.2530E+01  4.1723E+04  1.0000E+00
I05:   1.0100E+50 -1.2570E+01  4.1950E+04  1.0000E+01
I06:   2.0800E+50 -1.2550E+01  4.2103E+04  2.5000E+01
I07:   2.4700E+50 -1.2500E+01  4.2196E+04  5.0000E+01
I08:   2.5300E+50 -1.2470E+01  4.2251E+04  7.5000E+01
I09:   2.2400E+50 -1.2430E+01  4.2262E+04  1.0000E+02
1475. CCOONO(+M)=CCOONO_I(+M)                1.00E+00    0.0         0.0
I01:   1.2900E+52 -1.2820E+01  4.1644E+04  1.0000E-03
I02:   1.2900E+53 -1.2820E+01  4.1644E+04  1.0000E-02
I03:   1.3100E+54 -1.2820E+01  4.1649E+04  1.0000E-01
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I04:   1.4300E+55 -1.2830E+01  4.1693E+04  1.0000E+00
I05:   1.8200E+56 -1.2870E+01  4.1930E+04  1.0000E+01
I06:   3.6800E+56 -1.2850E+01  4.2087E+04  2.5000E+01
I07:   4.3000E+56 -1.2800E+01  4.2181E+04  5.0000E+01
I08:   4.3700E+56 -1.2760E+01  4.2235E+04  7.5000E+01
I09:   3.8500E+56 -1.2730E+01  4.2246E+04  1.0000E+02
1476. CCOONO_I(+M)=C2H5O+NO2(+M)             1.00E+00    0.0        0.0
I01:   6.3700E+52 -1.3100E+01  4.2526E+04  1.0000E-03
I02:   6.3700E+53 -1.3100E+01  4.2526E+04  1.0000E-02
I03:   6.3600E+54 -1.3100E+01  4.2527E+04  1.0000E-01
I04:   6.2500E+55 -1.3100E+01  4.2535E+04  1.0000E+00
I05:   5.1400E+56 -1.3070E+01  4.2597E+04  1.0000E+01
I06:   9.1400E+56 -1.3030E+01  4.2653E+04  2.5000E+01
I07:   1.1300E+57 -1.2970E+01  4.2702E+04  5.0000E+01
I08:   1.1500E+57 -1.2930E+01  4.2733E+04  7.5000E+01
I09:   1.1000E+57 -1.2890E+01  4.2754E+04  1.0000E+02
1477. CCOONO_I(+M)=C2H5O2+NO(+M)             1.00E+00    0.0        0.0
I01:   2.0800E+46 -1.1790E+01  4.2432E+04  1.0000E-03
I02:   2.0800E+47 -1.1790E+01  4.2432E+04  1.0000E-02
I03:   2.0700E+48 -1.1790E+01  4.2433E+04  1.0000E-01
I04:   2.0400E+49 -1.1780E+01  4.2441E+04  1.0000E+00
I05:   1.6400E+50 -1.1760E+01  4.2501E+04  1.0000E+01
I06:   2.7800E+50 -1.1710E+01  4.2552E+04  2.5000E+01
I07:   3.1500E+50 -1.1630E+01  4.2594E+04  5.0000E+01
I08:   2.9400E+50 -1.1580E+01  4.2617E+04  7.5000E+01
I09:   2.5800E+50 -1.1520E+01  4.2629E+04  1.0000E+02
1478. CCOONO_I(+M)=CH3CHO+HONO(+M)           1.00E+00    0.0        0.0
      Declared duplicate reaction...
I01:   1.6400E+39 -1.0560E+01  4.1915E+04  1.0000E-03
I02:   1.6400E+40 -1.0560E+01  4.1915E+04  1.0000E-02
I03:   1.6300E+41 -1.0560E+01  4.1916E+04  1.0000E-01
I04:   1.5900E+42 -1.0560E+01  4.1923E+04  1.0000E+00
I05:   1.1200E+43 -1.0510E+01  4.1972E+04  1.0000E+01
I06:   1.5100E+43 -1.0420E+01  4.2005E+04  2.5000E+01
I07:   1.1400E+43 -1.0280E+01  4.2014E+04  5.0000E+01
I08:   7.2300E+42 -1.0160E+01  4.2003E+04  7.5000E+01
I09:   4.3600E+42 -1.0050E+01  4.1983E+04  1.0000E+02
1479. CCOONO_I(+M)=CH3CHO+HONO(+M)           1.00E+00    0.0        0.0
      Declared duplicate reaction...
I01:   1.4400E+19 -5.9300E+00  4.5048E+04  1.0000E-03
I02:   1.4400E+20 -5.9300E+00  4.5046E+04  1.0000E-02
I03:   1.4000E+21 -5.9200E+00  4.5030E+04  1.0000E-01
I04:   1.1200E+22 -5.8900E+00  4.4873E+04  1.0000E+00
I05:   6.3200E+22 -5.8200E+00  4.3935E+04  1.0000E+01
I06:   5.0800E+23 -5.9500E+00  4.3417E+04  2.5000E+01
I07:   9.7900E+24 -6.1900E+00  4.3269E+04  5.0000E+01
I08:   8.4900E+25 -6.3800E+00  4.3330E+04  7.5000E+01
I09:   4.0700E+26 -6.5000E+00  4.3431E+04  1.0000E+02
1480. C2H5O+NO2=CH3CHO+HNO2                  2.93E+00    3.4     -917.0
1481. C2H5O+NO2=CH3CHO+HONO                  2.17E-01    3.6    -1048.4
1482. C2H5O+NO=CH3CHO+HNO                    1.06E+00    3.4     -923.7
1483. CH3CHO+NO2=CH3CO+HONO                  2.50E+07    1.3    15398.0
1484. CH3CHO+NO2=CH3CO+HNO2                  7.10E-03    4.6    19979.0
1485. CH3CHO+NO2=CH2CHO+HONO                 2.50E+07    1.3    22674.0
1486. CH3CHO+NO2=CH2CHO+HNO2                 1.42E-02    4.6    28799.0
1487. CH3CO+NO2=CH3CO2+NO                    4.51E+13    0.0        0.0
1488. CH2CHO+NO2=CDOCOJ+NO                   2.35E+13    0.0        0.0
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1489. CDOCOJ=HCO+CH2O                          2.53E+13    0.4     8090.3
1490. CDOCOJ+H=CHOCHO+H2                       1.73E+09    0.1     -300.6
1491. CDOCOJ+HO2=CHOCHO+H2O2                   1.86E+17   -1.3     4754.3
1492. CDOCOJ+NO2=CHOCHO+HNO2                   9.15E+15   -1.1     2130.8
1493. CDOCOJ+NO2=CHOCHO+HONO                   4.30E+17   -1.4     4832.3
1494. CDOCOJ+O2=CHOCHO+HO2                     1.70E+17   -1.5     4872.0
1495. CDOCOJ+O=CHOCHO+OH                       9.23E+15   -0.9      -54.4
1496. CDOCOJ+OH=CHOCHO+H2O                     1.26E+17   -1.2     1496.2
1497. CDOCOJ+NO=CHOCHO+HNO                     1.49E+17   -1.4     4953.7
1498. C2H5O+NO2(+M)=C2H5O2+NO(+M)              1.00E+00    0.0        0.0
I01:   1.9300E+04  2.0200E+00  6.2170E+03  1.0000E-03
I02:   1.9300E+04  2.0200E+00  6.2170E+03  1.0000E-02
I03:   1.9200E+04  2.0200E+00  6.2150E+03  1.0000E-01
I04:   2.5000E+04  1.9900E+00  6.2790E+03  1.0000E+00
I05:   3.8900E+05  1.6500E+00  7.0190E+03  1.0000E+01
I06:   2.6500E+06  1.4200E+00  7.6140E+03  2.5000E+01
I07:   1.1700E+07  1.2400E+00  8.1490E+03  5.0000E+01
I08:   2.5700E+07  1.1500E+00  8.4800E+03  7.5000E+01
I09:   4.1500E+07  1.0900E+00  8.7160E+03  1.0000E+02
1499. C2H5O+NO2(+M)=CH3CHO+HONO(+M)            1.00E+00    0.0        0.0
I01:   1.1800E+08  7.6000E-01  1.8420E+04  1.0000E-03
I02:   1.1800E+08  7.6000E-01  1.8420E+04  1.0000E-02
I03:   1.1800E+08  7.6000E-01  1.8420E+04  1.0000E-01
I04:   1.1800E+08  7.6000E-01  1.8420E+04  1.0000E+00
I05:   1.1800E+08  7.6000E-01  1.8419E+04  1.0000E+01
I06:   1.3700E+08  7.4000E-01  1.8456E+04  2.5000E+01
I07:   2.0200E+08  6.9000E-01  1.8562E+04  5.0000E+01
I08:   2.8400E+08  6.5000E-01  1.8666E+04  7.5000E+01
I09:   3.7300E+08  6.2000E-01  1.8758E+04  1.0000E+02
1500. C2H5O+NO2(+M)=CH3CHO+HNO2(+M)            1.00E+00    0.0        0.0
I01:   5.2300E+06  9.2000E-01  1.4471E+04  1.0000E-03
I02:   5.2300E+06  9.2000E-01  1.4471E+04  1.0000E-02
I03:   5.2300E+06  9.2000E-01  1.4471E+04  1.0000E-01
I04:   5.1700E+06  9.2000E-01  1.4468E+04  1.0000E+00
I05:   7.0700E+06  8.8000E-01  1.4539E+04  1.0000E+01
I06:   3.2300E+07  6.9000E-01  1.4923E+04  2.5000E+01
I07:   3.3500E+08  4.0000E-01  1.5557E+04  5.0000E+01
I08:   1.9400E+09  1.9000E-01  1.6069E+04  7.5000E+01
I09:   7.4400E+09  2.0000E-02  1.6486E+04  1.0000E+02
1501. CH3CHO=CH3+HCO                           2.61E+15    0.1    80550.0
1502. C2H5OH(+M)=CH3CHO+H2(+M)                 7.24E+11    0.1    91010.0
      Low pressure limit:  0.31100E+86 -0.18840E+02  0.11310E+06
      TROE centering:      0.50000E+00  0.55000E+03  0.82500E+03  0.61000E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    5.000E+00
      CO              Enhanced by    2.000E+00
      CO2             Enhanced by    3.000E+00
1503. SC2H4OH+M=CH3CHO+H+M                     1.00E+14    0.0    25000.0
      Reverse Arrhenius coefficients:          8.17E+12    0.4      730.0
1504. SC2H4OH+O2=CH3CHO+HO2                    3.81E+06    2.0     1641.0
1505. CH2O+OH(+M)=HOCH2O(+M)                   1.00E+00    0.0        0.0
I01:   3.1300E+08 -2.7700E+00  1.4790E+04  1.0000E-03
I02:   7.9700E+08 -2.6500E+00  1.2271E+04  1.0000E-02
I03:   3.8400E+10 -2.9300E+00  8.1500E+03  1.0000E-01
I04:   1.7800E+17 -4.6400E+00  4.4280E+03  1.0000E+00
I05:   1.6300E+31 -8.2800E+00  6.1650E+03  1.0000E+01
I06:   1.9400E+36 -9.5400E+00  7.8620E+03  2.5000E+01
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I07:   2.9500E+39 -1.0280E+01  9.2170E+03  5.0000E+01
I08:   1.0600E+41 -1.0630E+01  9.9940E+03  7.5000E+01
I09:   9.5900E+41 -1.0830E+01  1.0525E+04  1.0000E+02
1506. CH2O+OH(+M)=HOCHO+H(+M)                1.00E+00    0.0         0.0
I01:   6.3300E+06  1.6300E+00  4.2800E+03  1.0000E-03
I02:   6.3300E+06  1.6300E+00  4.2800E+03  1.0000E-02
I03:   6.3300E+06  1.6300E+00  4.2800E+03  1.0000E-01
I04:   6.3300E+06  1.6300E+00  4.2800E+03  1.0000E+00
I05:   7.2600E+06  1.6100E+00  4.3130E+03  1.0000E+01
I06:   1.4000E+07  1.5300E+00  4.4770E+03  2.5000E+01
I07:   4.5800E+07  1.3800E+00  4.7810E+03  5.0000E+01
I08:   1.2500E+08  1.2600E+00  5.0480E+03  7.5000E+01
I09:   2.8600E+08  1.1500E+00  5.2750E+03  1.0000E+02
1507. HOCH2O(+M)=HOCHO+H(+M)                 1.00E+00    0.0         0.0
I01:   1.5200E+17 -3.0900E+00  1.1241E+04  1.0000E-03
I02:   3.8000E+18 -3.2100E+00  1.1673E+04  1.0000E-02
I03:   9.0400E+20 -3.6200E+00  1.2744E+04  1.0000E-01
I04:   2.4600E+26 -4.9100E+00  1.5382E+04  1.0000E+00
I05:   1.2800E+28 -5.1100E+00  1.6886E+04  1.0000E+01
I06:   9.8300E+26 -4.6400E+00  1.6866E+04  2.5000E+01
I07:   1.7000E+27 -4.6400E+00  1.7220E+04  5.0000E+01
I08:   1.9900E+27 -4.6100E+00  1.7408E+04  7.5000E+01
I09:   2.3200E+27 -4.6000E+00  1.7542E+04  1.0000E+02
1508. CH3CO(+M)=CH3+CO(+M)                   3.00E+12    0.0     16720.0
      Low pressure limit:  0.12000E+16  0.00000E+00  0.12518E+05
1509. CH3CO+H=CH2CO+H2                       2.00E+13    0.0         0.0
1510. CH3CO+O=CH2CO+OH                       2.00E+13    0.0         0.0
1511. CH3CO+CH3=CH2CO+CH4                    5.00E+13    0.0         0.0
1512. CH3CO2+M=CH3+CO2+M                     4.40E+15    0.0     10500.0
      Reverse Arrhenius coefficients:        9.65E+12    0.2     21040.0
1513. C2H5+HO2=C2H5O+OH                      3.20E+13    0.0         0.0
1514. C2H5OH(+M)=CH2OH+CH3(+M)               5.71E+23   -1.7     94410.0
      Low pressure limit:  0.31100E+86 -0.18840E+02  0.11310E+06
      TROE centering:      0.50000E+00  0.55000E+03  0.82500E+03  0.61000E+04
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    5.000E+00
      CO              Enhanced by    2.000E+00
      CO2             Enhanced by    3.000E+00
1515. C2H5OH(+M)=C2H5+OH(+M)                 2.40E+23   -1.6     99540.0
      Low pressure limit:  0.51100E+86 -0.18800E+02  0.11877E+06
      TROE centering:      0.50000E+00  0.65000E+03  0.80000E+03  0.10000E+16
      H2              Enhanced by    2.000E+00
      H2O             Enhanced by    5.000E+00
      CO              Enhanced by    2.000E+00
      CO2             Enhanced by    3.000E+00
1516. C2H5OH(+M)=C2H4+H2O(+M)                2.79E+13    0.1     66140.0
      Low pressure limit:  0.25700E+84 -0.18850E+02  0.86453E+05
      TROE centering:      0.70000E+00  0.35000E+03  0.80000E+03  0.38000E+04
      H2O             Enhanced by    5.000E+00
1517. C2H5OH+O2=PC2H4OH+HO2                  2.00E+13    0.0     52800.0
1518. C2H5OH+O2=SC2H4OH+HO2                  1.50E+13    0.0     50150.0
1519. C2H5OH+OH=PC2H4OH+H2O                  1.74E+11    0.3       600.0
1520. C2H5OH+OH=SC2H4OH+H2O                  4.64E+11    0.1         0.0
1521. C2H5OH+OH=C2H5O+H2O                    7.46E+11    0.3      1634.0
1522. C2H5OH+H=PC2H4OH+H2                    1.23E+07    1.8      5098.0
1523. C2H5OH+H=SC2H4OH+H2                    2.58E+07    1.6      2827.0
1524. C2H5OH+H=C2H5O+H2                      1.50E+07    1.6      3038.0
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1525. C2H5OH+HO2=PC2H4OH+H2O2                1.23E+04    2.5    15750.0
1526. C2H5OH+HO2=SC2H4OH+H2O2                8.20E+03    2.5    10750.0
1527. C2H5OH+HO2=C2H5O+H2O2                  2.50E+12    0.0    24000.0
1528. C2H5OH+O=PC2H4OH+OH                    9.41E+07    1.7     5459.0
1529. C2H5OH+O=SC2H4OH+OH                    1.88E+07    1.9     1824.0
1530. C2H5OH+O=C2H5O+OH                      1.58E+07    2.0     4448.0
1531. C2H5OH+CH3=PC2H4OH+CH4                 1.33E+02    3.2     9362.0
1532. C2H5OH+CH3=SC2H4OH+CH4                 4.44E+02    2.9     7690.0
1533. C2H5OH+CH3=C2H5O+CH4                   1.34E+02    2.9     7452.0
1534. C2H5OH+C2H5=PC2H4OH+C2H6               5.00E+10    0.0    13400.0
1535. C2H5OH+C2H5=SC2H4OH+C2H6               5.00E+10    0.0    10400.0
1536. C2H5O(+M)=CH3+CH2O(+M)                 1.00E+00    0.0        0.0
I01:   1.9000E+12 -1.7400E+00  1.6096E+04  1.0000E-03
I02:   2.3800E+12 -1.5800E+00  1.3425E+04  1.0000E-02
I03:   3.4200E+23 -4.5600E+00  1.6708E+04  1.0000E-01
I04:   1.0000E+28 -5.4600E+00  1.8903E+04  1.0000E+00
I05:   3.2600E+27 -4.9300E+00  1.9638E+04  1.0000E+01
I06:   6.3300E+24 -3.9500E+00  1.9155E+04  2.5000E+01
I07:   5.4500E+24 -3.8300E+00  1.9472E+04  5.0000E+01
I08:   3.7300E+24 -3.7300E+00  1.9606E+04  7.5000E+01
I09:   3.0600E+24 -3.6700E+00  1.9706E+04  1.0000E+02
1537. C2H5O(+M)=CH3CHO+H(+M)                 1.00E+00    0.0        0.0
I01:   7.9800E+19 -3.8600E+00  1.4837E+04  1.0000E-03
I02:   2.1000E+22 -4.2600E+00  1.5949E+04  1.0000E-02
I03:   3.1800E+23 -4.2800E+00  1.7232E+04  1.0000E-01
I04:   2.4300E+21 -3.3700E+00  1.7357E+04  1.0000E+00
I05:   1.3200E+19 -2.4500E+00  1.7351E+04  1.0000E+01
I06:   1.4100E+16 -1.4300E+00  1.6684E+04  2.5000E+01
I07:   6.8400E+15 -1.2700E+00  1.6836E+04  5.0000E+01
I08:   3.5900E+15 -1.1500E+00  1.6882E+04  7.5000E+01
I09:   2.4500E+15 -1.0700E+00  1.6921E+04  1.0000E+02
1538. C2H5O+O2=CH3CHO+HO2                    4.28E+10    0.0     1097.0
1539. C2H5O2=C2H5+O2                         4.93E+50  -11.5    42250.0
1540. C2H5O2=C2H4O2H                         5.64E+47  -11.4    37320.0
1541. C2H5O2=C2H4+HO2                        3.37E+55  -13.4    44670.0
1542. C2H5O2+CH2O=C2H5O2H+HCO                1.99E+12    0.0    11670.0
1543. C2H5O2+C2H4=C2H3+C2H5O2H               1.13E+13    0.0    30430.0
1544. C2H5O2+CH4=CH3+C2H5O2H                 1.81E+11    0.0    18480.0
1545. C2H5O2+CH3OH=CH2OH+C2H5O2H             1.81E+12    0.0    13710.0
1546. C2H5O2+HO2=C2H5O2H+O2                  1.75E+10    0.0    -3275.0
1547. C2H5O2+C2H6=C2H5+C2H5O2H               1.70E+13    0.0    20460.0
1548. C2H5O2+C2H4=>C2H4O+C2H5O               2.82E+12    0.0    17110.0
1549. C2H5O2H=C2H5O+OH                       6.31E+14    0.0    42300.0
1550. PC2H4OH=C2H4+OH                        1.29E+12   -0.4    26850.0
1551. O2C2H4OH=PC2H4OH+O2                    3.90E+16   -1.0    30000.0
1552. O2C2H4OH=>OH+CH2O+CH2O                 1.25E+10    0.0    18900.0
1553. C2H4O2H=>C2H4O+OH                      4.25E+22   -4.2    22350.0
1554. C2H4O2H=C2H4+HO2                       9.29E+30   -6.1    19930.0
1555. C2H4O2H=C2H5+O2                        2.15E+37   -8.2    28020.0
1556. C2H5O+OH=CH3CHO+H2O                    1.00E+14    0.0        0.0
1557. C2H5O+H=CH3CHO+H2                      1.00E+14    0.0        0.0
1558. C2H5O+O=CH3CHO+OH                      1.21E+14    0.0        0.0
