

## Kinetic Model and Simulation of Promoted Selective Non-catalytic Reduction by Sodium Carbonate\*

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**Abstract** The detailed kinetic model of selective non-catalytic reduction (SNCR) of nitric oxide, including sodium species reactions, was developed on the basis of recent studies on thermal DeNO<sub>x</sub> mechanism, NO<sub>x</sub>OUT mechanism and promotion mechanism of Na<sub>2</sub>CO<sub>3</sub>. The model was validated by comparison with several experimental findings, thus providing an effective tool for the primary and promoted SNCR process simulation. Experimental and simulated results show part-per-million level of sodium carbonate enhances NO removal efficiency and extend the effective SNCR temperature range in comparison with use of a nitrogen agent alone. The kinetic modeling, sensitivity and rate-of-production analysis suggest that the performance improvement can be explained as homogeneous sodium species reactions producing more reactive OH radicals. The net result of sodium species reactions is conversion of H<sub>2</sub>O and inactive HO<sub>2</sub> radicals into reactive OH radicals, *i.e.* H<sub>2</sub>O+HO<sub>2</sub>=3OH, which enhances the SNCR performance of nitrogen agents by mainly increasing the production rate of NH<sub>2</sub> radicals. Moreover, N<sub>2</sub>O and CO are eliminated diversely *via* the reactions Na+N<sub>2</sub>O=NaO+N<sub>2</sub>, NaO+CO=Na+CO<sub>2</sub> and NaO<sub>2</sub>+CO=NaO+CO<sub>2</sub>, in the promoted SNCR process, especially in the NO<sub>x</sub>OUT process.

**Keywords** kinetic model, simulation, selective non-catalytic reduction, nitric oxide, sodium carbonate, mechanism

### 1 INTRODUCTION

Selective non-catalytic reduction (SNCR) is a more economical NO<sub>x</sub> control method with a considerable efficiency of 40%—70%, which involves injection of a nitrogen agent (N-agent) into the flue gas containing NO at temperatures near 1250K. The injected N-agent mainly generates NH<sub>i</sub> radicals (NH<sub>2</sub>, NH, and N) that react selectively with NO<sub>x</sub> to form N<sub>2</sub> in the typical temperature range of 1173—1373K. Several N-agents can be utilized in the SNCR process, including ammonia (NH<sub>3</sub>, thermal DeNO<sub>x</sub> process)[1], urea [CO(NH<sub>2</sub>)<sub>2</sub>, NO<sub>x</sub>OUT process][2], and cyanuric acid [(HOCN)<sub>3</sub>, RAPRENO<sub>x</sub> process][3]. There are some differences in their chemical mechanisms.

Although reasonably inexpensive, SNCR process has a serious limitation, *i.e.* the “temperature window” over which N-agents are effective is relatively narrow. At slightly higher or lower temperature, the NO<sub>x</sub> reduction rate drops off drastically. On the high temperature side of the optimum, the agent is oxidized to NO, reducing NO<sub>x</sub> reduction efficiency. On the low-temperature side, the injected agent does not effectively react and leads to “ammonia slip”, which decreases SNCR’s effectiveness to about 40%—50% typically[4]. In addition, the nonuniformity of the temperature profile in practical full-scale installations, together with difficulties of mixing the N-agent across the boiler cross section, reduced the effective residence time for reactions. And higher emission of N<sub>2</sub>O is also a major drawback in NO<sub>x</sub>OUT process.

To avoid such problems, various additives injected together with N-agent have been widely investigated to widen the SNCR temperature window. Some additives, such as hydrogen, hydrogen peroxide, hydrocarbons, alcohols, carbon monoxide, can shift

the active temperature window towards lower temperature. However, such additives can bring higher CO emission. The previous studies[5,6] show that a little addition of Na<sub>2</sub>CO<sub>3</sub> extended the SNCR temperature window to lower temperature and enhanced the NO<sub>x</sub> reduction efficiency of both NH<sub>3</sub> and (NH<sub>2</sub>)<sub>2</sub>CO, and the presence of Na<sub>2</sub>CO<sub>3</sub> also suppressed the formation of N<sub>2</sub>O.

The construction of a completely satisfactory chemical kinetic model for SNCR process has been a great challenge for many years. Yuan and Feng[7] and Wang *et al.*[8] adopted the MB Model[1] to analyze the DeNO<sub>x</sub> process. Calculated results[8] did not accord with experiments satisfactorily because of the limitation of adopted model itself and deficient mixing of aqueous NH<sub>3</sub> in the experiment. The more satisfactory MG model[9] of thermal DeNO<sub>x</sub> Process, an extension of the previous model[10], can be brought into better agreement with the experiments. Rota *et al.*[2] developed Urea2000 model of NO<sub>x</sub>OUT process based on the several detailed kinetic models, with which the simulation using perfectly stirred reactor agreed with experiments better. A more satisfactory kinetic model based on the experimental findings is desired as a useful tool to predict and analyze the trends and even range of parameters.

The objective of this work is to improve the MG model on the basis of the recent progress in the chemistry of NH<sub>3</sub>, decomposition of urea, and chain reactions of sodium compounds, and to validate the model by previous experimental data. The effect of additive amount and temperature on the NO reduction efficiency, N<sub>2</sub>O and CO emission is discussed by the updated model. The promotion mechanism of Na<sub>2</sub>CO<sub>3</sub> is identified through sensitivity and reaction path analysis.