1559. C2H5O+HO2=CH3CHO+H2O2                  1.00E+14    0.0        0.0
1560. SC2H4OH+H=CH3CHO+H2                    2.00E+13    0.0        0.0
1561. SC2H4OH+OH=CH3CHO+H2O                  1.50E+13    0.0        0.0
1562. SC2H4OH+O=CH3CHO+OH                    9.04E+13    0.0        0.0
1563. SC2H4OH+HO2=>CH3CHO+OH+OH              1.00E+13    0.0        0.0
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1564. PC2H4OH=H+CDCOH                          2.91E+09    1.1    33074.0
1565. PC2H4OH=SC2H4OH                          1.00E+11    0.0    27000.0
1566. C2H5OH=CH2OH+CH3                         3.10E+15    0.0    80600.0
1567. C2H5OH+H=>C2H5+H2O                       2.40E+10    0.0        0.0
1568. C2H5OH+CH3O=SC2H4OH+CH3OH                2.00E+11    0.0     7000.0
1569. C2H5OH+CH2O=C2H5O+CH3O                   1.50E+12    0.0    79500.0
1570. C2H5OH+C2H5O=C2H5OH+SC2H4OH              2.00E+11    0.0     7000.0
1571. C2H5OH=C2H5+OH                           5.00E+16    0.0    91212.0
1572. C2H5OH=C2H4+H2O                          1.00E+14    0.0    76706.0
1573. C2H5OH+O2=C2H5O+HO2                      2.00E+13    0.0    56000.0
1574. C2H5OH+CH2OH=SC2H4OH+CH3OH               4.00E+11    0.0     9700.0
1575. CH3CHO+C2H5O2=CH3CO+C2H5O2H              1.15E+11    0.0    10000.0
1576. C2H5O2H+O=OH+C2H5O2                      2.00E+13    0.0     4750.0
1577. C2H5O2H+OH=C2H5O2+H2O                    2.00E+12    0.0     -370.0
1578. C2H5OH+CH3O2=SC2H4OH+CH3O2H              1.00E+13    0.0    10000.0
1579. C2H5+NO2(+M)=C2H5ONO(+M)                 1.00E+00    0.0        0.0
I01:   8.8600E-38  1.0570E+01 -4.2130E+03  1.0000E-03
I02:   3.8800E-28  8.0800E+00 -7.4200E+02  1.0000E-02
I03:   2.8000E-06  2.0400E+00  7.0380E+03  1.0000E-01
I04:   1.0800E+12 -2.8000E+00  9.2120E+03  1.0000E+00
I05:   1.5800E+18 -4.2600E+00  2.8600E+03  1.0000E+01
I06:   1.5100E+23 -5.5200E+00  1.7980E+03  2.5000E+01
I07:   3.4800E+27 -6.6200E+00  1.8510E+03  5.0000E+01
I08:   1.0800E+30 -7.2300E+00  2.1450E+03  7.5000E+01
I09:   4.7800E+31 -7.6300E+00  2.4320E+03  1.0000E+02
1580. C2H5+NO2(+M)=C2H5O+NO(+M)                1.00E+00    0.0        0.0
I01:   2.0800E+13  0.0000E+00  3.0000E+00  1.0000E-03
I02:   2.0800E+13  0.0000E+00  3.0000E+00  1.0000E-02
I03:   2.0800E+13  0.0000E+00  3.0000E+00  1.0000E-01
I04:   2.0800E+13  0.0000E+00  3.0000E+00  1.0000E+00
I05:   2.0800E+13  0.0000E+00  3.0000E+00  1.0000E+01
I06:   2.0800E+13  0.0000E+00  3.0000E+00  2.5000E+01
I07:   2.0900E+13  0.0000E+00  3.0000E+00  5.0000E+01
I08:   2.1000E+13  0.0000E+00  5.0000E+00  7.5000E+01
I09:   2.1400E+13 -1.0000E-02  1.0000E+01  1.0000E+02
1581. C2H5+NO2(+M)=C2H4+HNO2(+M)               1.00E+00    0.0        0.0
I01:   3.3900E+02  1.5700E+00  4.6100E+02  1.0000E-03
I02:   3.3900E+02  1.5700E+00  4.6100E+02  1.0000E-02
I03:   3.3900E+02  1.5700E+00  4.6100E+02  1.0000E-01
I04:   3.3900E+02  1.5700E+00  4.6200E+02  1.0000E+00
I05:   3.4700E+02  1.5600E+00  4.6900E+02  1.0000E+01
I06:   3.6200E+02  1.5600E+00  4.8100E+02  2.5000E+01
I07:   3.9200E+02  1.5500E+00  5.0400E+02  5.0000E+01
I08:   4.2700E+02  1.5400E+00  5.3000E+02  7.5000E+01
I09:   4.6900E+02  1.5300E+00  5.5700E+02  1.0000E+02
1582. C2H5ONO(+M)=C2H5O+NO(+M)                 1.00E+00    0.0        0.0
I01:   6.2000E+48 -1.1660E+01  4.7370E+04  1.0000E-03
I02:   6.7700E+49 -1.1670E+01  4.7713E+04  1.0000E-02
I03:   6.2400E+50 -1.1660E+01  4.8404E+04  1.0000E-01
I04:   2.7800E+51 -1.1540E+01  4.9388E+04  1.0000E+00
I05:   3.1100E+50 -1.0950E+01  5.0064E+04  1.0000E+01
I06:   8.6700E+45 -9.4200E+00  4.8948E+04  2.5000E+01
I07:   3.1800E+44 -8.9000E+00  4.8771E+04  5.0000E+01
I08:   1.5600E+44 -8.7600E+00  4.8837E+04  7.5000E+01
I09:   9.0300E+43 -8.6500E+00  4.8874E+04  1.0000E+02
1583. C2H5ONO(+M)=C2H4+HNO2(+M)                1.00E+00    0.0        0.0
I01:   2.2800E+24 -6.7700E+00  6.3860E+04  1.0000E-03
```

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I02:   2.3800E+24 -6.5200E+00  6.1261E+04  1.0000E-02
I03:   1.6600E+26 -6.7900E+00  5.7668E+04  1.0000E-01
I04:   1.2700E+32 -8.1700E+00  5.5202E+04  1.0000E+00
I05:   1.9000E+40 -1.0060E+01  5.6368E+04  1.0000E+01
I06:   2.7300E+38 -9.2300E+00  5.5950E+04  2.5000E+01
I07:   1.0900E+39 -9.2300E+00  5.6470E+04  5.0000E+01
I08:   4.5800E+39 -9.3300E+00  5.6906E+04  7.5000E+01
I09:   1.2100E+40 -9.3900E+00  5.7219E+04  1.0000E+02
1584. C2H5ONO(+M)=C2H5NO2(+M)                1.00E+00    0.0         0.0
I01:   5.5300E+10 -3.4300E+00  8.9152E+04  1.0000E-03
I02:   5.0100E+10 -3.1600E+00  8.6499E+04  1.0000E-02
I03:   9.5300E+11 -3.2700E+00  8.2396E+04  1.0000E-01
I04:   3.6300E+14 -3.7400E+00  7.6445E+04  1.0000E+00
I05:   8.4600E+19 -4.9700E+00  6.9104E+04  1.0000E+01
I06:   3.6500E+20 -4.9000E+00  6.5928E+04  2.5000E+01
I07:   6.4700E+24 -5.9700E+00  6.5362E+04  5.0000E+01
I08:   6.7900E+27 -6.7500E+00  6.5513E+04  7.5000E+01
I09:   1.2200E+30 -7.3300E+00  6.5796E+04  1.0000E+02
1585. C2H5+NO2(+M)=C2H5NO2(+M)               1.00E+00    0.0         0.0
I01:   3.1000E+45 -1.1850E+01  5.3500E+03  1.0000E-03
I02:   6.2700E+46 -1.1630E+01  7.2750E+03  1.0000E-02
I03:   4.8000E+43 -1.0280E+01  7.5110E+03  1.0000E-01
I04:   4.5600E+38 -8.4400E+00  6.8770E+03  1.0000E+00
I05:   5.6100E+31 -6.1000E+00  5.3770E+03  1.0000E+01
I06:   3.7000E+28 -5.0500E+00  4.5680E+03  2.5000E+01
I07:   1.1300E+26 -4.2300E+00  3.8930E+03  5.0000E+01
I08:   3.6000E+24 -3.7500E+00  3.4790E+03  7.5000E+01
I09:   3.0900E+23 -3.4000E+00  3.1800E+03  1.0000E+02
1586. C2H5+NO2(+M)=C2H4+HONO(+M)             1.00E+00    0.0         0.0
I01:   9.8300E+17 -2.1600E+00  2.5200E+02  1.0000E-03
I02:   2.3900E+20 -2.8200E+00  2.0320E+03  1.0000E-02
I03:   1.5700E+21 -3.0000E+00  3.8050E+03  1.0000E-01
I04:   2.3400E+19 -2.3800E+00  4.8270E+03  1.0000E+00
I05:   3.4500E+14 -8.9000E-01  4.7510E+03  1.0000E+01
I06:   6.6600E+11 -7.0000E-02  4.3940E+03  2.5000E+01
I07:   3.3700E+09  6.2000E-01  4.0100E+03  5.0000E+01
I08:   1.2900E+08  1.0400E+00  3.7460E+03  7.5000E+01
I09:   1.2100E+07  1.3400E+00  3.5430E+03  1.0000E+02
1587. C2H5NO2(+M)=C2H4+HONO(+M)              1.00E+00    0.0         0.0
I01:   1.6400E+45 -1.0400E+01  5.5490E+04  1.0000E-03
I02:   7.2200E+37 -7.9300E+00  5.3777E+04  1.0000E-02
I03:   3.2800E+33 -6.4900E+00  5.2742E+04  1.0000E-01
I04:   2.0400E+29 -5.1200E+00  5.1608E+04  1.0000E+00
I05:   7.3100E+24 -3.6900E+00  5.0322E+04  1.0000E+01
I06:   1.0500E+23 -3.1000E+00  4.9770E+04  2.5000E+01
I07:   3.3400E+21 -2.6300E+00  4.9312E+04  5.0000E+01
I08:   3.7700E+20 -2.3300E+00  4.9020E+04  7.5000E+01
I09:   7.7300E+19 -2.1100E+00  4.8807E+04  1.0000E+02
1588. C2H5O+NO3=C2H5O2+NO2                   1.99E+12    0.0         0.0
1589. C2H5O+C2H5O=C2H5OH+CH3CHO              1.44E+13    0.0         0.0
1590. C2H5O+C2H5=C2H6+CH3CHO                 1.56E+12    0.0         0.0
1591. C2H5O+C2H5=C2H5OH+C2H4                 2.76E+12    0.0         0.0
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NOTE: A units mole-cm-sec-K, E units cal/mole

Table A-2 Coefficients for calculating thermodynamic property estimates for species in the NG mechanism

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THERMO
   300.000  1500.000  5000.000
CDOOHA    CONO2CDOOH_BHaC   2H   3N   1O   5G   300.000  5000.000 1406.000    21
 1.90622954E+01 9.56080594E-03-3.37066000E-06 5.34712293E-10-3.15133196E-14    2
-6.52289877E+04-7.11834364E+01-6.20401037E-01 5.86257336E-02-4.94836048E-05    3
 1.98913597E-08-3.08825327E-12-5.88810123E+04 3.31330974E+01                   4
CDOOJA    CONO2COHOJ_BH_C   2H   4N   1O   5G   300.000  5000.000 1399.000    41
 1.96506127E+01 1.05146339E-02-3.63642751E-06 5.68900696E-10-3.31866752E-14    2
-4.05144224E+04-6.90949928E+01 3.91525349E+00 5.53318964E-02-5.35492020E-05    3
 2.59099320E-08-4.90481630E-12-3.58496530E+04 1.25659979E+01                   4
CACACDOOH CONO2CONO2CDOOC   3H   4N   2O   8G   300.000  5000.000 1399.000    41
 3.15054374E+01 1.40834483E-02-5.07773126E-06 8.16709863E-10-4.85692860E-14    2
-8.27296674E+04-1.32418831E+02-7.01631142E-01 9.71657225E-02-8.70903349E-05    3
 3.74732923E-08-6.28261713E-12-7.25455460E+04 3.74122942E+01                   4
CACACDOOJ CONO2CONO2COHCC   3H   5N   2O   8G   300.000  5000.000 1398.000    61
 3.27612770E+01 1.43878706E-02-5.10753528E-06 8.13311886E-10-4.80388189E-14    2
-5.86666439E+04-1.34909692E+02 4.53609389E+00 8.76708299E-02-7.82648875E-05    3
 3.40086478E-08-5.79284579E-12-4.97555052E+04 1.38126648E+01                   4
DIOHCH2                C   1H   4O   2    0G   300.000  5000.000 1408.000    01
 7.23599163E+00 9.39087193E-03-3.11037208E-06 4.72375853E-10-2.69830566E-14    2
-5.06157972E+04-1.42438837E+01 8.23487237E-01 2.48484141E-02-1.73882425E-05    3
 6.47025502E-09-9.90888491E-13-4.84507250E+04 2.00011895E+01                   4
CACACOH   NG-NG1J+CACACOC   3H   6N   2O   7G   300.000  5000.000 1427.000    71
 2.89011195E+01 1.66482702E-02-5.76241823E-06 9.03027715E-10-5.27717758E-14    2
-6.07320627E+04-1.11657564E+02 9.67180613E-01 8.41292400E-02-6.63673956E-05    3
 2.48038614E-08-3.52589400E-12-5.15409878E+04 3.70960996E+01                   4
O2NCHO                 C   1H   1N   1O   3G   300.000  5000.000 1394.000    11
 9.91141295E+00 4.90047838E-03-1.72715003E-06 2.73638213E-10-1.61035429E-14    2
-2.00230456E+04-2.30177654E+01 2.62365244E+00 2.36338057E-02-2.04428729E-05    3
 8.85914610E-09-1.52941335E-12-1.76779234E+04 1.54916873E+01                   4
KIDOCDOOJ  6/ 7/10 THERMC   3H   1O   4    0G   300.000  5000.000 1379.000    11
 1.39779734E+01 6.82250399E-03-2.45597358E-06 3.94568912E-10-2.34447631E-14    2
-5.20723676E+04-4.04306309E+01 2.82318161E+00 3.29451351E-02-2.55860680E-05    3
 9.61145797E-09-1.42080813E-12-4.82482868E+04 1.93847130E+01                   4
HOCDONO                C   1H   1N   1O   3G   300.000  5000.000 1400.000    11
 9.84094437E+00 4.71273745E-03-1.60851575E-06 2.49577145E-10-1.44802858E-14    2
-3.14223386E+04-2.14472253E+01 3.38671948E+00 2.15074980E-02-1.84677705E-05    3
 7.96048213E-09-1.36107142E-12-2.93817859E+04 1.25584114E+01                   4
HOCDONO2               C   1H   1N   1O   4G   300.000  5000.000 1390.000    11
 1.28217298E+01 5.15487929E-03-1.85679871E-06 2.98434850E-10-1.77380555E-14    2
-5.13795098E+04-3.94584564E+01 2.21690968E+00 3.29433160E-02-3.01319912E-05    3
 1.34798396E-08-2.37261069E-12-4.80294458E+04 1.63761893E+01                   4
HOCDOONO               C   1H   1N   1O   4G   300.000  5000.000 1403.000    21
 1.45793492E+01 3.16593427E-03-1.15431568E-06 1.87028442E-10-1.11788182E-14    2
-5.60326833E+04-4.79836881E+01 9.10833792E-01 4.49883245E-02-5.01607294E-05    3
 2.58755678E-08-5.04053738E-12-5.23196233E+04 2.18428330E+01                   4
ONOCHO                 C   1H   1N   1O   3G   300.000  5000.000 1410.000    21
 1.22840065E+01 2.54240817E-03-9.33422794E-07 1.51922313E-10-9.10868201E-15    2
-2.83490847E+04-3.52608565E+01 8.67680831E-01 3.59748223E-02-3.83580776E-05    3
 1.89460479E-08-3.55203605E-12-2.51378321E+04 2.35246630E+01                   4
HCJOHONO               C   1H   2N   1O   3G   300.000  5000.000 1412.000    21
 1.33706500E+01 3.92433214E-03-1.35842931E-06 2.13037116E-10-1.24604744E-14    2
-1.13311362E+04-4.15839523E+01 2.27239807E+00 3.56275553E-02-3.60086850E-05    3
 1.72430523E-08-3.16347350E-12-8.13553697E+03 1.58365059E+01                   4
OJNHCHO                C   1H   2N   1O   3G   300.000  5000.000 1400.000    11
 1.08734861E+01 6.50228848E-03-2.25178564E-06 3.52675979E-10-2.05918430E-14    2
-2.03343514E+04-2.84424804E+01 1.95323752E+00 2.93851318E-02-2.49049976E-05    3
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 1.05847645E-08-1.78869460E-12-1.74760935E+04 1.86811328E+01                   4
HONJOCHO                C   1H   2N   1O   3G   300.000  5000.000 1401.000    21
 1.17747099E+01 5.21375906E-03-1.78777179E-06 2.78381747E-10-1.61956188E-14    2
-2.12687212E+04-3.21567860E+01 3.44111947E+00 2.68184766E-02-2.32741419E-05    3
 9.97076727E-09-1.68106597E-12-1.86392038E+04 1.17573165E+01                   4
OCHO                    C   1H   1O   2    0G   300.000  5000.000 1381.000    01
 6.68745467E+00 2.95190945E-03-1.05090800E-06 1.67601590E-10-9.90818539E-15    2
-1.85406254E+04-9.43952142E+00 2.80270641E+00 1.18925590E-02-8.84143783E-06    3
 3.23180648E-09-4.70421586E-13-1.71855715E+04 1.14598519E+01                   4
NG        [NG]_NG_IV_BK1C   3H   5N   3O   9G   300.000  5000.000 1679.000    81
 3.17905527E+01 2.15462327E-02-8.14853254E-06 1.35682759E-09-8.27426040E-14    2
-5.11450173E+04-1.21122161E+02 6.91509331E+00 7.78682750E-02-5.33692075E-05    3
 1.65762778E-08-1.87542834E-12-4.28737343E+04 1.23261411E+01                   4
NG1J      [NG1J]_NG_IV_CC   3H   4N   3O   9G   300.000  5000.000 1386.000    81
 3.67990247E+01 1.30405164E-02-4.73086307E-06 7.63951238E-10-4.55546633E-14    2
-2.91978669E+04-1.48407213E+02 8.83903344E+00 8.17316990E-02-6.88117192E-05    3
 2.77108938E-08-4.35242286E-12-2.00057403E+04 2.61786473E-01                   4
NG2J      [NG2J]_NG_IV_CC   3H   4N   3O   9G   300.000  5000.000 1374.000    81
 3.63643586E+01 1.34349717E-02-4.87285191E-06 7.86757584E-10-4.69094409E-14    2
-3.04688559E+04-1.44992375E+02 1.10424592E+01 7.06330837E-02-5.19874518E-05    3
 1.73565477E-08-2.09596494E-12-2.16876660E+04-8.64768101E+00                   4
DICACOJ   6_[DICACOJ]_DIC   3H   5N   2O   7G   300.000  5000.000 1385.000    61
 3.05153592E+01 1.40824518E-02-5.07818536E-06 8.16793469E-10-4.85723777E-14    2
-3.47650348E+04-1.20208144E+02 4.20794521E+00 7.82957908E-02-6.48587921E-05    3
 2.60375324E-08-4.11440660E-12-2.60329333E+04 1.98913671E+01                   4
CACACOJ   9_[CACACOJ]_COC   3H   5N   2O   7G   300.000  5000.000 1380.000    61
 3.04161121E+01 1.43066390E-02-5.18930099E-06 8.37883811E-10-4.99592011E-14    2
-3.53594673E+04-1.21140816E+02 2.35359482E+00 7.94117384E-02-6.11212416E-05    3
 2.18552653E-08-2.94533753E-12-2.57864720E+04 2.93734813E+01                   4
CACACDO   3_[CACACDO][NGC   3H   4N   2O   7G   300.000  5000.000 1398.000    61
 3.13808405E+01 1.07393812E-02-3.91192809E-06 6.33405898E-10-3.78405633E-14    2
-5.08171865E+04-1.27688926E+02 4.21832645E+00 7.89613443E-02-6.88048498E-05    3
 2.83391650E-08-4.51044334E-12-4.20894623E+04 1.61207745E+01                   4