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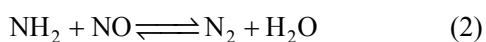
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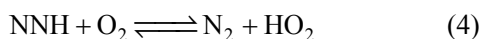
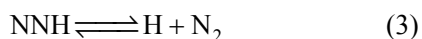
## 2 KINETIC MODEL AND CALCULATION PROCEDURE

The updated model for SNCR process in the present work includes thermal DeNO<sub>x</sub> mechanism, NO<sub>x</sub>OUT mechanism and promotion mechanism of Na<sub>2</sub>CO<sub>3</sub>. The thermodynamic data were drawn from the Sandia thermodynamic database[11]. The H/N/O subset was cited mainly from the previous model of thermal DeNO<sub>x</sub> by Miller *et al.*[1,9,10], and the extended chemistry of N<sub>2</sub>-amines was adopted from Skreiberg *et al.*[12]. The urea decomposition reactions are selected from Aoki *et al.*[13]. Reactions involving CO, HNCO and NCO are mainly from Glarborg *et al.*[14]. The mechanism includes a detailed subset for the chemistry of Na<sub>2</sub>CO<sub>3</sub> adopted from Zamansky[15]. The key reactions are discussed below.

In the thermal DeNO<sub>x</sub> process, the key species for NO abatement is the radical NH<sub>2</sub> that arises from NH<sub>3</sub> through hydrogen abstraction. There are two major reaction channels for NO and NH<sub>2</sub>:



but only one initiates the chain process through the decomposition reaction of NNH:



In spite of the large differences in terms of species and reactions among many detailed kinetic models previously presented in the literature, Miller and Glarborg[10] showed that the main differences among these models can be explained in terms of the values chosen for two key parameters: the chain branching ratio,  $\alpha$ , and the lifetime of the NNH radical,  $\tau_{\text{NNH}}$ . The chain branching parameter  $\alpha = k_1/(k_1+k_2)$  represents the ratio between the two major channels of reaction between NO and NH<sub>2</sub>, of which only the first one initiates the chain process. The value of  $\alpha$  determines the starting temperature of the reaction, *i.e.* for larger  $\alpha$  the first reaction prevails and the reduction process begins at lower temperature.

The second parameter is related to the rate constant of the decomposition reaction of NNH,  $\tau_{\text{NNH}} = 1/k_3$ . A short lifetime of NNH leads to the production of a large amount of H radicals, which induces an unconstrained growth of chain carrier. On the contrary, increasing the  $\tau_{\text{NNH}}$  value leads to a smoother transition from non-reactive to complete conversion conditions, while lower values induce a sharper profile.

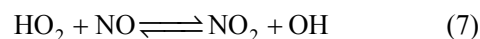
Miller and Glarborg[9] incorporated their experimental results for  $\alpha$  into the model. For the NH<sub>2</sub> + NO reaction the model used the following rate coefficients:

$$k_1 = 2.77 \times 10^{20} T^{-2.65} \exp(-5263/RT) \quad (5)$$

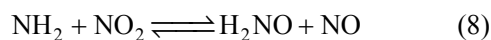
$$k_2 = 2.29 \times 10^{10} T^{0.425} \exp(3410/RT) \quad (6)$$

In addition, the observation that the process does not produce measurable quantities of NO<sub>2</sub> severely

limited the rate of the reaction (4) used in the model, because the formed HO<sub>2</sub> produces large quantities of NO<sub>2</sub> through reaction:

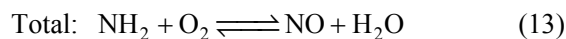
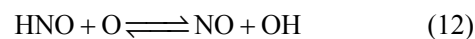
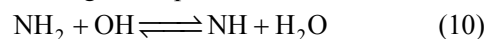


As a key breakthrough, the NH<sub>2</sub> + NO<sub>2</sub> reactions were adopted in the MG model:



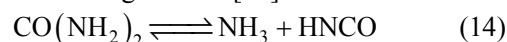
Thus recycling any NO<sub>2</sub> goes back to NO (H<sub>2</sub>NO ended up as NO through H<sub>2</sub>NO → HNO → NO). This allowed the construction of a model with a fast NNH+O<sub>2</sub> reaction, which allowed a smaller value of  $\tau_{\text{NNH}}$  without producing runaway chain branching[10,16]. The value of  $\tau_{\text{NNH}}$  used in the MG model was 10<sup>-7</sup>s, smaller than the upper limit of 0.5μs set by experiment[17], but still more than an order of magnitude larger than the 3 × 10<sup>-9</sup>s obtained from quantum scattering calculations.

On the other hand, NH<sub>2</sub> can also follow an oxidation channel leading to the production of NO:

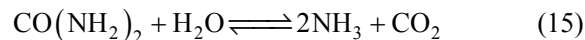


The curves of the outlet NO concentration as a function of temperature around the optimum temperature representing "valley shape", arises from the competition among reactions (1), (2) and (13) at different temperature.

In the NO<sub>x</sub>OUT process, the rates of the urea decomposition reactions and some detailed kinetic schemes for the HNCO/NO system are required. In SNCR processes instantaneous decomposition of urea is a common assumption[18]. In particular, up to about 600 K urea is believed to decompose mainly through the following reaction[19]:



Moreover, in the presence of water it has been proposed that urea decomposes through the following path[13]:



The rate constants parameters of above two reactions are listed in Table 1[13].

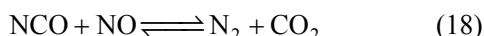
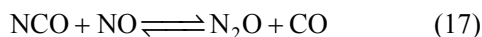
**Table 1** Rate constant parameters,  $k=A\exp(-E/RT)$ , for the urea decomposition reactions[13]

Reaction	$A, \text{s}^{-1}$	$E, \text{J}\cdot\text{mol}^{-1}$
$\text{CO}(\text{NH}_2)_2 \longrightarrow \text{NH}_3 + \text{HNCO}$	$1.27 \times 10^4$	60019
$\text{CO}(\text{NH}_2)_2 + \text{H}_2\text{O} \longrightarrow 2\text{NH}_3 + \text{CO}_2$	$6.13 \times 10^{10}$	87780

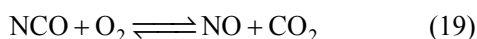
In the presence of oxygen and water the main radical reacting with HNCO is OH through the reaction:



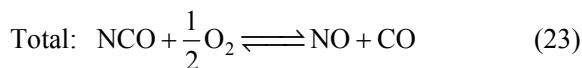
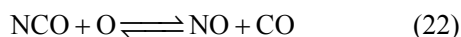
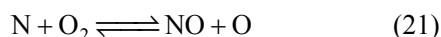
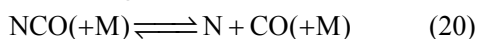
Also there are the two major channels of reaction between NO and NCO:



The above channel explains the formation of  $\text{N}_2\text{O}$  in large amount when HNCO is used as reducing agent. However, NCO can also undergo oxidation leading to the formation of NO either through oxidation:

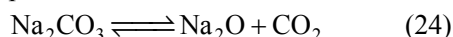


or through the following reactions:

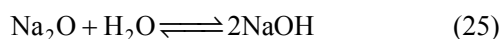


For the HNCO/NO system, the final NO reduction efficiency is decided by the balance between reactions (17), (18), (19) and (23) at different temperature.

Zamansky *et al.*[15] determined the reaction of  $\text{Na}_2\text{CO}_3$  decomposition is



that can also proceed as a reversible reaction, which in presence of water vapor can be followed by NaOH formation:



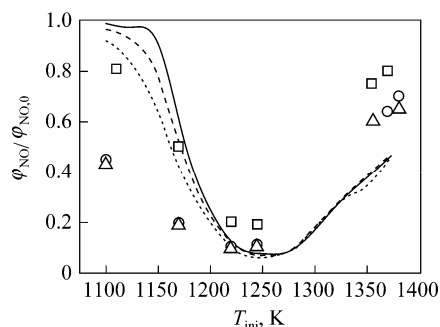
Other sodium species reactions were listed in the literature[5], most of which will be discussed in the following text.

On the whole, the mechanism involves 221 reactions and 38 species (available at <http://www.cjche.com.cn>). All the simulations discussed in the following have been performed using the plug flow reactor module of Chemkin 4.0[20]. Promotion mechanism for SNCR process is analyzed by species sensitivity and rate-of-production analysis of Chemkin 4.0[21]. In the following simulation with Chemkin 4.0, the solver step distance is 1cm, and the species of NO is selected in the panel of species sensitivity and rate-of-production (ROP). Other settings are default.

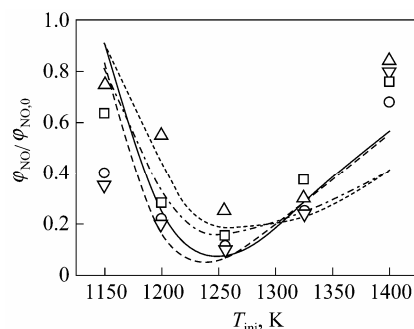
### 3 KINETIC MODEL VALIDATION

Miller and Glarborg had discussed and validated the MG model by comparing the calculation results with Kasuya *et al.*'s experiments[21], and got more satisfactory solution. Zamansky *et al.*[5,15] studied the promotion of  $\text{Na}_2\text{CO}_3$  on the NO reduction in a boiler simulator facility (BSF)[5]. The residence time-temperature profile of BSF under different experimental conditions could match that of a typical full scale boiler through controlling the heat extraction,

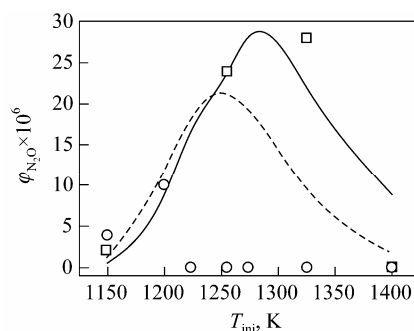
and the rate of temperature decrease at the reburning injection point was  $300\text{K}\cdot\text{s}^{-1}$ . All experimental data in Figs.1—3 are adopted from the Ref.[5]. The experimental initial conditions of SNCR process: the volume fraction of NO in the mixture was  $500 \times 10^{-6}$ , and  $N[(\text{NH}_3)/(\text{NO}) \text{ molar ratio}]$  was 1.5. The volume fraction of  $\text{O}_2$  in all experiments was 3.9%,  $\text{H}_2\text{O}$  15.0%,  $\text{CO}_2$  7.0%, and the pressure was 101.3kPa. All calculation in Figs.1—3 has been performed using the plug flow reactor module of Chemkin 4.0, and assumed the introduced N-agent and  $\text{Na}_2\text{CO}_3$  follow ideal mixing (instantaneous mixing). Mass spectrometric analysis and thermodynamic calculation confirmed that decomposition of