DICACDO   1_[DICACDO][NGC   3H   4N   2O   7G   300.000  5000.000 1387.000    61
 2.92779191E+01 1.25288956E-02-4.52904090E-06 7.29637295E-10-4.34374662E-14    2
-5.16259387E+04-1.13953816E+02 3.06088122E+00 7.98843834E-02-7.14728751E-05    3
 3.11796054E-08-5.35813029E-12-4.32265239E+04 2.45283463E+01                   4
HCOCDOCA  32_[HCOCDOCA][C   3H   3N   1O   5G   300.000  5000.000 1392.000    41
 2.30813845E+01 8.19508699E-03-2.97426305E-06 4.80425740E-10-2.86535960E-14    2
-4.81235439E+04-8.81349233E+01 3.12716159E+00 6.04246823E-02-5.56551631E-05    3
 2.46731882E-08-4.27013370E-12-4.18595469E+04 1.68690708E+01                   4
CDJOCA    48_[CDJOCA]_CDC   2H   2N   1O   4G   300.000  5000.000 1380.000    31
 1.50591976E+01 7.60669565E-03-2.72719133E-06 4.36966971E-10-2.59156551E-14    2
-1.40354249E+04-4.49275887E+01 3.60367542E+00 3.45323936E-02-2.68308746E-05    3
 1.02325623E-08-1.55413751E-12-1.01018471E+04 1.64924927E+01                   4
DICDOCA   22_[DICDOCA][NC   3H   3N   1O   5G   300.000  5000.000 1403.000    41
 2.39744985E+01 7.34620634E-03-2.66029618E-06 4.29123476E-10-2.55707116E-14    2
-4.73493560E+04-9.42016126E+01-5.82383341E-02 7.70462256E-02-8.05202073E-05    3
 3.96634392E-08-7.47106375E-12-4.04655827E+04 2.98840190E+01                   4
HCOCOJCA  51_[HCOCOJCA]_C   3H   4N   1O   5G   300.000  5000.000 1400.000    41
 2.28970349E+01 1.08387954E-02-3.87208293E-06 6.19047052E-10-3.66619218E-14    2
-3.15914496E+04-8.54092617E+01 1.15180629E+00 6.69868000E-02-5.95274230E-05    3
 2.56667302E-08-4.33387938E-12-2.47005913E+04 2.92699151E+01                   4
HCOCACOJ  17_[HCOCACOJ]_C   3H   4N   1O   5G   300.000  5000.000 1390.000    41
 2.14556617E+01 1.20558918E-02-4.28938143E-06 6.83841611E-10-4.04183193E-14    2
-3.02222874E+04-7.71899889E+01 2.79346249E+00 5.78968920E-02-4.75255696E-05    3
 1.92796670E-08-3.11075676E-12-2.40294954E+04 2.21370783E+01                   4
HCOCDOCJA 34_[HCOCDOCJA]C   3H   2N   1O   5G   300.000  5000.000 1405.000    31
 2.19682440E+01 6.97306006E-03-2.54271477E-06 4.12002424E-10-2.46259847E-14    2
-2.94472917E+04-8.24859077E+01 1.02646447E+00 6.29902545E-02-5.98766725E-05    3
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 2.69214472E-08-4.67149148E-12-2.30454657E+04 2.71998617E+01                   4
CDJOCDOCA 35_[CDJOCDOCA]C   3H   2N   1O   5G   300.000  5000.000 1385.000    31
 1.84276000E+01 9.92172196E-03-3.54456620E-06 5.66602984E-10-3.35497656E-14    2
-2.85281891E+04-5.97024161E+01 3.26461282E+00 4.70174413E-02-3.85914778E-05    3
 1.57665098E-08-2.57976007E-12-2.34566887E+04 2.10962443E+01                   4
DICDOCJA  24_[DICDOCJA]_C   3H   2N   1O   5G   300.000  5000.000 1415.000    41
 2.25118000E+01 6.03944140E-03-2.20960690E-06 3.58807693E-10-2.14786147E-14    2
-3.11996251E+04-8.43975158E+01 3.31423651E+00 5.65896691E-02-5.27747746E-05    3
 2.30807809E-08-3.87861591E-12-2.52852211E+04 1.63789292E+01                   4
DICDJOCA  25_[DICDJOCA]_C   3H   2N   1O   5G   300.000  5000.000 1374.000    41
 2.11475408E+01 7.17011333E-03-2.59195048E-06 4.17568260E-10-2.48589317E-14    2
-2.67195130E+04-7.58434453E+01 8.77961876E+00 3.54405169E-02-2.66033117E-05    3
 9.39215478E-09-1.26634511E-12-2.24307450E+04-9.31121536E+00                   4
CDOCACOJ  12A_CDOCONO2COC   3H   4N   1O   5G   300.000  5000.000 1395.000    41
 2.32322319E+01 1.06823475E-02-3.84799937E-06 6.18519692E-10-3.67657476E-14    2
-3.13856595E+04-8.79770656E+01 4.48154783E-01 6.92032620E-02-6.15669182E-05    3
 2.64881035E-08-4.46204482E-12-2.41299776E+04 3.22992281E+01                   4
HCOCONO2  45_[HCOCONO2]_C   2H   3N   1O   4G   300.000  5000.000 1389.000    31
 1.64587490E+01 8.97219876E-03-3.19981071E-06 5.10923846E-10-3.02300047E-14    2
-3.32876739E+04-5.46362076E+01 2.21337648E+00 4.43498011E-02-3.71160218E-05    3
 1.54053400E-08-2.54837362E-12-2.85881131E+04 2.10647711E+01                   4
CJACACOH  16A_CJONO2CDOCC   3H   5N   2O   7G   300.000  5000.000 1402.000    71
 2.94685926E+01 1.37385032E-02-4.77657052E-06 7.50326089E-10-4.39072111E-14    2
-3.65047519E+04-1.12955256E+02 5.32146673E+00 7.82336164E-02-7.12315061E-05    3
 3.18850209E-08-5.59604778E-12-2.90494830E+04 1.36591053E+01                   4
CDOCACOH  12_[CDOCACOH][C   3H   5N   1O   5G   300.000  5000.000 1400.000    51
 2.41709863E+01 1.15249857E-02-4.02655825E-06 6.34304719E-10-3.71828469E-14    2
-5.75786447E+04-9.40987496E+01 2.85153431E+00 7.25114875E-02-7.18599875E-05    3
 3.49017024E-08-6.58086546E-12-5.13249166E+04 1.63811759E+01                   4
CACDOCOJ  14_[CACDOCOJ]_C   3H   4N   1O   5G   300.000  5000.000 1391.000    41
 2.21025308E+01 1.15273747E-02-4.11177389E-06 6.56614178E-10-3.88531887E-14    2
-3.28508314E+04-8.18831713E+01 2.21771044E+00 6.31410447E-02-5.62591180E-05    3
 2.48612358E-08-4.35424256E-12-2.65002987E+04 2.30176059E+01                   4
DICJACDO  1A_DICJONO2CDOC   3H   3N   2O   7G   300.000  5000.000 1386.000    51
 2.75242677E+01 1.18470015E-02-4.28247248E-06 6.89909109E-10-4.10721672E-14    2
-3.13424767E+04-1.04808588E+02 3.65156226E+00 7.13788985E-02-6.12024307E-05    3
 2.54498014E-08-4.16518680E-12-2.35424178E+04 2.18814107E+01                   4
CJACDOCOH 11A_CJONO2CONOC   3H   4N   1O   5G   300.000  5000.000 1405.000    41
 2.11156492E+01 1.17132717E-02-4.03063765E-06 6.28743363E-10-3.66125928E-14    2
-3.86607403E+04-7.56518744E+01 1.96321739E+00 6.37918723E-02-5.87442478E-05    3
 2.67521678E-08-4.77521843E-12-3.28315088E+04 2.44587312E+01                   4
ODCCDOCOH 37_[ODCCDOCOH]C   3H   4O   3    0G   300.000  5000.000 1414.000    31
 1.80922178E+01 7.37963477E-03-2.60942961E-06 4.14835510E-10-2.44863777E-14    2
-5.82762377E+04-6.84278893E+01 8.47707722E-01 5.13597998E-02-4.50160357E-05    3
 1.87183592E-08-3.00190772E-12-5.28226069E+04 2.25994123E+01                   4
CACACDJO  3A_CONO2CONO2CC   3H   3N   2O   7G   300.000  5000.000 1396.000    61
 2.87579835E+01 1.03836158E-02-3.78069816E-06 6.11981894E-10-3.65533688E-14    2
-3.06582883E+04-1.09186553E+02 4.83442686E+00 6.73248632E-02-5.40224699E-05    3
 2.00179814E-08-2.78794465E-12-2.26912497E+04 1.85327407E+01                   4
CACJACDO  3B_CONO2CJONO2C   3H   3N   2O   7G   300.000  5000.000 1380.000    51
 2.83412521E+01 1.11591793E-02-4.04696225E-06 6.53363447E-10-3.89540210E-14    2
-3.07164606E+04-1.10004310E+02 6.45629275E+00 6.21818601E-02-4.82499017E-05    3
 1.74870385E-08-2.40645273E-12-2.32691964E+04 7.29902967E+00                   4
CJACACDO  3C_CJONO2CONO2C   3H   3N   2O   7G   300.000  5000.000 1392.000    61
 2.81004192E+01 1.08763518E-02-3.93437620E-06 6.34132529E-10-3.77642966E-14    2
-2.58519260E+04-1.04545423E+02 3.18919184E+00 7.64008081E-02-7.05787205E-05    3
 3.15710826E-08-5.52664917E-12-1.80405324E+04 2.64689376E+01                   4
ODCJCACOH 20_[ODCJCACOH]C   3H   4N   1O   5G   300.000  5000.000 1400.000    51
 2.36195291E+01 9.45058389E-03-3.31080941E-06 5.22453623E-10-3.06614870E-14    2
-3.85886383E+04-8.90116122E+01 2.78162272E+00 7.30919666E-02-7.84595973E-05    3
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 4.04022134E-08-7.94370898E-12-3.28369007E+04 1.76138025E+01                   4
COHCDO    [COHCDO]_COHCDC   2H   4O   2    0G   300.000  5000.000 1494.000    21
 9.75098946E+00 9.66217861E-03-3.36757878E-06 5.30101564E-10-3.10722665E-14    2
-4.31119186E+04-2.77155212E+01 3.45457001E-01 2.59812170E-02-1.05269047E-05    3
-5.02367723E-10 8.61680595E-13-3.93574474E+04 2.46765312E+01                   4
ODCICDO2  [ODCICDO2]_CDOC   3H   2O   3    0G   300.000  5000.000 1382.000    21
 1.20732619E+01 7.73300416E-03-2.70381548E-06 4.26060745E-10-2.49779691E-14    2
-4.07763355E+04-3.07218527E+01 4.89849412E+00 2.35737858E-02-1.59022207E-05    3
 5.39051954E-09-7.41311134E-13-3.81807922E+04 8.15830834E+00                   4
ODCCDOCOJ 38_[ODCCDOCOJ]C   3H   3O   3    0G   300.000  5000.000 1382.000    21
 1.31408492E+01 9.28247194E-03-3.21792127E-06 5.04181350E-10-2.94404565E-14    2
-2.76068420E+04-3.62338457E+01 5.86182642E+00 2.40831500E-02-1.38420320E-05    3
 3.55330676E-09-2.85086387E-13-2.48567189E+04 3.64434184E+00                   4
DICDOCOJ  27_[DICDOCOJ]_C   3H   3O   3    0G   300.000  5000.000 1374.000    21
 1.34378977E+01 9.04448041E-03-3.13791808E-06 4.91824770E-10-2.87235328E-14    2
-2.69201548E+04-3.85008826E+01 8.46745674E+00 1.71344268E-02-6.47792661E-06    3
 4.88568258E-11 3.38694343E-13-2.48044070E+04-1.04942446E+01                   4
HCOCJONO2 47_[HCOCJONO2]C   2H   2N   1O   4G   300.000  5000.000 1387.000    31
 1.63076789E+01 6.60963053E-03-2.39900630E-06 3.87520865E-10-2.31131218E-14    2
-1.48009746E+04-5.10349082E+01 2.33497221E+00 4.01051214E-02-3.25160527E-05    3
 1.24290743E-08-1.82736099E-12-1.01416639E+04 2.35263799E+01                   4
CDOCOJCOH 29_[CDOCOJCOH]C   3H   5O   3    0G   300.000  5000.000 1405.000    31
 1.58341657E+01 1.12732598E-02-3.81841297E-06 5.88990558E-10-3.40193615E-14    2
-3.91978927E+04-5.30030295E+01 1.67421441E+00 5.12488487E-02-4.77486008E-05    3
 2.25512609E-08-4.19106813E-12-3.49895961E+04 2.05649167E+01                   4
CDOCJACOH 12D_CDOCJONO2CC   3H   4N   1O   5G   300.000  5000.000 1403.000    41
 2.10369511E+01 1.17302538E-02-4.02756835E-06 6.27495379E-10-3.65137323E-14    2
-3.86997633E+04-7.48552361E+01 5.44710137E+00 4.92326451E-02-3.79148252E-05    3
 1.42539905E-08-2.08934876E-12-3.35095302E+04 8.29518859E+00                   4
ODCCDJO    4/ 4/10 THERMC   2H   1O   2    0G   300.000  5000.000 1415.000    01
 7.81525514E+00 4.02150430E-03-1.30901449E-06 1.96668239E-10-1.11562717E-14    2
-9.46292348E+03-1.41721698E+01 1.74810209E+00 2.13338176E-02-2.02387303E-05    3
 9.51144225E-09-1.73690014E-12-7.71019710E+03 1.72310520E+01                   4
OCJCDOCOH 41_[OCJCDOCOH]C   3H   3O   3    0G   300.000  5000.000 1399.000    21
 1.32306752E+01 8.94685700E-03-3.04587725E-06 4.71550476E-10-2.73093590E-14    2
-3.71690524E+04-3.74971443E+01 4.24201161E+00 3.09510544E-02-2.37297114E-05    3
 9.33238167E-09-1.48263634E-12-3.41747458E+04 1.03760498E+01                   4
COHCDJO                 C   2H   3O   2    0G   300.000  5000.000 1393.000    01
 9.35142631E+00 6.95596116E-03-2.41330436E-06 4.05176640E-10-2.53601772E-14    2
-2.19729685E+04-1.96039725E+01 4.20863539E+00 1.95296544E-02-1.44212705E-05    3
 5.72270774E-09-9.40316946E-13-2.02347759E+04 7.83116998E+00                   4
ODCJKIDO                C   3H   1O   3    0G   300.000  5000.000 1381.000    01
 1.30307103E+01 5.42479998E-03-1.95526257E-06 3.14387723E-10-1.86913541E-14    2
-2.88753573E+04-3.91025938E+01 3.60290349E+00 2.77762170E-02-2.20066382E-05    3
 8.40888328E-09-1.26071797E-12-2.56784293E+04 1.13420481E+01                   4
ODCKCJOH  37A_ODCCDOCJOHC   3H   3O   3    0G   300.000  5000.000 1391.000    11
 1.47379258E+01 8.60329122E-03-3.04384973E-06 4.83626506E-10-2.85222632E-14    2
-4.53900896E+04-5.06293206E+01 9.94680663E-01 4.16337513E-02-3.30424009E-05    3
 1.27055346E-08-1.91237883E-12-4.07922665E+04 2.27161010E+01                   4
COHONOKK                C   3H   3N   1O   5G   300.000  5000.000 1410.000    41
 2.46446049E+01 6.85351864E-03-2.50901308E-06 4.07594746E-10-2.44060332E-14    2
-6.56977256E+04-9.82610471E+01 5.80609559E-01 7.28628153E-02-7.17225736E-05    3
 3.31135397E-08-5.86566179E-12-5.85175387E+04 2.71752039E+01                   4
COHOJKK                 C   3H   3O   4    0G   300.000  5000.000 1410.000    31
 1.80530976E+01 6.91276994E-03-2.33534757E-06 3.60083460E-10-2.08076402E-14    2
-5.49213408E+04-6.13522944E+01 2.70196058E+00 5.17526430E-02-5.25413743E-05    3
 2.56215352E-08-4.79547331E-12-5.05762631E+04 1.77607148E+01                   4
COHONOK                 C   2H   3N   1O   4G   300.000  5000.000 1369.000    31
 1.66294866E+01 1.11977321E-02-5.07462258E-06 9.12519618E-10-5.53542619E-14    2
-5.02001079E+04-5.77839366E+01-1.75979717E+00 7.07210084E-02-7.64687174E-05    3
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 3.85000533E-08-7.38160215E-12-4.57046255E+04 3.47219816E+01                   4
COHOJK                  C   2H   3O   3    0G   300.000  5000.000 1413.000    21
 1.36557474E+01 6.00410874E-03-2.02464947E-06 3.11607545E-10-1.79777976E-14    2
-4.11029061E+04-4.33031972E+01 7.26791575E-01 4.46454223E-02-4.62115436E-05    3
 2.29443103E-08-4.35766644E-12-3.75230169E+04 2.30288969E+01                   4
NO2               121286N   1O   2          G  0300.00   5000.00  1000.00     1
 0.04682859E+02 0.02462429E-01-0.01042259E-04 0.01976902E-08-0.01391717E-12    2
 0.02261292E+05 0.09885985E+01 0.02670600E+02 0.07838501E-01-0.08063865E-04    3
 0.06161715E-07-0.02320150E-10 0.02896291E+05 0.01161207E+03                   4
NO                MCB93 N   1O   1    0    0G   200.000  6000.000 1000.000    01
 3.26071234E+00 1.19101135E-03-4.29122646E-07 6.94481463E-11-4.03295681E-15    2
 9.92143132E+03 6.36900518E+00 4.21859896E+00-4.63988124E-03 1.10443049E-05    3
-9.34055507E-09 2.80554874E-12 9.84509964E+03 2.28061001E+00 1.09770882E+04    4
O                 120186O   1              G  0300.00   5000.00  1000.00     1
 0.02542060E+02-0.02755062E-03-0.03102803E-07 0.04551067E-10-0.04368052E-14    2
 0.02923080E+06 0.04920308E+02 0.02946429E+02-0.01638166E-01 0.02421032E-04    3
-0.01602843E-07 0.03890696E-11 0.02914764E+06 0.02963995E+02                   4
N2O               121286N   2O   1          G  0300.00   5000.00  1000.00     1
 0.04718977E+02 0.02873714E-01-0.01197496E-04 0.02250552E-08-0.01575337E-12    2
 0.08165811E+05-0.01657250E+02 0.02543058E+02 0.09492193E-01-0.09792775E-04    3
 0.06263845E-07-0.01901826E-10 0.08765100E+05 0.09511222E+02                   4
H2O                20387H   2O   1          G  0300.00   5000.00  1000.00     1
 0.02672146E+02 0.03056293E-01-0.08730260E-05 0.01200996E-08-0.06391618E-13    2
-0.02989921E+06 0.06862817E+02 0.03386842E+02 0.03474982E-01-0.06354696E-04    3
 0.06968581E-07-0.02506588E-10-0.03020811E+06 0.02590233E+02                   4
N2                121286N   2              G  0300.00   5000.00  1000.00     1
 0.02926640E+02 0.01487977E-01-0.05684761E-05 0.01009704E-08-0.06753351E-13    2
-0.09227977E+04 0.05980528E+02 0.03298677E+02 0.01408240E-01-0.03963222E-04    3
 0.05641515E-07-0.02444855E-10-0.01020900E+05 0.03950372E+02                   4
CO2               121286C   1O   2          G  0300.00   5000.00  1000.00     1
 0.04453623E+02 0.03140169E-01-0.01278411E-04 0.02393997E-08-0.01669033E-12    2
-0.04896696E+06-0.09553959E+01 0.02275725E+02 0.09922072E-01-0.01040911E-03    3
 0.06866687E-07-0.02117280E-10-0.04837314E+06 0.01018849E+03                   4
O2                121386O   2              G  0300.00   5000.00  1000.00     1
 0.03697578E+02 0.06135197E-02-0.01258842E-05 0.01775281E-09-0.01136435E-13    2
-0.01233930E+05 0.03189166E+02 0.03212936E+02 0.01127486E-01-0.05756150E-05    3
 0.01313877E-07-0.08768554E-11-0.01005249E+05 0.06034738E+02                   4
H                 120186H   1              G  0300.00   5000.00  1000.00     1
 0.02500000E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.02547163E+06-0.04601176E+01 0.02500000E+02 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.02547163E+06-0.04601176E+01                   4
HNO       RFITHNO_200_60H   1N   1O   1    0G   300.000  5000.000 1000.00    0 1
 3.32506061D+00 3.28074885D-03-1.17988827D-06 1.90627500D-10-1.14185005D-14    2
 1.16469551D+04 6.44374561D+00 4.30275249D+00-3.27872764D-03 1.00572297D-05    3
-6.51594911D-09 1.03982469D-12 1.16696904D+04 2.60372138D+00                   4
OH          Sand/Rusc01 O   1H   1          G  0300.00   5000.00  1000.00     1
 0.02882730E+02 0.01013974E-01-0.02276877E-05 0.02174684E-09-0.05126305E-14    2
 0.03672089E+05 0.05595712E+02 0.03637266E+02 0.01850910E-02-0.01676165E-04    3
 0.02387203E-07-0.08431442E-11 0.03391983E+05 0.01358860E+02                   4
HONO               31787H   1N   1O   2     G  0300.00   5000.00  1000.00     1
 0.05486893E+02 0.04218065E-01-0.01649143E-04 0.02971877E-08-0.02021148E-12    2
-0.01126865E+06-0.02997002E+02 0.02290413E+02 0.01409922E+00-0.01367872E-03    3
 0.07498780E-07-0.01876905E-10-0.01043195E+06 0.01328077E+03                   4
HCN          McB93/GM94 H   1C   1N   1    0G   200.000  6000.000 1000.000    01
 3.80231733E+00 3.14630009E-03-1.06315698E-06 1.66185395E-10-9.79891789E-15    2
 1.47215128E+04 1.57503584E+00 2.25901123E+00 1.00510591E-02-1.33514911E-05    3
 1.00920882E-08-3.00882048E-12 1.50268794E+04 8.91634590E+00 1.60477053E+04    4
CN                121286C   1N   1          G  0300.00   5000.00  1000.00     1
 0.03720120E+02 0.01518351E-02 0.01987381E-05-0.03798371E-09 0.01328230E-13    2
 0.05111626E+06 0.02888597E+02 0.03663204E+02-0.01156529E-01 0.02163409E-04    3
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 0.01854208E-08-0.08214695E-11 0.05128118E+06 0.03739016E+02                   4
C2N2              121286C   2N   2          G  0300.00   5000.00  1000.00     1
 0.06548003E+02 0.03984707E-01-0.01634216E-04 0.03038597E-08-0.02111069E-12    2
 0.03490716E+06-0.09735790E+02 0.04265459E+02 0.01192257E+00-0.01342014E-03    3
 0.09192297E-07-0.02778942E-10 0.03547888E+06 0.01713212E+02                   4
HNCO         McB93/GM94 H   1N   1C   1O   1G   200.000  6000.000 1000.000    01
 5.29404664E+00 4.03039650E-03-1.41290348E-06 2.24428234E-10-1.32859380E-14    2
-1.61346328E+04-3.08763130E+00 2.24322454E+00 1.44986380E-02-1.52609054E-05    3
 8.36364453E-09-1.72191967E-12-1.53950081E+04 1.21565469E+01-1.42008857E+04    4
NH          McB93/WRA00 N   1H   1    0    0G   200.000  6000.000 1000.000    01
 2.78372645E+00 1.32985886E-03-4.24785565E-07 7.83494425E-11-5.50451298E-15    2
 4.22190438E+04 5.74084857E+00 3.49295037E+00 3.11795722E-04-1.48906628E-06    3
 2.48167403E-09-1.03570916E-12 4.19788215E+04 1.84834974E+00 4.30253623E+04    4
CO                121286C   1O   1          G  0300.00   5000.00  1000.00     1
 0.03025078E+02 0.01442689E-01-0.05630828E-05 0.01018581E-08-0.06910952E-13    2
-0.01426835E+06 0.06108218E+02 0.03262452E+02 0.01511941E-01-0.03881755E-04    3
 0.05581944E-07-0.02474951E-10-0.01431054E+06 0.04848897E+02                   4
H2CN               41687H   2C   1N   1     G  0300.00   4000.00  1000.00     1
 0.05209703E+02 0.02969291E-01-0.02855589E-05-0.01635550E-08 0.03043259E-12    2
 0.02767711E+06-0.04444478E+02 0.02851661E+02 0.05695233E-01 0.01071140E-04    3
-0.01622612E-07-0.02351108E-11 0.02863782E+06 0.08992751E+02                   4
NCNO               92789C   1N   2O   1    0G   300.000  4000.000 1000.00    0 1
 0.73266358E+01 0.17882655E-02-0.20288753E-06-0.94724527E-10 0.18667134E-13    2
 0.36704793E+05-0.10886014E+02 0.49251637E+01 0.53706546E-02 0.27844874E-06    3
-0.21986761E-08 0.46036536E-12 0.37592273E+05 0.24706030E+01                   4
C                 121086C   1               G  0300.00   5000.00  1000.00     1
 0.02602087E+02-0.01787081E-02 0.09087041E-06-0.01149933E-09 0.03310844E-14    2
 0.08542154E+06 0.04195177E+02 0.02498585E+02 0.08085777E-03-0.02697697E-05    3
 0.03040729E-08-0.01106652E-11 0.08545878E+06 0.04753459E+02                   4
N                 120186N   1               G  0300.00   5000.00  1000.00     1
 0.02450268E+02 0.01066146E-02-0.07465337E-06 0.01879652E-09-0.01025984E-13    2
 0.05611604E+06 0.04448758E+02 0.02503071E+02-0.02180018E-03 0.05420529E-06    3
-0.05647560E-09 0.02099904E-12 0.05609890E+06 0.04167566E+02                   4
NO3               121286N   1O   3          G  0300.00   5000.00  1000.00     1
 0.07120307E+02 0.03246228E-01-0.01431613E-04 0.02797053E-08-0.02013008E-12    2
 0.05864479E+05-0.01213730E+03 0.01221076E+02 0.01878797E+00-0.01344321E-03    3
 0.01274601E-07 0.01354060E-10 0.07473144E+05 0.01840203E+03                   4
HO2          McB93/WRA00 H   1O   2    0    0G   200.000  6000.000 1000.000    01
 4.17228728E+00 1.88117647E-03-3.46277408E-07 1.94657853E-11 1.76254294E-16    2
 2.13417795E+02 2.95767746E+00 4.30179801E+00-4.74912051E-03 2.11582891E-05    3
-2.42763894E-08 9.29225124E-12 4.46415539E+02 3.71666245E+00 1.66125750E+03    4
NH2               McB93 N   1H   2    0    0G   200.000  6000.000 1000.000    01
 2.84768992E+00 3.14280035E-03-8.98641458E-07 1.30318284E-10-7.48812926E-15    2
 2.18239049E+04 6.47165433E+00 4.20556857E+00-2.13561363E-03 7.26851301E-06    3
-5.93069876E-09 1.80690978E-12 2.15352231E+04-1.46662770E-01 2.27475415E+04    4
NH3               121386N   1H   3          G  0300.00   5000.00  1000.00     1
 0.02461904E+02 0.06059166E-01-0.02004977E-04 0.03136003E-08-0.01938317E-12    2
-0.06493270E+05 0.07472097E+02 0.02204352E+02 0.01011476E+00-0.01465265E-03    3
 0.01447235E-06-0.05328509E-10-0.06525488E+05 0.08127138E+02                   4
CH                121286C   1H   1          G  0300.00   5000.00  1000.00     1
 0.02196223E+02 0.02340381E-01-0.07058201E-05 0.09007582E-09-0.03855040E-13    2
 0.07086723E+06 0.09178373E+02 0.03200202E+02 0.02072876E-01-0.05134431E-04    3
 0.05733890E-07-0.01955533E-10 0.07045259E+06 0.03331588E+02                   4
HCO          McB93 L12/89H   1C   1O   1    0G   200.000  6000.000 1000.000    01
 3.64896209E+00 3.08090819E-03-1.12429876E-06 1.86308085E-10-1.13951828E-14    2
 3.71209048E+03 5.06147406E+00 4.22118584E+00-3.24392532E-03 1.37799446E-05    3
-1.33144093E-08 4.33768865E-12 3.83956496E+03 3.39437243E+00 5.05141013E+03    4
H2                121286H   2               G  0300.00   5000.00  1000.00     1
 0.02991423E+02 0.07000644E-02-0.05633829E-06-0.09231578E-10 0.01582752E-13    2
-0.08350340E+04-0.01355110E+02 0.03298124E+02 0.08249442E-02-0.08143015E-05    3
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-0.09475434E-09 0.04134872E-11-0.01012521E+05-0.03294094E+02                   4
HCCO               32387H   1C   2O   1     G  0300.00   4000.00  1000.00     1
 0.06758073E+02 0.02000400E-01-0.02027607E-05-0.01041132E-08 0.01965165E-12    2
 0.01901513E+06-0.09071262E+02 0.05047965E+02 0.04453478E-01 0.02268283E-05    3
-0.01482095E-07 0.02250742E-11 0.01965892E+06 0.04818439E+01                   4
H2O2               120186H   2O   2          G  0300.00   5000.00  1000.00     1
 0.04573167E+02 0.04336136E-01-0.01474689E-04 0.02348904E-08-0.01431654E-12    2
-0.01800696E+06 0.05011370E+01 0.03388754E+02 0.06569226E-01-0.01485013E-05    3
-0.04625806E-07 0.02471515E-10-0.01766315E+06 0.06785363E+02                   4
NCN                103190C   1N   2          G  0300.00   4000.00  1500.00     1
 0.06652121E+02 0.06108034E-02-0.01389727E-05 0.02695549E-10 0.01669944E-13    2
 0.05172403E+06-0.01138517E+03 0.03101270E+02 0.09981674E-01-0.09920701E-04    3
 0.04758919E-07-0.08968626E-11 0.05285757E+06 0.07317579E+02                   4
HCNO               120186H   1C   1N   1O   1G  0250.00   4000.00  1000.00     1
 0.06692412E+02 0.02368360E-01-0.02371510E-05-0.01275503E-08 0.02407137E-12    2
 0.01694737E+06-0.01245434E+03 0.03184859E+02 0.09752316E-01-0.01280203E-04    3
-0.06163104E-07 0.03226275E-10 0.01797907E+06 0.06123844E+02                   4
NCO         McB93/WRA98 N   1C   1O   1    0G   200.000  6000.000 1000.000    01
 5.15255717E+00 2.30945594E-03-8.83699519E-07 1.48525346E-10-9.08857905E-15    2
 1.39030086E+04-2.56406350E+00 2.75452392E+00 9.23008037E-03-9.28006629E-06    3
 5.62521381E-09-1.61200144E-12 1.45909290E+04 9.85368773E+00 1.57508051E+04    4
NNH                120186N   2H   1          G  0250.00   4000.00  1000.00     1
 0.04415342E+02 0.01614388E-01-0.01632894E-05-0.08559846E-09 0.01614791E-12    2
 0.02788029E+06 0.09042888E+01 0.03501344E+02 0.02053587E-01 0.07170410E-05    3
 0.04921348E-08-0.09671170E-11 0.02833347E+06 0.06391837E+02                   4
N2H2       RB91/Gurvich N   2H   2    0    0G   200.000  6000.000 1000.00     01
 1.43773356D+00 8.72166734D-03-2.99323466D-06 4.50029732D-10-2.50422693D-14    2
 2.22727357D+04 1.57453260D+01 4.74387065D+00-9.15242446D-03 3.35349897D-05    3
-3.22086920D-08 1.06734098D-11 2.17525597D+04 7.28947240D-01 2.29978160D+04    4
N2H3          DB00/RB91 N   2H   3    0    0G   300.000  5000.000 1385.000    11
 5.56523220E+00 5.92789098E-03-2.05378972E-06 3.21563158E-10-1.87648230E-14    2
 2.40692822E+04-7.11150205E+00 1.68398813E+00 1.46455461E-02-9.84764677E-06    3
 3.66967922E-09-5.99668094E-13 2.54978433E+04 1.39338819E+01 2.65708384E+04    4
N2H4               121286N   2H   4          G  0300.00   5000.00  1000.00     1
 0.04977317E+02 0.09595519E-01-0.03547639E-04 0.06124299E-08-0.04029795E-12    2
 0.09341219E+05-0.02962990E+02 0.06442606E+00 0.02749730E+00-0.02899451E-03    3
 0.01745240E-06-0.04422282E-10 0.01045192E+06 0.02127789E+03                   4
HNC          MEL/LIN92  H   1C   1N   1    0G   300.000  5000.000 1394.000    01
 4.14927436E+00 2.75915497E-03-9.32137975E-07 1.43421369E-10-8.26579656E-15    2
 2.12186267E+04-2.04087166E-02 2.85596031E+00 6.10771202E-03-4.55238112E-06    3
 2.02415456E-09-3.88077938E-13 2.16612862E+04 6.85303990E+00                   4
HOCO               103190C   1H   1O   2     G  0300.00   4000.00  1500.00     1
 0.07517634E+02 0.01259029E-01-0.01910901E-05-0.03136391E-09 0.07547673E-13    2
-0.02634121E+06-0.01448392E+03 0.02285122E+02 0.01351435E+00-0.01160407E-03    3
 0.05047011E-07-0.09032231E-11-0.02448416E+06 0.01367874E+03                   4
HNNO          MELIUS    N   2H   1O   1    0G   300.000  5000.000 1389.000    01
 6.24922910E+00 3.26983002E-03-1.14794284E-06 1.81383141E-10-1.06538637E-14    2
 2.53822106E+04-7.09495778E+00 2.40143922E+00 1.26718648E-02-1.00828306E-05    3
 4.10522736E-09-6.79228705E-13 2.66782646E+04 1.34257436E+01                   4
HNO3               121286H   1N   1O   3     G  0300.00   5000.00  1000.00     1
 0.07003845E+02 0.05811493E-01-0.02333789E-04 0.04288814E-08-0.02959385E-12    2
-0.01889952E+06-0.01047863E+03 0.01353185E+02 0.02220025E+00-0.01978812E-03    3
 0.08773908E-07-0.01658384E-10-0.01738563E+06 0.01851868E+03                   4
CH2                120186C   1H   2          G  0250.00   4000.00  1000.00     1
 0.03636408E+02 0.01933057E-01-0.01687016E-05-0.01009899E-08 0.01808256E-12    2
 0.04534134E+06 0.02156561E+02 0.03762237E+02 0.01159819E-01 0.02489585E-05    3
 0.08800836E-08-0.07332435E-11 0.04536791E+06 0.01712578E+02                   4
CH3                121286C   1H   3          G  0300.00   5000.00  1000.00     1
 0.02844052E+02 0.06137974E-01-0.02230345E-04 0.03785161E-08-0.02452159E-12    2
 0.01643781E+06 0.05452697E+02 0.02430443E+02 0.01112410E+00-0.01680220E-03    3
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 0.01621829E-06-0.05864953E-10 0.01642378E+06 0.06789794E+02                   4
CH2O              L 8/88H   2C   1O   1   00G   200.000  3500.000  1000.000    1
 1.76069008E+00 9.20000082E-03-4.42258813E-06 1.00641212E-09-8.83855640E-14    2
-1.39958323E+04 1.36563230E+01 4.79372315E+00-9.90833369E-03 3.73220008E-05    3
-3.79285261E-08 1.31772652E-11-1.43089567E+04 6.02812900E-01 1.00197170E+04    4
CH4               121286C   1H   4          G  0300.00   5000.00  1000.00     1
 0.01683479E+02 0.01023724E+00-0.03875129E-04 0.06785585E-08-0.04503423E-12    2
-0.01008079E+06 0.09623395E+02 0.07787415E+01 0.01747668E+00-0.02783409E-03    3
 0.03049708E-06-0.01223931E-09-0.09825229E+05 0.01372219E+03                   4
CH2OH             120186H   3C   1O   1     G  0250.00   4000.00  1000.00     1
 0.06327520E+02 0.03608271E-01-0.03201547E-05-0.01938750E-08 0.03509705E-12    2
-0.04474509E+05-0.08329366E+02 0.02862628E+02 0.01001527E+00-0.05285436E-05    3
-0.05138540E-07 0.02246041E-10-0.03349679E+05 0.01039794E+03                   4
CH3O              121686C   1H   3O   1     G  0300.00   3000.00  1000.00     1
 0.03770800E+02 0.07871497E-01-0.02656384E-04 0.03944431E-08-0.02112616E-12    2
 0.01278325E+04 0.02929575E+02 0.02106204E+02 0.07216595E-01 0.05338472E-04    3
-0.07377636E-07 0.02075611E-10 0.09786011E+04 0.01315218E+03                   4
CH3OH             121686C   1H   4O   1     G  0300.00   5000.00  1000.00     1
 0.04029061E+02 0.09376593E-01-0.03050254E-04 0.04358793E-08-0.02224723E-12    2
-0.02615791E+06 0.02378196E+02 0.02660115E+02 0.07341508E-01 0.07170051E-04    3
-0.08793194E-07 0.02390570E-10-0.02535348E+06 0.01123263E+03                   4
C2H                81193C   2H   1          G  0300.00   4000.00  1000.00     1
 0.03986367E+02 0.03143123E-01-0.01267243E-04 0.02924363E-08-0.02716320E-12    2
 0.06655884E+06 0.01191063E+02 0.02737704E+02 0.08048446E-01-0.09244310E-04    3
 0.06525259E-07-0.01939580E-10 0.06683813E+06 0.07300220E+02                   4