**Figure 1** Effect of  $\text{Na}_2\text{CO}_3$  upon  $\text{NH}_3$  performance[5]  
exp.:  $\square \beta=0$ ;  $\circ \beta=5 \times 10^{-6}$ ;  $\triangle \beta=15 \times 10^{-6}$   
cal.: —  $\beta=0$ ; - - -  $\beta=5 \times 10^{-6}$ ; ····  $\beta=15 \times 10^{-6}$



**Figure 2** Effect of  $\text{Na}_2\text{CO}_3$  upon  $\text{NH}_3$  and urea performance[5]  
exp.:  $\square \text{NH}_3, \beta=0$ ;  $\circ \text{NH}_3, \beta=30 \times 10^{-6}$ ;  $\triangle \text{urea}, \beta=0$ ;  $\nabla \text{urea}, \beta=30 \times 10^{-6}$   
cal.: —  $\text{NH}_3, \beta=0$ ; - - -  $\text{NH}_3, \beta=30 \times 10^{-6}$ ; ····  $\text{urea}, \beta=0$ ; - · -  $\text{urea}, \beta=30 \times 10^{-6}$



**Figure 3** Effect of additives on  $\text{N}_2\text{O}$  formation with urea as N-agent[5]  
exp.:  $\square \beta=0$ ;  $\circ \beta=30 \times 10^{-6}$   
cal.: —  $\beta=0$ ; - - -  $\beta=30 \times 10^{-6}$

$\text{Na}_2\text{CO}_3$  in the presence of water into gaseous  $\text{NaOH}$  and  $\text{CO}_2$  occurs in the temperature range from 1000K to 1500K.  $\beta$  is defined as the molar fraction of  $\text{Na}_2\text{CO}_3$  added into the flue gas. The calculation data were modeled assuming a linear temperature decrease at  $300\text{K}\cdot\text{s}^{-1}$  from the N-agent injection temperature to 900K, at which reaction is practically frozen.

It is clear that modeling the mixing of  $\text{NH}_3$  with the main gas stream in the furnace in addition to modeling the chemical reactions can significantly affect the results. In fact, there is non-ideal mixing at the injection stage in the experiment, and mixing has a distinct (but not drastic) effect on the SNCR chemistry at higher temperature. The data[22, 23] show that the effective temperature range becomes narrower when the mixing rate decreases. So the model significantly overpredicts the efficiency of NO removal at high temperature as shown in Figs.1 and 2. The predicted NO removal efficiencies are below the measured values at the lower temperature, it is probably due to the model limitation from the chain branching parameter  $\alpha$  and incomplete subset for the chemistry of  $\text{Na}_2\text{CO}_3$ . The promotion by additives is clearly predicted by the model that sodium compounds enhance the reduction efficiency and widen the temperature window, and shift it toward lower temperature in comparison with injection of  $\text{NH}_3$  or urea alone.

Moreover, additive can obviously decrease the  $\text{N}_2\text{O}$  emission especially in  $\text{NO}_x\text{OUT}$  process, as Fig.3 shows. However, the injection of additive stimulates slightly  $\text{N}_2\text{O}$  production at lower temperature; the predicted  $\text{N}_2\text{O}$  formation with additive injection is more in comparison with experimental data at higher temperature as a result of the non-ideal mixing at the injection stage and incomplete subset for the chemistry of  $\text{Na}_2\text{CO}_3$ . At least, the model can predict the main trend of additive influence and  $\text{N}_2\text{O}$  production.

The injection of  $\text{Na}_2\text{CO}_3$  and N-agent with overfire air led to higher CO emission in the advanced re-burning process, but injection of  $\text{Na}_2\text{CO}_3$  with urea or ammonia did not increase CO production in SNCR[15]. Since the  $\text{NO}_2$  production was little in the flue gas, it was not notable or measured in the promoted SNCR experiments, and the modeling[15] indicated the  $\text{NO}_2$  production was reduced in the promoted SNCR. Though there is considerable difficulty in the real time detection of all kinds of nitrogenous compounds in the flue gas at present, it is necessary to further study the effect of sodium compounds on CO,  $\text{NO}_2$  emission and  $\text{NH}_3$  escape in the promoted SNCR.

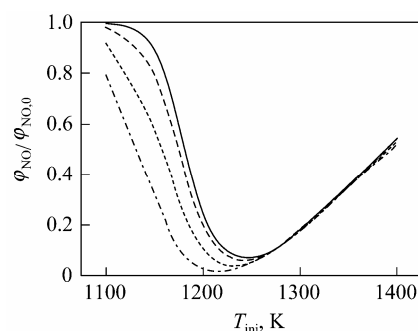
#### 4 MODELING RESULTS AND DISCUSSION

All simulations in the following text were performed in a conventional atmospheric pressure plug flow system with a 5cm i.d., 100cm long reactor, at temperature in the range between 900K and 1450K. A constant flow rate,  $2000\text{cm}^3\cdot\text{s}^{-1}$  (293K, 101.3kPa), was used in the experiment, corresponding to a residence time varying with injection temperature around 1s (the residence time can be expressed as  $t = 4.2979 \times 10^{-4} T_{\text{inj}} + 0.6129\text{s}$ ). The calculation data were modeled assuming a linear temperature decrease at