C2H2              121386C   2H   2          G  0300.00   5000.00  1000.00     1
 0.04436770E+02 0.05376039E-01-0.01912817E-04 0.03286379E-08-0.02156710E-12    2
 0.02566766E+06-0.02800338E+02 0.02013562E+02 0.01519045E+00-0.01616319E-03    3
 0.09078992E-07-0.01912746E-10 0.02612444E+06 0.08805378E+02                   4
C2H5      12387         C   2H   5N   0O   0G   300.000  5000.000 1460.000    11
 5.57508447E+00 1.05558254E-02-3.55403212E-06 5.46155407E-10-3.14675617E-14    2
 1.10133650E+04-6.48758419E+00 1.60717554E+00 1.33592058E-02 1.85866156E-06    3
-5.67582851E-09 1.66338686E-12 1.30227172E+04 1.70908946E+01                   4
C2H6              121686C   2H   6          G  0300.00   4000.00  1000.00     1
 0.04825938E+02 0.01384043E+00-0.04557259E-04 0.06724967E-08-0.03598161E-12    2
-0.01271779E+06-0.05239507E+02 0.01462539E+02 0.01549467E+00 0.05780507E-04    3
-0.01257832E-06 0.04586267E-10-0.01123918E+06 0.01443229E+03                   4
CH2CO             121686C   2H   2O   1     G  0300.00   5000.00  1000.00     1
 0.06038817E+02 0.05804840E-01-0.01920954E-04 0.02794485E-08-0.01458868E-12    2
-0.08583402E+05-0.07657581E+02 0.02974971E+02 0.01211871E+00-0.02345046E-04    3
-0.06466685E-07 0.03905649E-10-0.07632637E+05 0.08673553E+02                   4
C2H3               12787C   2H   3          G  0300.00   5000.00  1000.00     1
 0.05933468E+02 0.04017746E-01-0.03966740E-05-0.01441267E-08 0.02378644E-12    2
 0.03185435E+06-0.08530313E+02 0.02459276E+02 0.07371476E-01 0.02109873E-04    3
-0.01321642E-07-0.01184784E-10 0.03335225E+06 0.01155620E+03                   4
C2H4              121286C   2H   4          G  0300.00   5000.00  1000.00     1
 0.03528419E+02 0.01148518E+00-0.04418385E-04 0.07844601E-08-0.05266848E-12    2
 0.04428289E+05 0.02230389E+02-0.08614880E+01 0.02796163E+00-0.03388677E-03    3
 0.02785152E-06-0.09737879E-10 0.05573046E+05 0.02421149E+03                   4
HCCOH              32387H   2C   2O   1     G  0300.00   4000.00  1000.00     1
 0.07328324E+02 0.03336416E-01-0.03024705E-05-0.01781106E-08 0.03245168E-12    2
 0.07598258E+05-0.01401214E+03 0.03899465E+02 0.09701075E-01-0.03119309E-05    3
-0.05537732E-07 0.02465732E-10 0.08701190E+05 0.04491875E+02                   4
HNO2      G2MP2//B3DP   C   0H   1N   1O   2G   300.000  5000.000 1432.000    11
 5.86536159E+00 3.31399617E-03-1.19686495E-06 1.92694936E-10-1.14665018E-14    2
-7.43588573E+03-7.16262271E+00 2.33853317E+00 7.87822298E-03-4.64351984E-07    3
-2.66198709E-09 9.09206462E-13-5.88999705E+03 1.30055842E+01                   4
HNOH        JWB/94      N   1H   2O   1    0G   300.000  5000.000 1375.000    11
 5.24159962E+00 3.64132385E-03-1.26199882E-06 1.97647403E-10-1.15363360E-14    2
 8.79675199E+03-2.52971854E+00 3.42226363E+00 6.62639079E-03-2.62136579E-06    3
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 1.83974483E-10 7.81187077E-14 9.57854837E+03 7.72947399E+00                   4
NH2O        M/JB86      N   1H   2O   1    0G   300.000  5000.000 1398.000    01
 4.26222939E+00 4.60071183E-03-1.52686779E-06 2.32081624E-10-1.32607907E-14    2
 6.26937941E+03 1.89523882E+00 2.62132814E+00 8.05594293E-03-4.34199752E-06    3
 1.31067689E-09-1.79413169E-13 6.89825870E+03 1.08768221E+01                   4
C2H4O         Chase98   C   2H   4O   1    0G   300.000  5000.000 1400.000    01
 7.04272994E+00 1.00110676E-02-3.42398623E-06 5.31623557E-10-3.08469387E-14    2
-1.00228712E+04-1.61926118E+01-1.42915337E+00 2.91826985E-02-1.96414512E-05    3
 6.60926623E-09-8.79248471E-13-7.04124488E+03 2.94882584E+01                   4
CH2CHO            SAND86O   1H   3C   2     G   300.000  5000.000  1000.000    1
 0.05975670E+02 0.08130591E-01-0.02743624E-04 0.04070304E-08-0.02176017E-12    2
 0.04903218E+04-0.05045251E+02 0.03409062E+02 0.10738574E-01 0.01891492E-04    3
-0.07158583E-07 0.02867385E-10 0.15214766E+04 0.09558290E+02                   4
CH3CHO            L 8/88C   2H   4O   1     G   200.000  6000.000  1000.000    1
 0.54041108E+01 0.11723059E-01-0.42263137E-05 0.68372451E-09-0.40984863E-13    2
-0.22593122E+05-0.34807917E+01 0.47294595E+01-0.31932858E-02 0.47534921E-04    3
-0.57458611E-07 0.21931112E-10-0.21572878E+05 0.41030159E+01                   4
HOCN              110193H   1C   1N   1O   1G  0300.00   4000.00  1400.00     1
 0.06022112E+02 0.01929530E-01-0.01455029E-05-0.01045811E-08 0.01794814E-12    2
-0.04040321E+05-0.05866433E+02 0.03789424E+02 0.05387981E-01-0.06518270E-05    3
-0.01420164E-07 0.05367969E-11-0.03135335E+05 0.06667052E+02                   4
CH3NHNH2               0C   1H   6N   2    0G   298.150  6000.000 1000.00    0 1
 6.46195602D+00 1.54661452D-02-5.29188310D-06 8.22877488D-10-4.78182997D-14    2
 8.08517920D+03-1.06506405D+01-1.55617356D-01 3.41164172D-02-3.21289044D-05    3
 2.50164209D-08-9.43703969D-12 1.01527490D+04 2.41129608D+01                   4
CH3NH         Burcat-03 C   1H   4N   1    0G   200.000  6000.000  1000.00     1
 0.43023153D+01 0.10277337D-01-0.36593760D-05 0.58702457D-09-0.34979453D-13    2
 0.20473126D+05 0.13025403D+00 0.47462749D+01-0.71705198D-02 0.50242579D-04    3
-0.58589231D-07 0.22243219D-10 0.21124201D+05 0.17162390D+01 0.22559203D+05    4
CH3NNH2                0C   1H   5N   2O   0G   200.000  6000.000 1000.00    0 1
 6.48248625D+00 1.31416200D-02-4.55408099D-06 7.15495219D-10-4.19235501D-14    2
 2.18344199D+04-9.10020638D+00 2.89725447D+00 1.52571928D-02 5.46573210D-06    3
-1.13299263D-08 3.45334525D-12 2.33342324D+04 1.16815443D+01                   4
CH3NNH                 0C   1H   4N   2O   0G   200.000  6000.000 1000.00    0 1
 5.48334026D+00 1.17117818D-02-4.12106147D-06 6.54262200D-10-3.86199590D-14    2
 1.86890527D+04-4.73384237D+00 3.51484036D+00 5.56200324D-03 2.14472257D-05    3
-2.41589770D-08 7.32461054D-12 1.99403457D+04 8.65997982D+00                   4
CH2NH       MELIUS 88   H   3C   1N   1    0G   300.000  5000.000 1577.000    01
 4.54737795E+00 7.17720948E-03-2.47935299E-06 3.87692351E-10-2.26113075E-14    2
 8.64056516E+03-1.16687427E+00 2.81849510E+00 5.11983235E-03 6.38887146E-06    3
-6.61374671E-09 1.65531940E-12 9.88442597E+03 1.03390629E+01 1.09953704E+04    4
CH3NN                  0C   1H   3N   2    0G   200.000  6000.000 1000.00    0 1
 5.67013311D+00 8.94569233D-03-3.14525028D-06 4.98943442D-10-2.94305257D-14    2
 2.57493809D+04-3.74855208D+00 3.61245823D+00 8.93290434D-03 4.69342467D-06    3
-6.90933755D-09 1.61064066D-12 2.67246172D+04 8.61822414D+00                   4
CH3NNCH3        C&S-02  C   2N   2H   6    0G   300.000  4000.000  1000.00     1
 0.49863152E+01 0.24070809E-01-0.10732555E-04 0.22441162E-08-0.17961655E-12    2
 0.15409582E+05-0.15606158E+01 0.19013815E+01 0.27280859E-01-0.53752194E-05    3
-0.57609693E-08 0.23430172E-11 0.16600457E+05 0.15898338E+02 1.83222625E+04    4
N2O4              121286N   2O   4          G  0300.00   5000.00  1000.00     1
 0.01048220E+03 0.05972272E-01-0.02564044E-04 0.04916885E-08-0.03490969E-12    2
-0.02849989E+05-0.02612289E+03 0.03624593E+02 0.02474708E+00-0.02172875E-03    3
 0.09927104E-07-0.02222817E-10-0.09128241E+04 0.09457174E+02                   4
NAMMH                  0C   1H   7N   3O   3G   200.000  6000.000 1000.00    0 1
 1.50959778D+01 2.14520842D-02-7.50972231D-06 1.18712673D-09-6.98257234D-14    2
-1.84746328D+04-4.69501419D+01 5.71540308D+00 3.20207886D-02 4.71338672D-06    3
-1.74429253D-08 5.14898454D-12-1.48390283D+04 6.07362127D+00                   4
CH3NO2            103190C   1H   3N   1O   2G  0300.00   4000.00  1500.00     1
 0.01090158E+03 0.04326381E-01-0.04203548E-05-0.01893071E-08 0.03417444E-12    2
-0.01370862E+06-0.03073183E+03 0.03224717E+01 0.02665147E+00-0.01930574E-03    3
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 0.07762620E-07-0.01398746E-10-0.09597527E+05 0.02726156E+03                   4
CH3NO             103190C   1H   3N   1O   1G  0300.00   4000.00  1500.00     1
 0.08820547E+02 0.03706233E-01-0.02894741E-05-0.01897910E-08 0.03237544E-12    2
 0.05362862E+05-0.02213220E+03 0.02109955E+02 0.01517822E+00-0.07071789E-04    3
 0.01510611E-07-0.01604204E-11 0.08293612E+05 0.01569702E+03                   4
H2CNO2            103190C   1H   2N   1O   2G  0300.00   4000.00  1500.00     1
 0.01127481E+03 0.02584711E-01-0.03934331E-05-0.05614969E-09 0.01392400E-12    2
 0.01360470E+06-0.03461951E+03 0.01165696E+02 0.02890490E+00-0.02817663E-03    3
 0.01387569E-06-0.02727595E-10 0.01694546E+06 0.01888293E+03                   4
CH3ONO            103190C   1H   3N   1O   2G  0300.00   4000.00  1500.00     1
 0.01136129E+03 0.04159349E-01-0.04145670E-05-0.01695140E-08 0.03028732E-12    2
-0.01281482E+06-0.03545435E+03 0.01490345E+02 0.02645433E+00-0.02112332E-03    3
 0.09414399E-07-0.01811205E-10-0.09125782E+05 0.01813766E+03                   4
CHOCHO     2/ 7/ 7      C   2H   2O   2    0G   300.000  5000.000 1386.000    11
 9.75438561E+00 4.97645947E-03-1.74410483E-06 2.75586994E-10-1.61969892E-14    2
-2.95832896E+04-2.61878329E+01 1.88105120E+00 2.36386368E-02-1.83443295E-05    3
 6.84842963E-09-9.92733674E-13-2.69280190E+04 1.59154793E+01                   4
C3H8              L 4/85C   3H   8          G   300.000  5000.000  1000.000    1
 0.75341368E+01 0.18872239E-01-0.62718491E-05 0.91475649E-09-0.47838069E-13    2
-0.16467516E+05-0.17892349E+02 0.93355381E+00 0.26424579E-01 0.61059727E-05    3
-0.21977499E-07 0.95149253E-11-0.13958520E+05 0.19201691E+02                   4
C3H7              L 9/84C   3H   7          G   300.000  5000.000  1000.000    1
 0.77026987E+01 0.16044203E-01-0.52833220E-05 0.76298590E-09-0.39392284E-13    2
 0.82984336E+04-0.15480180E+02 0.10515518E+01 0.25991980E-01 0.23800540E-05    3
-0.19609569E-07 0.93732470E-11 0.10631863E+05 0.21122559E+02                   4
CH3ONO2   CH3ONO2_G3MP2BC   1H   3N   1O   3G   300.000  5000.000 1382.000    21
 1.13980493E+01 8.43730296E-03-2.97734215E-06 4.72072167E-10-2.77953870E-14    2
-1.99184963E+04-3.29755758E+01 2.00735388E+00 2.89172145E-02-1.93690231E-05    3
 6.14043414E-09-7.31614920E-13-1.65357106E+04 1.79360405E+01                   4
CH3OONO   CH3OONO_G4.outC   1H   3N   1O   3G   300.000  5000.000 1494.000    01
 1.21875552E+01 8.17408541E-03-2.79386939E-06 4.34165217E-10-2.52247350E-14    2
-4.81404643E+03-3.43126278E+01 5.48691449E+00 1.95385444E-02-7.35972144E-06    3
-6.65431141E-10 6.93373477E-13-2.11121372E+03 3.10809865E+00                   4
CH3OONOI  CH3OONO_I_BK1.C   1H   3N   1O   3G   300.000  5000.000 1359.000    31
 1.17404835E+01 7.79729216E-03-2.77331328E-06 4.41968769E-10-2.61130780E-14    2
-5.41338875E+03-3.12701889E+01 5.79625109E+00 1.77190906E-02-7.29923824E-06    3
 3.03861648E-10 3.15712663E-13-2.90994810E+03 2.13425651E+00                   4
CH3O2      9/23/96      C   1H   3O   2    0G   300.000  5000.000 1385.000    11
 5.95787891E+00 7.90728626E-03-2.68246234E-06 4.13891337E-10-2.39007330E-14    2
-1.72699146E+03-4.22643302E+00 4.26146906E+00 1.00873599E-02-3.21506184E-06    3
 2.09409266E-10 4.18339104E-14-8.75637340E+02 5.65650904E+00                   4
CH3O2H     9/23/96      C   1H   4O   2    0G   300.000  5000.000 1390.000    21
 8.43117091E+00 8.06817909E-03-2.77094921E-06 4.31332243E-10-2.50692146E-14    2
-1.96678771E+04-1.93032733E+01 3.23442817E+00 1.90129767E-02-1.13386287E-05    3
 3.40306653E-09-4.11830222E-13-1.77197926E+04 9.07002912E+00                   4
C2H5O     1/ 2/97 THERM C   2H   5N   0O   1G   300.000  5000.000 1397.000    11
 7.99494328E+00 1.16435818E-02-4.95527268E-06 9.40395740E-10-6.27179768E-14    2
-6.03840830E+03-1.80274987E+01-2.06105850E+00 3.90869199E-02-3.39343824E-05    3
 1.48663223E-08-2.60789426E-12-2.98499617E+03 3.45061278E+01                   4
CH3CO             120186C   2H   3O   1     G  0300.00   5000.00  1000.00     1
 0.05612279e+02 0.08449886e-01-0.02854147e-04 0.04238376e-08-0.02268404e-12    2
-0.05187863e+05-0.03274949e+02 0.03125278e+02 0.09778220e-01 0.04521448e-04    3
-0.09009462e-07 0.03193718e-10-0.04108508e+05 0.01122885e+03                   4
CDCONO2   CDCONO2_BK1_G3C   2H   3N   1O   3G   300.000  5000.000 1405.000    21
 1.40417680E+01 8.50005220E-03-2.94750572E-06 4.62179339E-10-2.70114913E-14    2
-8.41498031E+03-4.53161830E+01-5.64762170E-01 4.73860351E-02-4.28030522E-05    3
 1.90078671E-08-3.30897487E-12-3.90059834E+03 3.13037825E+01                   4
CONOCDO   CONOCDO_BH_B3GC   2H   3N   1O   3G   300.000  5000.000 1382.000    31
 1.30878363E+01 9.21480731E-03-3.26600326E-06 5.19315520E-10-3.06363437E-14    2
-2.53124989E+04-3.80804493E+01 2.19236648E+00 3.43529991E-02-2.54449832E-05    3
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 9.46261573E-09-1.42638896E-12-2.14956513E+04 2.05511241E+01                   4
CNO2CDO   CNO2CDO_BH_B3GC   2H   3N   1O   3G   300.000  5000.000 1371.000    21
 1.32288746E+01 9.26849853E-03-3.22656841E-06 5.06934833E-10-2.96576108E-14    2
-2.46158782E+04-3.63830375E+01 7.03685016E+00 1.96126610E-02-7.54117304E-06    3
-1.86582837E-10 5.10199439E-13-2.20524759E+04-1.66421396E+00                   4
CDCJONO2  CDCJONO2_BH_M0C   2H   2N   1O   3G   300.000  5000.000 1402.000    11
 1.36529858E+01 6.71971893E-03-2.33498422E-06 3.66637602E-10-2.14480539E-14    2
 2.06425576E+04-4.21413165E+01 1.20749335E+00 4.09753525E-02-3.88019995E-05    3
 1.80063308E-08-3.25998536E-12 2.43932553E+04 2.27723030E+01                   4
CJONOCDO  CJONOCDO_BH_M0C   2H   2N   1O   3G   300.000  5000.000 1375.000    11
 1.34535802E+01 7.24208738E-03-2.59433195E-06 4.15447751E-10-2.46297107E-14    2
-8.09453912E+03-4.08933250E+01 3.65447382E+00 2.90824004E-02-2.07328745E-05    3
 7.08587430E-09-9.41862910E-13-4.60815891E+03 1.20727129E+01                   4
CONOCDJO  CONOCDJO_BH_M0C   2H   2N   1O   3G   300.000  5000.000 1366.000    31
 1.39088821E+01 5.94382215E-03-2.13176154E-06 3.41631286E-10-2.02638895E-14    2
-6.21034387E+03-3.96279186E+01 6.71739835E+00 2.09518687E-02-1.34157463E-05    3
 3.90160946E-09-4.01687769E-13-3.53767575E+03-3.73924051E-01                   4
CJNO2CDO  CJNO2CDO_BH_M0C   2H   2N   1O   3G   300.000  5000.000 1399.000    11
 1.28968517E+01 7.45254331E-03-2.60772639E-06 4.11283037E-10-2.41313131E-14    2
-3.39664734E+03-3.81364573E+01 1.39610524E+00 3.65374276E-02-3.08201666E-05    3
 1.28427252E-08-2.11530240E-12 3.16396708E+02 2.27446553E+01                   4
CNO2CDJO  CNO2CDJO_BH_M0C   2H   2N   1O   3G   300.000  5000.000 1396.000    21
 1.18614720E+01 7.83770281E-03-2.72398742E-06 4.27604948E-10-2.50047534E-14    2
-4.92420844E+03-2.91567336E+01 1.80409610E+00 3.33483988E-02-2.78101648E-05    3
 1.17427155E-08-1.98673347E-12-1.65577401E+03 2.41051570E+01                   4
KDCNOHOJ  ODCDCNOHOJ_BH_C   2H   2N   1O   3G   300.000  5000.000 1396.000    01
-9.65312027E+00 4.32964389E-02-2.40839754E-05 5.09433831E-09-3.56342414E-13    2
 1.00680962E+04 8.79883253E+01 3.53211000E+00 2.98609574E-02-2.75856633E-05    3
 1.22751216E-08-2.23653225E-12 3.10440800E+03 9.95054749E+00                   4
ETONO2    FREQ_CCONO2_I_C   2H   5N   1O   3G   300.000  5000.000 1386.000    31
 1.46515723E+01 1.28951427E-02-4.51624920E-06 7.12471272E-10-4.18026785E-14    2
-2.58655638E+04-4.85145617E+01 1.50837107E+00 4.21061803E-02-2.87403500E-05    3
 9.61518131E-09-1.26461213E-12-2.11697401E+04 2.25733412E+01                   4
CJCONO2                 C   2H   4N   1O   3G   300.000  5000.000 1399.000    01
 1.38517581E+01 1.18591964E-02-4.06013780E-06 6.30897516E-10-3.66300367E-14    2
 2.33167020E+02-4.36638294E+01 1.49800776E+00 4.26286420E-02-3.36922236E-05    3
 1.37060312E-08-2.25507906E-12 4.30675402E+03 2.19629786E+01                   4
YC2JO     YCJ2O_B3GTBas3C   2H   3N   0O   1G   300.000  5000.000 1406.000    01
 6.81683925E+00 7.62002526E-03-2.59113313E-06 4.00752133E-10-2.31905993E-14    2
 1.60615293E+04-1.25713586E+01-6.16869600E-01 2.60165534E-02-2.00834274E-05    3
 7.97480374E-09-1.27809428E-12 1.85154616E+04 2.69449080E+01                   4
COJCONO2  FREQ_COJCONO2_C   2H   4N   1O   4G   300.000  5000.000 1381.000    31
 1.67734530E+01 1.12681466E-02-3.99562895E-06 6.35582533E-10-3.75073915E-14    2
-1.64575681E+04-5.54185115E+01 3.05340507E+00 4.11055238E-02-2.75745073E-05    3
 8.54264158E-09-9.56389649E-13-1.15288168E+04 1.89578134E+01                   4
CQJCONO2  FREQ_CQJCONO2_C   2H   4N   1O   5G   300.000  5000.000 1382.000    51
 2.15148604E+01 9.18513166E-03-3.33580359E-06 5.39057118E-10-3.21599762E-14    2
-1.93264084E+04-7.56925008E+01 2.69814934E+00 5.29722849E-02-4.09820481E-05    3
 1.46458085E-08-1.95953941E-12-1.29355694E+04 2.51594423E+01                   4
CDOCQ     FREQ_CDOCOOH_IC   2H   4O   3    0G   300.000  5000.000 1418.000    31
 1.59083418E+01 6.44259253E-03-2.23012225E-06 3.49619204E-10-2.04405575E-14    2
-3.53786109E+04-5.68289201E+01-7.05853704E-01 5.28285000E-02-5.16967689E-05    3
 2.40768348E-08-4.31137688E-12-3.05034699E+04 2.94836893E+01                   4
CDOCOJ    CDOCOJ_BK1_G3MC   2H   3N   0O   2G   300.000  5000.000 1400.000    11
 9.27571884E+00 7.75575520E-03-2.66050704E-06 4.13950919E-10-2.40557083E-14    2
-1.43202812E+04-2.15954698E+01 7.35801911E-01 2.94411702E-02-2.40116195E-05    3
 1.00523052E-08-1.69503344E-12-1.15462450E+04 2.36230662E+01                   4
CDJOCQ    CDJOCOOH_I_B3GC   2H   3O   3    0G   300.000  5000.000 1407.000    31
 1.48670719E+01 4.65146202E-03-1.57814245E-06 2.43830428E-10-1.41036785E-14    2
-1.58396780E+04-4.86539425E+01 1.59661371E+00 4.76893967E-02-5.44409850E-05    3
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 2.89550619E-08-5.78228861E-12-1.24560480E+04 1.83113216E+01                   4
CCOONO    FREQ_CCOONO_G4C   2H   5N   1O   3G   300.000  5000.000 1372.000    41
 1.52531777E+01 1.20289859E-02-4.23177954E-06 6.69469748E-10-3.93526998E-14    2
-1.05877371E+04-4.81975762E+01 6.75177828E+00 2.78319082E-02-1.41234387E-05    3
 2.85712283E-09-9.87063015E-14-7.16210614E+03-9.85637250E-01                   4
CCOONO_I  FREQ_CCOONO_I_C   2H   5N   1O   3G   300.000  5000.000 1374.000    41
 1.47574518E+01 1.24935145E-02-4.40217099E-06 6.97166259E-10-4.10112045E-14    2
-1.14047761E+04-4.52509519E+01 5.01498966E+00 3.21521432E-02-1.89965715E-05    3
 5.47531077E-09-6.33172616E-13-7.63360176E+03 8.30449907E+00                   4
C2H5O2     1/ 2/97 THERMC   2H   5O   2    0G   300.000  5000.000 1386.000    21
 9.15255914E+00 1.24709284E-02-4.27100650E-06 6.63470012E-10-3.85024363E-14    2
-7.91818201E+03-2.00995359E+01 3.25121168E+00 2.36765869E-02-1.18477606E-05    3
 2.79401564E-09-2.41043601E-13-5.53591951E+03 1.26342679E+01                   4
C2H5OH     3/12/95 tHermC   2H   6O   1    0G   300.000  5000.000 1391.000    11
 7.95264841e+00 1.31574144e-02-4.43693359e-06 6.82201160e-10-3.93096335e-14    2
-3.23602958e+04-1.76537972e+01 4.23149045e-01 2.92858167e-02-1.73845099e-05    3
 5.33639892e-09-6.74917252e-13-2.95683054e+04 2.33538763e+01                   4
SC2H4OH    4/ 3/ 0 tHermC   2H   5O   1    0G   300.000  5000.000 1392.000    21
 7.83524517e+00 1.08808198e-02-3.68694127e-06 5.68601361e-10-3.28288951e-14    2
-1.07534311e+04-1.53495702e+01 1.91496477e+00 2.45693145e-02-1.63075399e-05    3
 6.12282361e-09-1.00784363e-12-8.62161551e+03 1.65987309e+01                   4
HOCHO     HCOOH   103190C   1H   2O   2     G  0300.00   4000.00  1500.00     1
 0.07959698E+02 0.03024532E-01-0.03434242E-05-0.01326767E-08 0.02520240E-12    2
-0.05027445E+06-0.01872208E+03 0.09326031E+01 0.01891002E+00-0.01554964E-03    3
 0.07290031E-07-0.01483695E-10-0.04760071E+06 0.01950653E+03                   4
HOCH2O     4/ 9/98 tHermC   1H   3O   2    0G   300.000  5000.000 1452.000    11
 6.39521515e+00 7.43673043e-03-2.50422354e-06 3.84879712e-10-2.21778689e-14    2
-2.25557758e+04-6.63865583e+00 4.11183145e+00 7.53850697e-03 3.77337370e-06    3
-5.38746005e-09 1.45615887e-12-2.12471918e+04 7.46807254e+00                   4
OCHO       2/14/95 tHermC   1H   1O   2    0G   300.000  5000.000 1690.00     01
 6.12628782e+00 3.75602932e-03-1.42010352e-06 2.36429200e-10-1.44167651e-14    2
-2.17698466e+04-8.01574694e+00 1.35213452e+00 1.50082004e-02-1.09896141e-05    3
 3.73679840e-09-4.81014498e-13-2.02253647e+04 1.74373147e+01                   4
CH3CO2                  C   2H   3O   2    0G   300.000  5000.000 1402.000    01
 8.66668933E+00 8.12452077E-03-2.66950784E-06 4.03691210E-10-2.30057984E-14    2
-2.73530000E+04-1.77978225E+01 9.48577764E-01 2.69496305E-02-2.00635163E-05    3
 7.62275527E-09-1.15644350E-12-2.48005404E+04 2.32904248E+01                   4
PC2H4OH    3/12/95 tHermC   2H   5O   1     G  0300.00   5000.00  1391.00     1
 7.52241939e+00 1.10492715e-02-3.72576465e-06 5.72827397e-10-3.30061759e-14    2
-7.29333590e+03-1.24958732e+01 1.17714711e+00 2.48115685e-02-1.50299503e-05    3
 4.79006785e-09-6.40994211e-13-4.95369043e+03 2.20081586e+01                   4
C2H4O2H    7/27/98 tHermC   2H   5O   2    0G   300.000  5000.000 1388.000    31
 1.11476965e+01 1.04949968e-02-3.62326819e-06 5.66061229e-10-3.29857328e-14    2
-8.35606734e+02-2.87480538e+01 3.40977031e+00 2.65939711e-02-1.57408161e-05    3
 4.41132564e-09-4.49209001e-13 2.05874655e+03 1.35264941e+01                   4
C2H5O2H    7/27/98 tHermC   2H   6O   2    0G   300.000  5000.000 1389.000    31
 1.15361794e+01 1.26680904e-02-4.36302927e-06 6.80516196e-10-3.96092541e-14    2
-2.58990676e+04-3.37584606e+01 2.55448138e+00 3.13447282e-02-1.84312866e-05    3
 5.15917791e-09-5.28572992e-13-2.25353676e+04 1.53197322e+01                   4
O2C2H4OH   2/14/95 tHermC   2H   5O   3    0G   300.000  5000.000 1392.000    31
 1.07432659e+01 1.30957787e-02-4.45370088e-06 6.88548738e-10-3.98230113e-14    2
-2.55911274e+04-2.33254953e+01 4.11839445e+00 2.72240632e-02-1.60824430e-05    3
 5.17033408e-09-7.31610168e-13-2.30857785e+04 1.28482112e+01                   4
C2H5ONO     b3lyp/6-31g*C   2H   5N   1O   2G   300.000  5000.000 1394.000    21
 1.17299657E+01 1.27562764E-02-4.35584164E-06 6.75510485E-10-3.91616614E-14    2
-1.71362413E+04-3.31116039E+01 1.84941267E+00 3.53907948E-02-2.41398149E-05    3
 8.54918027E-09-1.24564972E-12-1.36536655E+04 2.01222696E+01                   4
C2H5NO2     b3lyp/6-31g*C   2H   5N   1O   2G   300.000  5000.000 1391.000    21
 1.07740191E+01 1.35779965E-02-4.64194704E-06 7.20484469E-10-4.17943130E-14    2
-1.80929868E+04-2.85409960E+01 8.60265707E-01 3.50853856E-02-2.19669529E-05    3
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 6.86630898E-09-8.49036070E-13-1.44784977E+04 2.52985528E+01                   4
HN3                 82687H   1N   3          G  0300.00   4000.00  1000.00     1
 0.06023015E+02 0.02454362E-01-0.02404279E-05-0.01322973E-08 0.02474146E-12    2
 0.03394051E+06-0.07015537E+02 0.03621003E+02 0.06030785E-01 0.04054460E-05    3
-0.02545271E-07 0.06174280E-11 0.03482373E+06 0.06333769E+02                   4
N3                121286N   3              G  0300.00   5000.00  1000.00     1
 0.05208505E+02 0.02444507E-01-0.01038941E-04 0.01977417E-08-0.01395644E-12    2
 0.04796178E+06-0.03612756E+02 0.02882219E+02 0.08930338E-01-0.08539038E-04    3
 0.05045585E-07-0.01521248E-10 0.04863468E+06 0.08481757E+02                   4
UREA      DINH2CDO_G4.ouC   1H   4N   2O   1G   300.000  5000.000 1384.000    21
 1.06924114E+01 9.03197857E-03-3.18041785E-06 5.03472894E-10-2.96090144E-14    2
-3.15706761E+04-3.12332635E+01 1.09896186E+00 3.29842120E-02-2.70702970E-05    3
 1.17452535E-08-2.10059659E-12-2.83306555E+04 1.98493573E+01                   4
UREA_R    NH2CDONJH_G4.oC   1H   3N   2O   1G   300.000  5000.000 1404.000    11
 1.01779438E+01 6.93707173E-03-2.36611010E-06 3.66716002E-10-2.12524657E-14    2
-2.67505892E+03-2.63048475E+01 2.10893731E+00 2.84672848E-02-2.47379135E-05    3
 1.10087727E-08-1.95461698E-12-1.56325945E+02 1.60538101E+01                   4
AKNHNO2   NH2CDONHNO2_G4C   1H   3N   3O   3G   300.000  5000.000 1413.000    11
 1.51882443E+01 9.94368482E-03-3.33129729E-06 5.10845889E-10-2.94100342E-14    2
-2.59946005E+04-5.35561801E+01 7.83346325E-01 4.64838523E-02-3.84467378E-05    3
 1.56472290E-08-2.49235247E-12-2.14058927E+04 2.25737511E+01                   4
NHNDOOH   NHNDOOH_G4.outH   2N   2O   2    0G   300.000  5000.000 1408.000    01
 8.52452944E+00 6.05439415E-03-2.02678193E-06 3.10221946E-10-1.78233555E-14    2
 7.12350730E+02-1.96332204E+01 4.65476826E-01 2.89531465E-02-2.72116908E-05    3
 1.28599296E-08-2.38014270E-12 3.07833613E+03 2.21613254E+01                   4
NH2NO2    NH2NO2_G4.out H   2N   2O   2    0G   300.000  5000.000 1418.000    11
 7.27751089E+00 6.28128963E-03-2.02071859E-06 3.00926641E-10-1.69572656E-14    2
-3.23090757E+03-1.27133820E+01 1.32649973E+00 2.19573388E-02-1.78160018E-05    3
 7.48794685E-09-1.25597926E-12-1.38424624E+03 1.85462469E+01                   4
NHNDOOJ   NHNDOOJ_I_G4.oH   1N   2O   2    0G   300.000  5000.000 1403.000    01
 8.38088627E+00 3.90673020E-03-1.34627504E-06 2.10187437E-10-1.22461403E-14    2
 2.34070748E+04-1.62703621E+01 2.41434891E+00 1.99333656E-02-1.80103744E-05    3
 8.10435675E-09-1.43642413E-12 2.52465752E+04 1.49933672E+01                   4
NJNDOOH   NJNDOOH_G4.outH   1N   2O   2    0G   300.000  5000.000 1407.000    01
 8.39160051E+00 3.81971841E-03-1.29942663E-06 2.01151846E-10-1.16512270E-14    2
 2.37930409E+04-1.71433547E+01 1.71936362E+00 2.29140657E-02-2.23909638E-05    3
 1.07332170E-08-1.99564555E-12 2.57325267E+04 1.74015699E+01                   4
NJHKNHNO2 NJHCDONHNO2_I_C   1H   2N   3O   3G   300.000  5000.000 1403.000    01
 1.54238760E+01 8.02123449E-03-2.74804602E-06 4.27457085E-10-2.48439283E-14    2
 6.19264173E+03-5.12081681E+01 1.94594282E+00 4.54119047E-02-4.28837557E-05    3
 1.99933821E-08-3.64133276E-12 1.02286438E+04 1.89920816E+01                   4
AKNHNO    NH2CDONHNO_G4.C   1H   3N   3O   2G   300.000  5000.000 1405.000    01
 1.32947700E+01 9.50038998E-03-3.18543411E-06 4.88136327E-10-2.80694537E-14    2
-1.24232081E+04-4.25328295E+01 1.48918746E+00 4.21981829E-02-3.83398087E-05    3
 1.76885346E-08-3.22160075E-12-8.86883815E+03 1.89983126E+01                   4
HNNOH     ZHNNOH_G4.out H   2N   2O   1    0G   300.000  5000.000 1408.000    01
 6.18343716E+00 5.53975709E-03-1.85812260E-06 2.84733163E-10-1.63704594E-14    2
 8.96889486E+03-8.31777817E+00 1.06506457E+00 1.84281221E-02-1.43549250E-05    3
 5.80640281E-09-9.49315494E-13 1.06349398E+04 1.88095484E+01                   4
ACONODNH  NH2CONODNH_I_GC   1H   3N   3O   2G   300.000  5000.000 1404.000    01
 1.36812586E+01 9.14222104E-03-3.05461489E-06 4.66907563E-10-2.67990149E-14    2
 7.12412764E+02-4.37719489E+01 2.19576266E+00 4.20043658E-02-3.95758518E-05    3
 1.88830772E-08-3.53459484E-12 4.07823125E+03 1.57396399E+01                   4
NH2NO     H2NNO_G4.out  H   2N   2O   1    0G   300.000  5000.000 1393.000    11
 5.58336257E+00 5.09204279E-03-1.73536968E-06 2.83666022E-10-1.73828574E-14    2
 9.12692776E+03-4.61046368E+00 1.64587862E+00 1.47076327E-02-1.09035730E-05    3
 4.33657169E-09-7.13659773E-13 1.04585192E+04 1.63982286E+01                   4
NJHKNHNO  NJHCDONHNO_II_C   1H   2N   3O   2G   300.000  5000.000 1405.000    01
 1.34386799E+01 7.08798652E-03-2.40905719E-06 3.72663423E-10-2.15741564E-14    2
 2.03779850E+04-4.23071249E+01 1.89876520E+00 3.99355900E-02-3.85836860E-05    3
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 1.84185027E-08-3.42222512E-12 2.37576251E+04 1.75151951E+01                   4
NH2OH     NH2OH_G4.out  H   3N   1O   1    0G   300.000  5000.000 1420.000    01
 4.63525852E+00 6.45493945E-03-2.08558973E-06 3.11059157E-10-1.75319478E-14    2
-7.64275787E+03-7.73608271E-01 2.09386013E+00 1.24417866E-02-7.51044198E-06    3
 2.55541054E-09-3.73533556E-13-6.76250551E+03 1.28607110E+01                   4
H2NN       M93/JBPM3 96 N   2H   2    0    0G   300.000  5000.000 1695.000    01
 3.13531032E+00 5.68632569E-03-1.93983467E-06 3.01290501E-10-1.74978144E-14    2
 3.33678346E+04 7.04815840E+00 2.88544262E+00 4.69495999E-03 7.01983230E-07    3
-1.53359038E-09 3.79345858E-13 3.36030690E+04 8.95096779E+00                   4
H2NONO      H2NONO_I_B 0H   2N   2O   2    0G   300.000  5000.000 1000.00    0 1
 1.06022091D+01 2.97922175D-03-4.11380626D-07-7.63555677D-11 1.51623624D-14    2
 7.04965039D+03-2.60694790D+01 4.11092949D+00 2.01979112D-02-2.22550043D-05    3
 1.79199517D-08-6.86493007D-12 9.08973535D+03 8.19506931D+00                   4
H2NNO2         RE-FIT  0H   2N   2O   2    0G   300.000  4500.000 1000.00    0 1
 9.45441628E+00 3.80055304E-03-5.10139330E-07-7.97079347E-11 1.62415349E-14    2
-3.15945020E+03-2.53962326E+01 4.51412708E-01 3.07305455E-02-3.94054223E-05    3