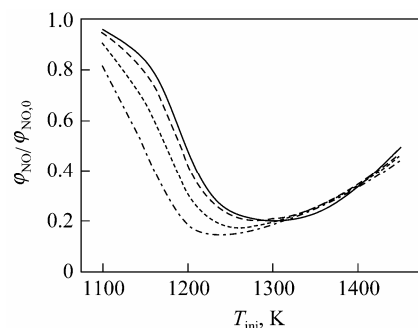
about  $300\text{K}\cdot\text{s}^{-1}$  from the inlet temperature to 900K, which keeps the residence time-temperature profile in the modeling similar to that of a typical full scale boiler. The initial volume fractions of gas were fixed to be:  $\text{NO}$ ,  $500 \times 10^{-6}$ ,  $\text{O}_2$  4%,  $\text{H}_2\text{O}$  8%,  $\text{CO}_2$  10% and  $\text{N}_2$  balance. The molar fraction of  $\text{Na}_2\text{CO}_3$  varies from 0 to  $550 \times 10^{-6}$ , and  $N$  is 1.5.

#### 4.1 Effect of $\text{Na}_2\text{CO}_3$ amount on SNCR process

As previously mentioned, the additive activates the initiation reactions at lower temperature without modifying significantly the main reaction paths at higher temperature. This is confirmed by the prediction of the detailed kinetic model when additive are involved. The simulations are reported for thermal  $\text{DeNO}_x$  process and  $\text{NO}_x\text{OUT}$  process in Figs.4—7. From Fig.4, it can be seen that the main trends are quite similar to the experiments[5]. The additive induces a precocious ignition of the  $\text{NH}_3$ —NO and urea—NO reactions thus enlarging the temperature windows towards low temperature without modifying the higher temperature behavior. Obviously, the optimum temperature of NO reduction for promoted SNCR process is lowered diversely with different additive amount. At the same time, the maximum NO reduction efficiency is differently enhanced corresponding to the increase of additive amount. The comparison of Fig.4 with Fig.2 shows that the efficiency of the  $\text{DeNO}_x$  process is higher than that of the  $\text{NO}_x\text{OUT}$  process at the same value of  $N$ , because the  $\text{HNCO}$  from urea decomposition forms  $\text{NCO}$  via reaction (16), then  $\text{NCO}$  undergoes oxidation leading to the NO formation through reactions (19)—(22).



(a)  $\text{NH}_3$  as N-agent

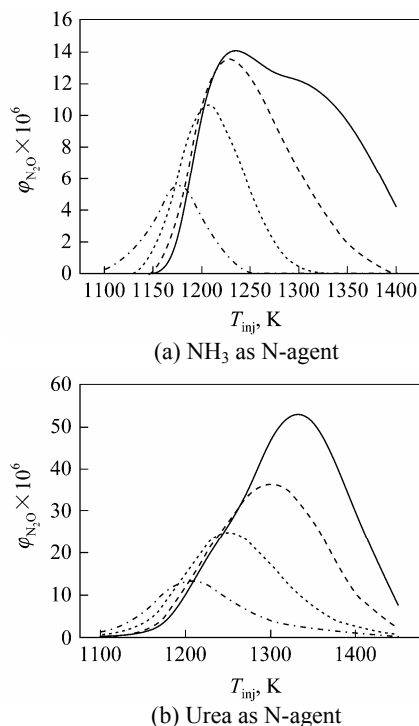


(b) Urea as N-agent

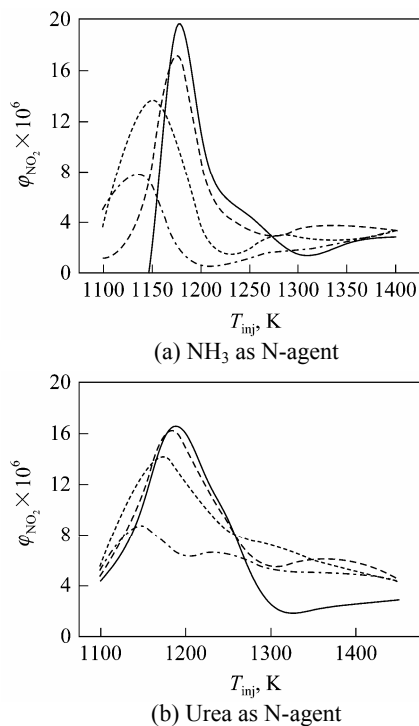
**Figure 4 Effect of  $\text{Na}_2\text{CO}_3$  on NO reduction with  $\text{NH}_3$  and urea as N-agents, respectively**

$\beta$ : — 0; - - -  $10 \times 10^{-6}$ ; ····  $50 \times 10^{-6}$ ; - · - ·  $150 \times 10^{-6}$

As analyzed previously, the notable  $N_2O$  emission from the  $NO_x$ OUT process can not be ignored because of reaction (17) between  $NO$  and  $NCO$ . The additive can destroy the  $N_2O$  formation remarkably in Figs.3 and 5, especially at higher temperature and higher additive concentration. Similarly in Fig.6, the