 3.29329026E-08-1.20280756E-11-5.00637573E+02 2.13188362E+01                   4
HOONO     HOONO_G4.out  H   1N   1O   3    0G   300.000  5000.000 1404.000    01
 8.67045892E+00 3.50845701E-03-1.17567986E-06 1.80133633E-10-1.03585545E-14    2
-2.82263590E+03-1.77656079E+01 3.85889794E+00 1.70164941E-02-1.58784450E-05    3
 7.44850623E-09-1.37103894E-12-1.39312875E+03 7.24655237E+00                   4
NH2QJ     NH2QJ_B3GTBas3H   2N   1O   2    0G   300.000  5000.000 1413.000    01
 6.78804822E+00 4.91007717E-03-1.61681265E-06 2.44675423E-10-1.39448536E-14    2
 1.58745596E+04-8.94756826E+00 2.49242794E+00 1.56153048E-02-1.17850476E-05    3
 4.60380239E-09-7.23142624E-13 1.72741990E+04 1.38424043E+01                   4
HNNDOOH_Z     RE-FIT   0H   2N   2O   2    0G   300.000  4500.000 1000.00    0 1
 9.55833721E+00 3.74337588E-03-5.07222978E-07-7.66333663E-11 1.58003832E-14    2
 1.40625635E+03-2.53437691E+01 1.88560843E-01 3.19484882E-02-4.05696737E-05    3
 3.29120518E-08-1.17457684E-11 4.13276953E+03 2.31506348E+01                   4
HNNDOOH       RE-FIT   0H   2N   2O   2    0G   300.000  4500.000 1000.00    0 1
 9.63997173E+00 3.70860961E-03-5.18303239E-07-6.96194283E-11 1.49814243E-14    2
 1.57270654E+03-2.55737362E+01 1.26449108E-01 3.37673463E-02-4.51127307E-05    3
 3.69971254E-08-1.30025522E-11 4.25849072E+03 2.32806358E+01                   4
N2O5      NIST CHASE 199N   2O   5    0    0G   300.000  5000.000 1397.000    01
 1.40972974E+01 4.27467371E-03-1.50087100E-06 2.37166589E-10-1.39312162E-14    2
-3.83999936E+03-4.16508426E+01 2.56982614E+00 4.24349709E-02-4.97133469E-05    3
 2.71882048E-08-5.57217535E-12-9.05347260E+02 1.63675147E+01                   4
HNJNO2    HNJNO2_G4.chk H   1N   2O   2    0G   300.000  5000.000 1393.000    11
 8.58829360E+00 3.55783685E-03-1.37988061E-06 2.34140297E-10-1.42057446E-14    2
 2.48692567E+04-1.72810309E+01 2.38719149E+00 2.06880667E-02-1.97118815E-05    3
 9.16137562E-09-1.66604445E-12 2.67339286E+04 1.50451867E+01                   4
NJH2Q     NJH2Q_II_B3GTBH   2N   1O   2    0G   300.000  5000.000 1411.000    01
 7.28155470E+00 4.47144130E-03-1.45944647E-06 2.19345201E-10-1.24347586E-14    2
 1.57203916E+04-1.09774221E+01 3.16360542E+00 1.64448333E-02-1.49603801E-05    3
 7.10451904E-09-1.33414813E-12 1.69096365E+04 1.02938463E+01                   4
HNOJNO2   HNOJNO2_B3d_B3H   1N   2O   3    0G   300.000  5000.000 1392.000    01
 1.03253946E+01 4.98675264E-03-1.80524376E-06 2.92271754E-10-1.73600960E-14    2
 1.02125162E+04-2.57969338E+01 2.76417845E+00 2.48231368E-02-2.20842798E-05    3
 9.81343839E-09-1.73206394E-12 1.26074164E+04 1.40188663E+01                   4
N2O3      NIST CHASE 199N   2O   3    0    0G   300.000  5000.000 1385.000    01
 9.47187957E+00 3.20342454E-03-1.15394851E-06 1.85472586E-10-1.10239650E-14    2
 6.29102106E+03-1.92801187E+01 3.42941189E+00 1.86131141E-02-1.64162298E-05    3
 7.13285223E-09-1.22878517E-12 8.24651782E+03 1.26913770E+01                   4
ONONO2    t_ONONO2_BHa_BN   2O   4    0    0G   300.000  5000.000 1394.000    01
 1.22043664E+01 3.45851420E-03-1.24871388E-06 2.01018965E-10-1.19612560E-14    2
-4.93024132E+02-3.16697375E+01 4.21575317E+00 2.46409530E-02-2.29584816E-05    3
 1.03444807E-08-1.82063749E-12 1.99316683E+03 1.02809212E+01                   4
HONNH     HONNH_G4      H   2N   2O   1    0G   300.000  5000.000 1410.000    01
 6.28422378E+00 5.37598499E-03-1.78502698E-06 2.71645903E-10-1.55420951E-14    2
 6.70148292E+03-8.61273360E+00 1.39096839E+00 1.79340781E-02-1.42097587E-05    3
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 5.87052739E-09-9.78695345E-13 8.26845062E+03 1.72339344E+01                   4
O3                121286O   3               G  0300.00   5000.00  1000.00     1
 0.05429371E+02 0.01820380E-01-0.07705607E-05 0.01499293E-08-0.01075563E-12    2
 0.01523527E+06-0.03266387E+02 0.02462609E+02 0.09582781E-01-0.07087359E-04    3
 0.01363368E-07 0.02969647E-11 0.01606152E+06 0.01214187E+03                   4
CH2(S)             31287C   1H   2          G  0300.00   4000.00  1000.00     1
 0.03552889E+02 0.02066788E-01-0.01914116E-05-0.01104673E-08 0.02021350E-12    2
 0.04984975E+06 0.01686570E+02 0.03971265E+02-0.01699089E-02 0.01025369E-04    3
 0.02492551E-07-0.01981266E-10 0.04989368E+06 0.05753207E+00                   4
CH3N(NH2)NO2           0C   1H   5N   3O   2G   200.000  6000.000 1000.00    0 1
 1.21984835D+01 1.62617248D-02-5.71988812D-06 9.08210118D-10-5.36252527D-14    2
 6.79844434D+03-3.67869301D+01 2.88978982D+00 3.53801027D-02-1.65682595D-05    3
 2.48456899D-09-5.91301368D-13 9.87751953D+03 1.34300222D+01                   4
CH3N(NH2)ONO           0C   1H   5N   3O   2G   200.000  6000.000 1000.00    0 1
 1.30544300D+01 1.54322572D-02-5.40527844D-06 8.55610804D-10-5.04036781D-14    2
 1.38417080D+04-4.07214851D+01 2.03535080D+00 4.72689942D-02-4.53003959D-05    3
 2.92119520D-08-9.32928127D-12 1.70074824D+04 1.63740444D+01                   4
ACCJA                  C   2H   3N   2O   6G   300.000  5000.000 1386.000    01
 1.86910132E+01 1.80443954E-02-8.07957324E-06 1.52616905E-09-9.95108875E-14    2
-1.08160042E+04-5.66085026E+01 9.98953377E-01 7.03029807E-02-6.66538442E-05    3
 3.08745239E-08-5.61607056E-12-5.93685691E+03 3.42517321E+01                   4
Y3COCA                 C   2H   3N   1O   4G   300.000  5000.000 1451.000    01
 1.68115792E+01 9.78948072E-03-3.45294759E-06 5.47901688E-10-3.22948472E-14    2
-2.52265373E+04-6.14702701E+01 2.54040884E+00 3.91378691E-02-2.35751154E-05    3
 5.18530257E-09-5.82503482E-14-2.00291603E+04 1.63285136E+01                   4
Y3COCOJ                C   2H   3O   2    0G   300.000  5000.000 1401.000    01
 9.17383335E+00 8.22812313E-03-2.81507219E-06 4.37221828E-10-2.53766092E-14    2
-1.03631874E+04-2.37823010E+01-1.29779828E-01 3.23807857E-02-2.71929856E-05    3
 1.17196115E-08-2.02680010E-12-7.39285304E+03 2.52943587E+01                   4
HOYCCO                 C   2H   4O   2    0G   300.000  5000.000 1418.000    01
 9.24063528E+00 9.80909716E-03-3.17075113E-06 4.73865566E-10-2.67729880E-14    2
-3.36102874E+04-2.41243631E+01-5.84104386E-01 3.55391645E-02-2.89141357E-05    3
 1.20968983E-08-2.01472680E-12-3.05488976E+04 2.75327581E+01                   4
CJOCDO                 C   2H   3O   2    0G   300.000  5000.000 1460.000    01
 1.08037367E+01 7.08996206E-03-2.48244812E-06 3.91976878E-10-2.30254771E-14    2
-2.41177064E+04-3.02291920E+01 3.15810251E+00 2.05547121E-02-8.59630180E-06    3
-3.19285417E-10 6.88498091E-13-2.10995109E+04 1.22655826E+01                   4
HOYCJCO                C   2H   3O   2    0G   300.000  5000.000 1393.000    01
 9.37106475E+00 7.84114656E-03-2.95589992E-06 5.12247312E-10-3.22484874E-14    2
-8.30584148E+03-2.34768760E+01 1.19797435E+00 2.90866328E-02-2.44729181E-05    3
 1.05281226E-08-1.82292888E-12-5.69629080E+03 1.96324341E+01                   4
CJCDOOH                C   2H   3O   2    0G   300.000  5000.000 1408.000    01
 9.92268798E+00 7.12175837E-03-2.33698653E-06 3.53122426E-10-2.01136310E-14    2
-3.42214024E+04-2.58304681E+01 7.81452443E-01 3.20323232E-02-2.84753333E-05    3
 1.27826432E-08-2.26150853E-12-3.14545057E+04 2.19152825E+01                   4
HOYCCJO                C   2H   3O   2    0G   300.000  5000.000 1393.000    01
 9.45126897E+00 7.85895317E-03-3.01074991E-06 5.27488064E-10-3.34089308E-14    2
-8.25767435E+03-2.42588526E+01 1.20153762E+00 2.94790106E-02-2.50682496E-05    3
 1.08554718E-08-1.88783739E-12-5.64472445E+03 1.91866823E+01                   4
CJOHCDO                C   2H   3O   2    0G   300.000  5000.000 1395.000    01
 9.44921414E+00 7.74500666E-03-2.60081773E-06 3.99391492E-10-2.30137072E-14    2
-2.91259253E+04-2.47737731E+01 8.11786303E-01 2.79549459E-02-2.02061959E-05    3
 7.15156504E-09-9.80241885E-13-2.61913594E+04 2.15004101E+01                   4
COCDO                  C   2H   4O   2    0G   300.000  5000.000 1463.000    01
 9.23259738E+00 1.05475892E-02-3.58559093E-06 5.55173899E-10-3.21739348E-14    2
-4.76258476E+04-2.25965404E+01 7.93074690E-01 2.48049082E-02-9.12231430E-06    3
-1.03961513E-09 9.33858527E-13-4.42260474E+04 2.45378489E+01                   4
COCDJO                 C   2H   3O   2    0G   300.000  5000.000 1541.000    01
 7.73793939E+00 8.89639270E-03-2.93211762E-06 4.44309261E-10-2.53559030E-14    2
-2.29909114E+04-1.21558332E+01 2.53422865E+00 1.79992156E-02-7.09392427E-06    3
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 3.41229579E-11 4.28677995E-13-2.09144223E+04 1.68146636E+01                   4
CCDOOH                   C   2H   4O   2    0G   300.000  5000.000 1406.000    01
 8.47880563E+00 1.04358500E-02-3.38181696E-06 5.06226275E-10-2.86319822E-14    2
-5.69628340E+04-1.79972281E+01 3.13389685E-01 3.06447963E-02-2.24672836E-05    3
 8.65714199E-09-1.35274380E-12-5.42830370E+04 2.53824436E+01                   4
C2H2OH    CDJCOH_B3GTBasC   2H   3O   1    0G   300.000  5000.000 1391.000    11
 9.34909932E+00 5.25044090E-03-1.82394986E-06 2.86589639E-10-1.67805710E-14    2
 1.15682550E+04-2.53098042E+01 1.26743959E+00 2.39821817E-02-1.78083709E-05    3
 6.19704804E-09-8.05764086E-13 1.43181570E+04 1.80275157E+01                   4
SC2H2OH    9/25/15      C   2H   3O   1    0G   300.000  5000.000 1410.000    11
+7.99235139E+00+5.83109353E-03-1.89242965E-06+2.83129118E-10-1.59933287E-14    2
+9.51237374E+03-1.62058375E+01+1.63791895E+00+2.64968839E-02-2.74821415E-05    3
+1.43110557E-08-2.85794966E-12+1.11467016E+04+1.58714777E+01+0.00000000E+00    4
OH*                      C   0H   1N   0O   1G   300.000  5000.000 1360.000    01
 2.34769505E+00 1.68959247E-03-4.96196365E-07 6.44214778E-11-3.12846870E-15    2
 5.05933255E+04 8.74832296E+00 3.79519890E+00-9.60320738E-04 1.07935821E-06    3
-2.21198282E-10-1.46184056E-14 5.00092499E+04 7.00359228E-01                   4
HE                120186HE  1               G  0300.00   5000.00  1000.00     1
 0.02500000E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-0.07453750E+04 0.09153489E+01 0.02500000E+02 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-0.07453750E+04 0.09153488E+01                   4
AR                120186AR  1               G  0300.00   5000.00  1000.00     1
 0.02500000E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-0.07453750E+04 0.04366001E+02 0.02500000E+02 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-0.07453750E+04 0.04366001E+02                   4
H2NCHO    H2NCHO_BH_B3LYC   1H   3N   1O   1G   300.000  5000.000 1398.000    01
 6.53544538E+00 7.60189660E-03-2.52847333E-06 3.85128016E-10-2.20452362E-14    2
-2.41589832E+04-9.39315303E+00 2.19118782E+00 1.71525883E-02-1.03704040E-05    3
 3.23947452E-09-4.09547394E-13-2.25884461E+04 1.41531425E+01                   4
C3H3       9/29/ 9 THERMC   3H   3    0    0G   300.000  5000.000 1395.000    01
 7.33864676E+00 7.21591641E-03-2.45847585E-06 3.80595652E-10-2.20344486E-14    2
 3.78839243E+04-1.52993244E+01 1.97162626E+00 2.08254354E-02-1.62243553E-05    3
 6.91470764E-09-1.22819424E-12 3.96736606E+04 1.31996920E+01                   4
CDCJCDO   CDCJCDO_I_BH_BC   3H   3O   1    0G   300.000  5000.000 1394.000    01
 9.16948946E+00 8.26011971E-03-2.83138627E-06 4.40239395E-10-2.55688961E-14    2
 1.63611269E+04-2.19787415E+01 2.06423047E+00 2.53895107E-02-1.89080978E-05    3
 7.42682956E-09-1.20612383E-12 1.87864637E+04 1.60108083E+01                   4
H2CC              L12/89H   2C   2    0    0G   200.000  6000.000  1000.000    1
 0.42780340E+01 0.47562804E-02-0.16301009E-05 0.25462806E-09-0.14886379E-13    2
 0.48316688E+05 0.64023701E+00 0.32815483E+01 0.69764791E-02-0.23855244E-05    3
-0.12104432E-08 0.98189545E-12 0.48621794E+05 0.59203910E+01 0.49887266E+05    4
VCDO      VCDO_G3MP2_G3_C   3H   4N   0O   1G   300.000  5000.000 1392.000    01
 9.39918255E+00 1.01168249E-02-3.36959545E-06 5.14172946E-10-2.94835284E-14    2
-1.23594302E+04-2.47300373E+01 1.13047846E+00 2.92269879E-02-1.99974542E-05    3
 6.98466320E-09-9.79237748E-13-9.49490843E+03 1.97052158E+01                   4
VCDJO     VCDJO_G3MP2_G3C   3H   3N   0O   1G   300.000  5000.000 1403.000    01
 8.76612341E+00 7.77928992E-03-2.49026790E-06 3.69252827E-10-2.07329959E-14    2
 7.79908556E+03-1.86491247E+01 2.10804239E+00 2.79698291E-02-2.62572868E-05    3
 1.29707093E-08-2.52092364E-12 9.65945852E+03 1.54835048E+01                   4
VJCDO     VCDO_+VIN     C   3H   3N   0O   1G   300.000  5000.000 1395.000    01
 9.34060960E+00 7.65330442E-03-2.52804099E-06 3.83705175E-10-2.19238512E-14    2
 1.77304831E+04-2.25416414E+01 1.89761455E+00 2.64954324E-02-2.09589509E-05    3
 8.62975143E-09-1.43738860E-12 2.01465708E+04 1.68774509E+01                   4
CDCOH     SmallC_OH_OJ_QC   2H   4N   0O   1G   300.000  5000.000 1410.000    11
 9.77956215E+00 6.84812705E-03-2.24091841E-06 3.37327909E-10-1.91426269E-14    2
-1.89257556E+04-2.92498906E+01-2.40062821E+00 4.77910119E-02-5.39966347E-05    3
 2.90602124E-08-5.88121059E-12-1.59381982E+04 3.17448264E+01                   4
CACACOONO                C   3H   5N   3O   9G   300.000  5000.000 1398.000    01
3.32789518E+01 2.13657403E-02-7.46467185E-06 1.17607053E-09-6.89524669E-14    2
-3.85446861E+04-1.43478361E+02 5.98806506E-01 1.05488581E-01-9.10328773E-05    3
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 3.90510284E-08-6.63538551E-12-2.81077518E+04 2.90523541E+01                   4
CACACQJ                 C   3H   5N   2O   8G   300.000  5000.000 1399.000    01
 2.87733204E+01 1.99781800E-02-6.95867503E-06 1.09414324E-09-6.40598993E-14    2
-3.45876565E+04-1.20113095E+02 5.73380652E-02 9.24809249E-02-7.73047832E-05    3
 3.21587787E-08-5.30925182E-12-2.52872258E+04 3.19710541E+01                   4
DICACOONO               C   3H   5N   3O   9G   300.000  5000.000 1398.000    01
 3.32070410E+01 2.14299058E-02-7.48744073E-06 1.17968689E-09-6.91654363E-14    2
-3.83204493E+04-1.39260568E+02 9.81300107E-01 1.03726642E-01-8.84800288E-05    3
 3.75231956E-08-6.30857134E-12-2.79668931E+04 3.10974661E+01                   4
DICACQJ                 C   3H   5N   2O   8G   300.000  5000.000 1398.000    01
 2.82371381E+01 2.03716159E-02-7.08073630E-06 1.11177760E-09-6.50293844E-14    2
-3.41158200E+04-1.14435212E+02 8.28454776E-01 8.79858891E-02-7.08399967E-05    3
 2.83777261E-08-4.51617489E-12-2.50855303E+04 3.12792462E+01                   4
CACACONO                C   3H   5N   3O   8G   300.000  5000.000 1398.000    01
 3.07138893E+01 2.09668937E-02-7.31986268E-06 1.15265674E-09-6.75545540E-14    2
-4.52711522E+04-1.29976175E+02 3.90908834E-01 9.75023055E-02-8.16287121E-05    3
 3.40230114E-08-5.63185676E-12-3.54393116E+04 3.06420299E+01                   4
DICACONO                C   3H   5N   3O   8G   300.000  5000.000 1397.000    01
 3.07079963E+01 2.09610758E-02-7.31533278E-06 1.15167638E-09-6.74860754E-14    2
-4.51510786E+04-1.26439729E+02 1.07318223E+00 9.52451368E-02-7.88803872E-05    3
 3.25552108E-08-5.34250737E-12-3.54884338E+04 3.07200415E+01                   4
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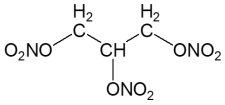
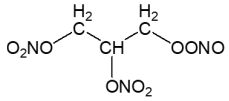
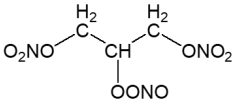
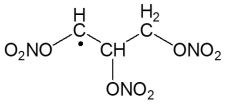
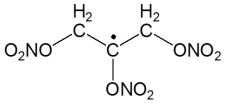
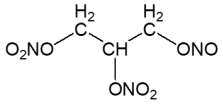
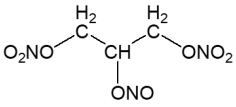
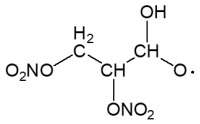
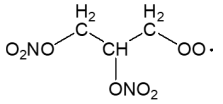
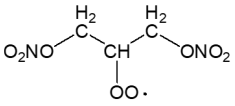
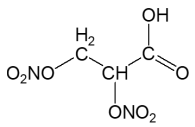
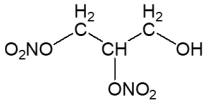
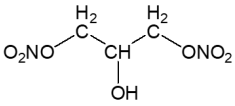
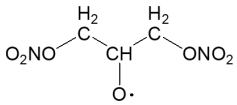
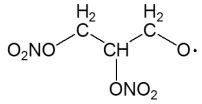
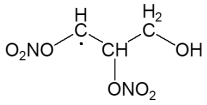
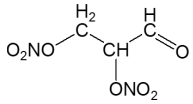
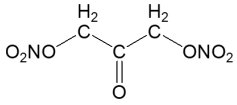
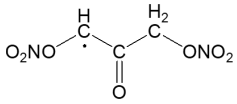
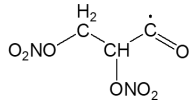
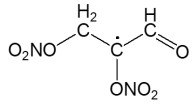
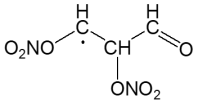
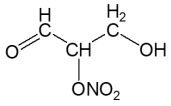
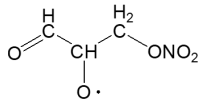
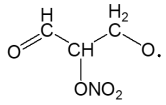
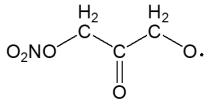
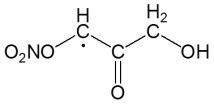
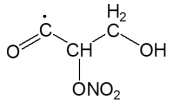
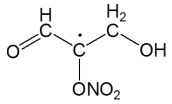
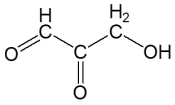
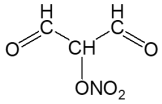
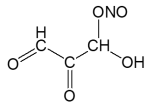
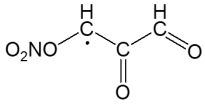
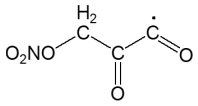
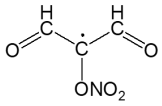
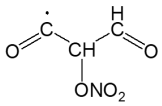
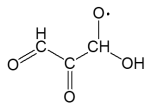
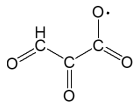
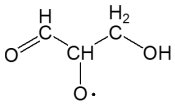
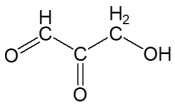
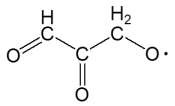
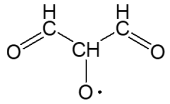
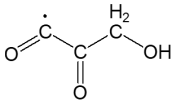
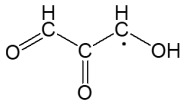
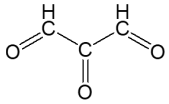
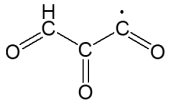
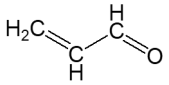
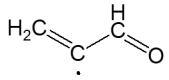
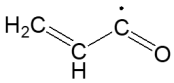
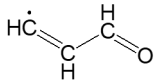
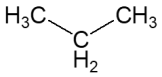
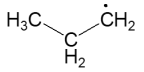
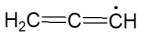
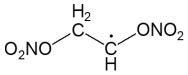
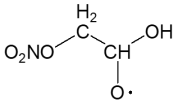
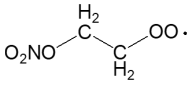
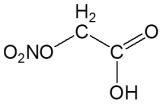
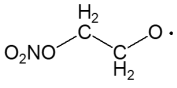
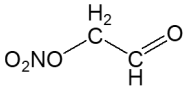
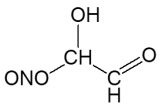
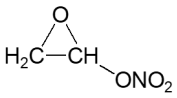
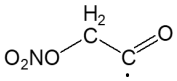
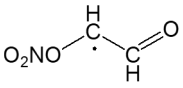
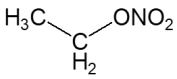
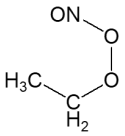
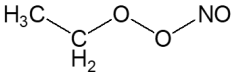
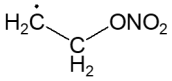
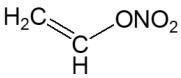
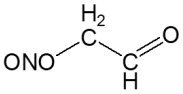
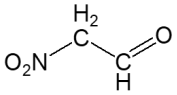
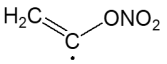
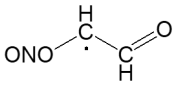
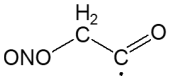
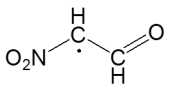
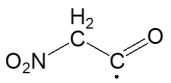
Table A-3 Molecular structures of species in the NG mechanism

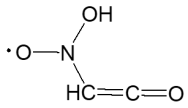
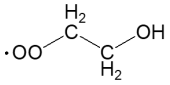
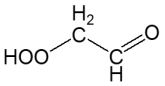
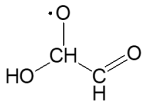
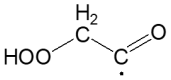
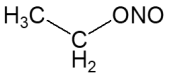
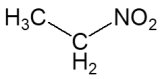
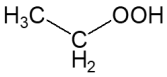
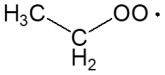
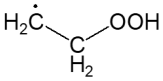
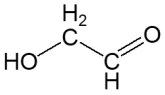
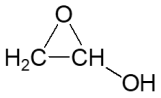
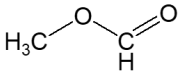
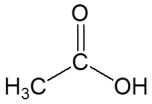
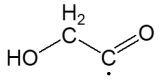
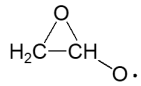
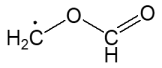
Species	Structure	Molecule weight	C	H	O	N
NG		227.088	3	5	3	9
CACACOONO		227.088	3	5	3	9
DICACOONO		227.088	3	5	3	9
NG1J		226.08	3	4	3	9
NG2J		226.08	3	4	3	9
CACACONO		211.0886	3	5	3	8
DICACONO		211.0886	3	5	3	8
CACACDOOJ		197.0819	3	5	2	8
CACACQJ		197.0819	3	5	2	8
DICACQJ		197.0819	3	5	2	8
CACACDOOH		196.0739	3	4	2	8
CACACOH		182.0905	3	6	2	7
DICACOH		182.0905	3	6	2	7

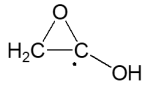
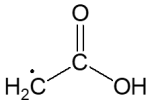
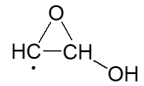
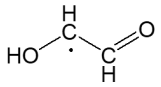
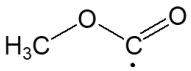
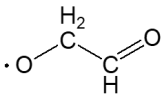
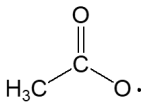
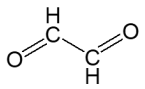
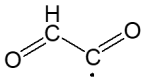
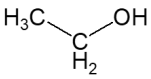
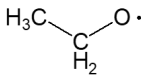
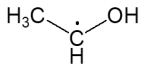
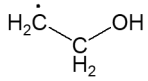
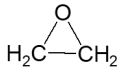
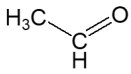
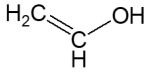
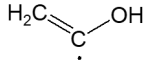
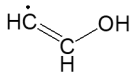
DICACOJ		181.0825	3	5	2	7
CACACOJ		181.0825	3	5	2	7
CJACACOH		181.0825	3	5	2	7
CACACDO		180.0745	3	4	2	7
DICACDO		180.0745	3	4	2	7
DICJACDO		179.0666	3	3	2	7
CACACDJO		179.0666	3	3	2	7
CACJACDO		179.0666	3	3	2	7
CJACACDO		179.0666	3	3	2	7
CDOCACOH		135.077	3	5	1	5
HCOCOJCA		134.069	3	4	1	5
HCOCACOJ		134.069	3	4	1	5
CACDOCOJ		134.069	3	4	1	5
CJACDOCOH		134.069	3	4	1	5

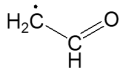
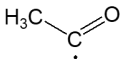
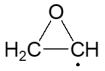
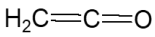
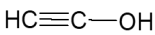
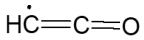
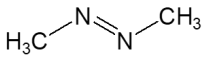
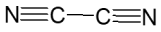
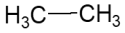
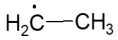
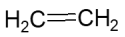
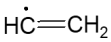
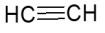
ODCJCACOH		134.069	3	4	1	5
CDOCJACOH		134.069	3	4	1	5
HCOCDOCA		133.0611	3	3	1	5
DICDOCA		133.0611	3	3	1	5
COHONOKK		133.0611	3	3	1	5
HCOCDOCJA		132.0531	3	2	1	5
CDJOCDOCA		132.0531	3	2	1	5
DICDOCJA		132.0531	3	2	1	5
DICDJOCA		132.0531	3	2	1	5
COHOJKK		103.055	3	3	0	4
KIDOCDOOJ		101.039	3	1	0	4
CDOCOJCOH		89.0715	3	5	0	3
ODCCDOCOH		88.06353	3	4	0	3
ODCCDOCOJ		87.05556	3	3	0	3

DICDOCOJ		87.05556	3	3	0	3
OCJCDOCOH		87.05556	3	3	0	3
ODCKCJOH		87.05556	3	3	0	3
ODCICDO2		86.04759	3	2	0	3
ODCJKIDO		85.03962	3	1	0	3
VCDO		56.06473	3	4	0	1
CDCJCDO		55.05676	3	3	0	1
VCDJO		55.05676	3	3	0	1
VJCDO		55.05676	3	3	0	1
C3H8		44.09721	3	8	0	0
C3H7		43.08924	3	7	0	0
C3H3		39.05736	3	3	0	0
ACCJA		151.056	2	3	2	6
CDOOJA		122.0579	2	4	1	5
CQJCONO2		122.0579	2	4	1	5
CDOOHA		121.0499	2	3	1	5
COJCONO2		106.0585	2	4	1	4

HCOCONO2		105.0505	2	3	1	4
COHONOK		105.0505	2	3	1	4
Y3COCA		105.0505	2	3	1	4
CDJOCA		104.0425	2	2	1	4
HCOCJONO2		104.0425	2	2	1	4
ETONO2		91.06705	2	5	1	3
CCOONO		91.06705	2	5	1	3
CCOONO_I		91.06705	2	5	1	3
CJCONO2		90.05908	2	4	1	3
CDCONO2		89.05111	2	3	1	3
CONOCDO		89.05111	2	3	1	3
CNO2CDO		89.05111	2	3	1	3
CDCJONO2		88.04314	2	2	1	3
CJONOCDO		88.04314	2	2	1	3
CONOCDJO		88.04314	2	2	1	3
CJNO2CDO		88.04314	2	2	1	3
CNO2CDJO		88.04314	2	2	1	3

KDCNOHOJ		88.04314	2	2	1	3
O2C2H4OH		77.06035	2	5	0	3
CDOCQ		76.05238	2	4	0	3
COHOJK		75.04441	2	3	0	3
CDJOCQ		75.04441	2	3	0	3
C2H5ONO		75.06765	2	5	1	2
C2H5NO2		75.06765	2	5	1	2
C2H5O2H		62.06892	2	6	0	2
C2H5O2		61.06095	2	5	0	2
C2H4O2H		61.06095	2	5	0	2
COHCDO		60.05298	2	4	0	2
HOYCCO		60.05298	2	4	0	2
COCDO		60.05298	2	4	0	2
CCDOOH		60.05298	2	4	0	2
COHCDJO		59.04501	2	3	0	2
Y3COCOJ		59.04501	2	3	0	2
CJOCDO		59.04501	2	3	0	2

HOYCJCO		59.04501	2	3	0	2
CJCDOOH		59.04501	2	3	0	2
HOYCCJO		59.04501	2	3	0	2
CJOHCDO		59.04501	2	3	0	2
COCDJO		59.04501	2	3	0	2
CDOCOJ		59.04501	2	3	0	2
CH3CO2		59.04501	2	3	0	2
CHOCHO		58.03704	2	2	0	2
ODCCDJO		57.02907	2	1	0	2
C2H5OH		46.06952	2	6	0	1
C2H5O		45.06155	2	5	0	1
SC2H4OH		45.06155	2	5	0	1
PC2H4OH		45.06155	2	5	0	1
C2H4O		44.05358	2	4	0	1
CH3CHO		44.05358	2	4	0	1
CDCOH		44.05358	2	4	0	1
C2H2OH		43.04561	2	3	0	1
SC2H2OH		43.04561	2	3	0	1

CH2CHO		43.04561	2	3	0	1
CH3CO		43.04561	2	3	0	1
YC2JO		43.04561	2	3	0	1
CH2CO		42.03764	2	2	0	1
HCCOH		42.03764	2	2	0	1
HCCO		41.02967	2	1	0	1
CH3NNCH3		58.08352	2	6	2	0
C2N2		52.0357	2	0	2	0
C2H6		30.07012	2	6	0	0
C2H5		29.06215	2	5	0	0
C2H4		28.05418	2	4	0	0
C2H3		27.04621	2	3	0	0
C2H2		26.03824	2	2	0	0
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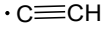
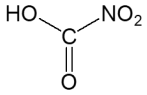
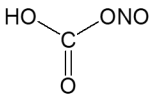
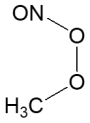
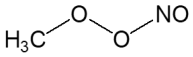
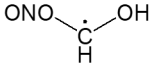
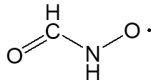
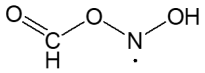
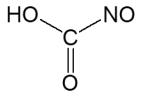
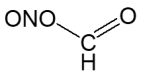
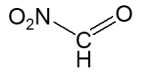
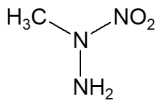
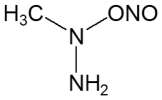
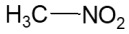
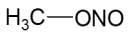
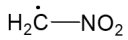
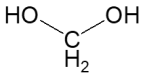
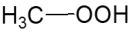
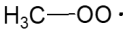
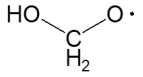
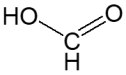
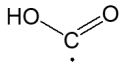
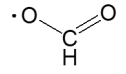
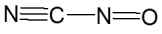
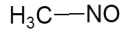
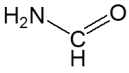
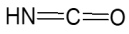
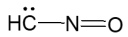
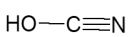
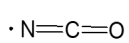
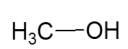
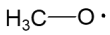
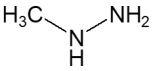
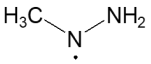
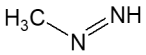
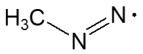
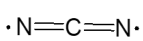
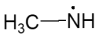
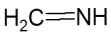
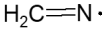
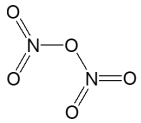
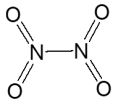
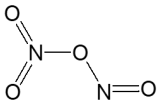
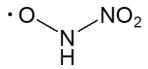
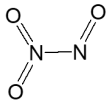
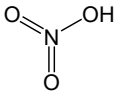
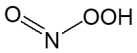
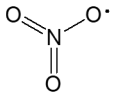
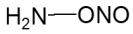
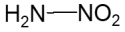
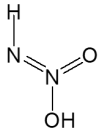
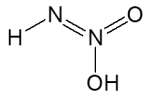
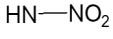
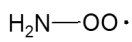
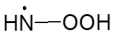
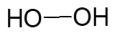
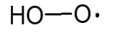
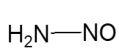
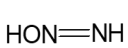
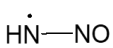
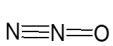
C2H		25.03027	2	1	0	0
HOCDONO2		91.02342	1	1	1	4
HOCDOONO		91.02342	1	1	1	4
NAMMH	[CH_3NHNH_2-HNO_3]	109.0852	1	7	3	3
CH3ONO2		77.03996	1	3	1	3
CH3OONO		77.03996	1	3	1	3
CH3OONOI		77.03996	1	3	1	3
HCJOHONO		76.03199	1	2	1	3
OJNHCHO		76.03199	1	2	1	3
HONJOCHO		76.03199	1	2	1	3

HOCDONO		75.02402	1	1	1	3
ONOCHO		75.02402	1	1	1	3
O2NCHO		75.02402	1	1	1	3
CH3N(NH2)NO2		91.0699	1	5	3	2
CH3N(NH2)ONO		91.0699	1	5	3	2
CH3NO2		61.04056	1	3	1	2
CH3ONO		61.04056	1	3	1	2
H2CNO2		60.03259	1	2	1	2
DIOHCH2		48.04183	1	4	0	2
CH3O2H		48.04183	1	4	0	2
CH3O2		47.03386	1	3	0	2
HOCH2O		47.03386	1	3	0	2
HOCHO		46.02589	1	2	0	2
HOCO		45.01792	1	1	0	2
OCHO		45.01792	1	1	0	2
NCNO		56.02395	1	0	2	1
CH3NO		45.04116	1	3	1	1
H2NCHO		45.04116	1	3	1	1
HNCO		43.02522	1	1	1	1
HCNO		43.02522	1	1	1	1
HOCN		43.02522	1	1	1	1
NCO		42.01725	1	0	1	1
CH3OH		32.04243	1	4	0	1
CH2OH		31.03446	1	3	0	1

CH3O		31.03446	1	3	0	1
CH3NHNH2		46.07237	1	6	2	0
CH3NNH2		45.0644	1	5	2	0
CH3NNH		44.05643	1	4	2	0
CH3NN		43.04846	1	3	2	0
NCN		40.02455	1	0	2	0
CH3NH		30.04973	1	4	1	0
CH2NH		29.04176	1	3	1	0
H2CN		28.03379	1	2	1	0
N2O5		108.0104	0	0	2	5
N2O4		92.011	0	0	2	4
ONONO2		92.011	0	0	2	4
HNOJNO2		77.01957	0	1	2	3
N2O3		76.0116	0	0	2	3
HNO3		63.01287	0	1	1	3
HOONO		63.01287	0	1	1	3
NO3		62.0049	0	0	1	3
H2NONO		62.02814	0	2	2	2
H2NNO2		62.02814	0	2	2	2
HNNDOOH_Z		62.02814	0	2	2	2

HNNDOOH		62.02814	0	2	2	2
HNJNO2		61.02017	0	1	2	2
NH2QJ		48.02144	0	2	1	2
NJH2Q		48.02144	0	2	1	2
H2O2		34.01474	0	2	0	2
HO2		33.00677	0	1	0	2
NH2NO		46.02874	0	2	2	1
HONNH		46.02874	0	2	2	1
HNNO		45.02077	0	1	2	1
N2O		44.0128	0	0	2	1
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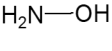
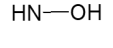
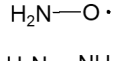
HNOH		32.02204	0	2	1	1
NH2O		32.02204	0	2	1	1
N2H4		32.04528	0	4	2	0
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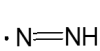
NNH		29.02137	0	1	2	0

List of Symbols, Abbreviations, and Acronyms

1-D	one-dimensional
ARL	Army Research Laboratory
BDE	bond dissociation energy
C	carbon
CO	carbon monoxide
CO_2	carbon dioxide
DEVCOM	US Army Combat Capabilities Development Command
DFT	density functional theory
DOD	Department of Defense
EGDN	ethylene glycol dinitrate
H	hydrogen
HCOOH	formic acid
HLK	Hertz–Langmuir–Knudson
HONO	nitrous acid
HR	homogeneous reactor
MEP	minimum energy path
N	nitrogen
NASA	National Aeronautics and Space Administration
NG	nitroglycerin
NG_g	gaseous nitroglycerin
NO	nitric oxide
NO_2	nitrogen dioxide
O	oxygen
PGDN	propylene glycol dinitrate
PL	pyrolysis law

QM-ESMs	quantum mechanics-based electronic structure methods
QRRK	quantum Rice–Ramsperger–Kassel
TS	transition state
VTST	variational transition state theory

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