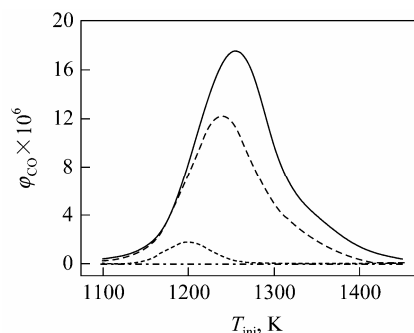
**Figure 5** Effect of  $Na_2CO_3$  on  $N_2O$  production with  $NH_3$  and urea as N-agents, respectively  
 $\beta$ : — 0; ----  $10 \times 10^{-6}$ ; .....  $50 \times 10^{-6}$ ; -.-.-  $150 \times 10^{-6}$



**Figure 6** Effect of  $Na_2CO_3$  on  $NO_2$  production with  $NH_3$  and urea as N-agents, respectively  
 $\beta$ : — 0; ----  $10 \times 10^{-6}$ ; .....  $50 \times 10^{-6}$ ; -.-.-  $150 \times 10^{-6}$

$NO_2$  production can be suppressed by the additive distinctly within the temperature window, although  $NO_2$  emission increases outside temperature window slightly in the presence of  $Na_2CO_3$ .

As the current model predicts, the promoted  $NO_x$ OUT process shows lower  $CO$  emission in Fig.7. With the increase of  $Na_2CO_3$  amount, the final  $CO$  emission decreases obviously. When the molar fraction of  $Na_2CO_3$  is above  $50 \times 10^{-6}$ , almost there is no additional  $CO$  emission with urea as N-agent. Though the result is the same as that in the Ref.[15], it is necessary to further validate the practical effect of  $Na_2CO_3$  on the  $CO$  emission in promoted SNCR.



**Figure 7** Effect of  $Na_2CO_3$  on  $CO$  emission with urea as N-agent  
 $\beta$ : — 0; ----  $10 \times 10^{-6}$ ; .....  $50 \times 10^{-6}$ ; -.-.-  $150 \times 10^{-6}$

Figure 8 shows the effect of  $Na_2CO_3$  concentration on the  $NO$ ,  $N_2O$ ,  $NO_2$  and total  $NO_x$  (defined as the sum of  $NO$ ,  $N_2O$  and  $NO_2$ ) emission at the optimum temperature (1250K  $NH_3$  as N-agent, and 1275K urea as N-agent). From the trend of curves, it can be seen the molar fraction of  $Na_2CO_3$  less than  $200 \times 10^{-6}$  evidently affects the  $N_2O$  formation for the thermal  $DeNO_x$  process and  $NO_x$ OUT processes. For the thermal  $DeNO_x$  process, when the molar fraction of  $Na_2CO_3$  reaches  $50 \times 10^{-6}$ , the  $NO$  reduction efficiency is about 95%, the  $NO_x$  reduction efficiency 94%,  $N_2O$  fraction about  $5 \times 10^{-6}$  and  $NO_2$  fraction  $2 \times 10^{-6}$ . In the  $NO_x$ OUT process, only when the  $Na_2CO_3$  concentration reaches  $100 \times 10^{-6}$ , the  $NO$  reduction efficiency tends toward steady value about 85%, the  $NO_x$  reduction efficiency 80%,  $N_2O$  fraction about  $11 \times 10^{-6}$  and  $NO_2$  fraction  $7 \times 10^{-6}$ , respectively.

#### 4.2 Promotion mechanism analysis

The promotion mechanism of  $Na_2CO_3$  helps us not only to understand experimental and simulated results, but also to further improve the SNCR process by seeking more effective additives.

The results presented in Fig.9 show that there is a significant increase in the concentration of  $OH$  produced in the presence of  $Na_2CO_3$  additive; however  $NH_3$  and  $NH_2$  concentrations decrease faster in comparison with the nonpromoted process. As a result, the concentration of  $NO$  decreases much faster;  $CO$  and  $N_2O$  emission amounts is also lower than that of nonpromoted process.

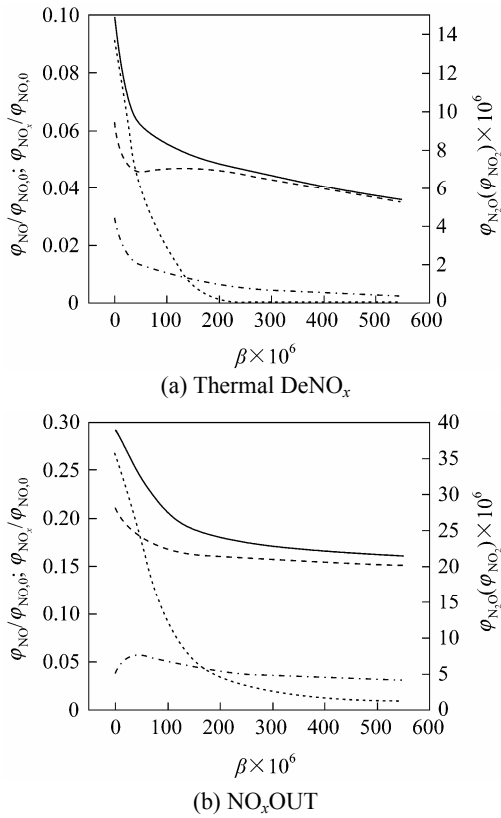


Figure 8 Dependence of NO, NO<sub>x</sub> removal efficiency and N<sub>2</sub>O, NO<sub>2</sub> emission in thermal DeNO<sub>x</sub> and NO<sub>x</sub>OUT processes on the amount of Na<sub>2</sub>CO<sub>3</sub> at optimum temperature — NO<sub>x</sub>; - - - NO; ···· N<sub>2</sub>O; - - - NO<sub>2</sub>

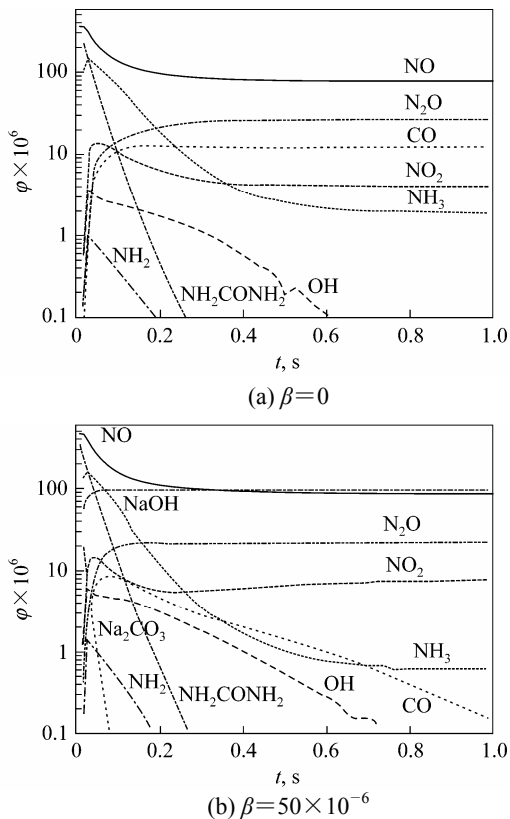


Figure 9 Changes of partial species and radical volume fraction for NO<sub>x</sub>OUT process ( $T=1275\text{K}$ )

Figures 10 and 11 show the sensitivity spectrum calculated for  $T = 1250\text{K}$ , corresponding to the Na<sub>2</sub>CO<sub>3</sub> concentration at  $50 \times 10^{-6}$ . Since there are many reactions in the N-O-H system that are quite sensitive in the promoted SNCR process, and since the primary interest of this study is in reactions of Na species, in Fig.10 the cut-off value for sensitivities of N-O-H reactions shown is 2 and the cut-off value for reactions of Na species is 0.4. Sensitivities less than 2 for N-H-O reactions are not shown in Fig.10. In order to explore the effect of Na species reactions on NO reduction, the cut-off value for Na species reactions in Fig.11 is 0.008. Sensitivities less than 0.008 for Na species reactions are not shown in Fig.11.

As previously analyzed reaction (1) and (2) play an important role for NO reduction, as Fig.10 shows. In all Na species reactions, the Na<sub>2</sub>CO<sub>3</sub> decomposition (24), OH formation mostly by reaction (26) and direct consumption of NO by reaction (35) are more sensitive for NO removal. Most of Na species reactions with higher sensitivities were drawn in Fig.11. These reactions bring on the main promotion of Na<sub>2</sub>CO<sub>3</sub> for SNCR process. The reactions are below:

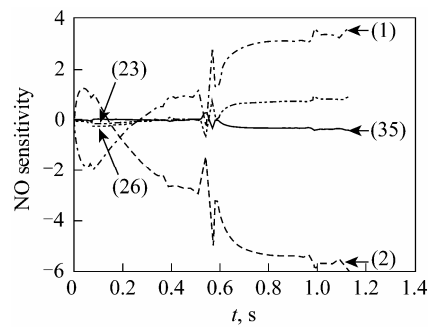
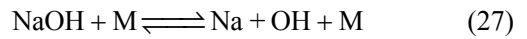
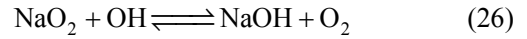


Figure 10 Sensitivity analysis for NO in the promoted SNCR process with NH<sub>3</sub> as N-agent ( $\beta = 50 \times 10^{-6}$ ,  $T = 1250\text{K}$ , numbers in the graph correspond to reaction numbers in text)

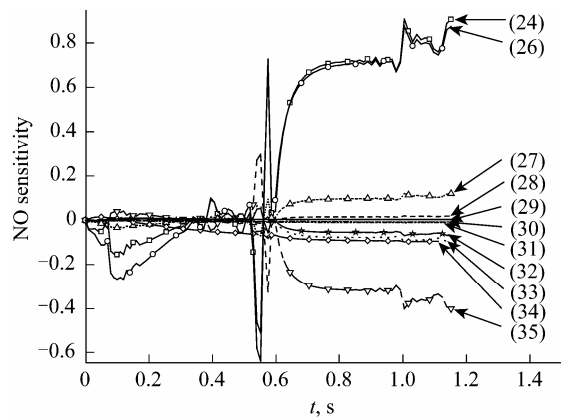
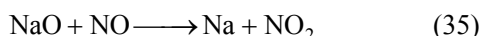
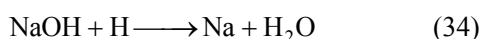
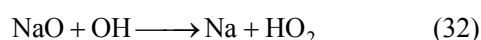
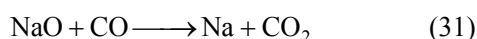
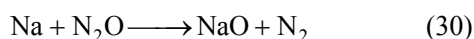


Figure 11 Sensitivity analysis for NO in the promoted SNCR process with NH<sub>3</sub> as N-agent ( $\beta = 50 \times 10^{-6}$ ,  $T = 1250\text{K}$ , numbers on the graph correspond to reaction numbers in text)



Based on the sensitivity analysis, the transformation of sodium-containing species (see Fig.12) was further drawn according to the rate-of-production analysis of sodium reactions, which determines the contribution of each reaction to the net production or destruction rates of a species. Width of arrows shows relative rates of chemical reactions, and numbers on the diagram correspond to reaction numbers in text. Some amount of  $\text{NH}_2$  radicals is produced in the reaction between  $\text{NaO}$  and  $\text{NH}_3$  through the rate-of-production analysis, so the reaction



was appended to the flux diagram, though it is a minor contribution to the total radical pool formed by the  $\text{NaOH}$  additive. As the transformation diagram of sodium species shows, the main conversion of sodium goes through the chain sequence  $\text{NaOH} \rightarrow \text{NaO}_2 \rightarrow \text{Na} \rightarrow \text{NaO} \rightarrow \text{NaOH}$ , corresponding to reactions (26), (28), (35), and (33). When these reactions are added together, the net reaction is

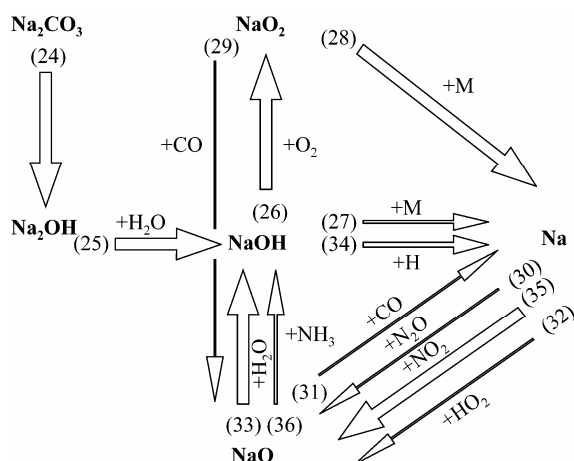
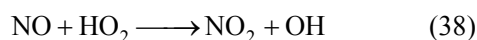
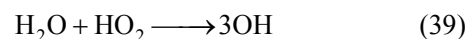


Figure 12 Transformation diagram for sodium-containing species ( $\beta=50 \times 10^{-6}$ ,  $T=1250\text{K}$ )

Since  $\text{NO}_2$  is mainly produced in the fast reaction



The net action of sodium species is equivalent to the conversion of  $\text{H}_2\text{O}$  and inactive  $\text{HO}_2$  radicals into reactive  $\text{OH}$  radicals:



Zamansky *et al.*[5] did the above similar analysis about production of  $\text{OH}$  radicals by the chain reactions of sodium species. Thus the net result of sodium conversion through the chain reaction is production of  $\text{OH}$  radicals. That explains the curves changes in Fig.9, because the additive also can produce a large  $\text{OH}$  radicals that are responsible for the formation of both  $\text{NH}_2$  and  $\text{NCO}$  in the promoted  $\text{NO}_x$ OUT process. Chain initiation is the rate limiting step in this sequence, and the converse reaction (26) is responsible for it with higher sensitivity in the sensitivity analysis (Figs.10 and 11). An alternative initiation approach would be reactions (27) and (34), but because of their high activation energy, they do not significantly contribute to production of active centers. However, it does become significant at higher temperature. That is why additive  $\text{Na}_2\text{CO}_3$  hardly enhances  $\text{NO}$  removal efficiency at higher temperature. At low temperature the  $\text{OH}$  radicals are mainly formed in reactions (26) and (33). Then more  $\text{OH}$  radicals react with  $\text{NH}_3$  by reaction



The efficiency of  $\text{NH}_3$  is enhanced through reactions (1) and (2) in the promoted SNCR. In addition,  $\text{N}_2\text{O}$  and  $\text{CO}$  are eliminated diversely *via* reactions (30), (29) and (31), which explains the lower emission of  $\text{N}_2\text{O}$  and  $\text{CO}$  in the promoted SNCR process. It is considered that this model needs be further validated using more experiments under a wider range of initial conditions.

## 5 CONCLUSIONS

A detailed kinetic model of selective non-catalytic reduction of nitric oxide, including sodium species reactions, has been developed on the basis of recent studies on thermal  $\text{DeNO}_x$  mechanism,  $\text{NO}_x$ OUT mechanism and promotion mechanism of  $\text{Na}_2\text{CO}_3$ . The detailed updated model has been validated by previous experiments, thus providing an effective tool for primary and promoted SNCR process simulation. Experimental and simulated results show parts per million levels of sodium carbonate enhance  $\text{NO}$  removal efficiency and extend the effective SNCR temperature range in comparison with use of a nitrogen agent alone. The modeling analysis suggests that the performance improvement can be explained as homogeneous sodium species reactions producing more reactive  $\text{OH}$  radicals. The net result of sodium species reactions is the conversion of  $\text{H}_2\text{O}$  and inactive  $\text{HO}_2$  radicals into reactive  $\text{OH}$  radicals, which enhances the SNCR performance of nitrogen agents by mainly increasing the production rate of  $\text{NH}_2$  radicals. Moreover, the experiments and modeling analysis show that  $\text{Na}_2\text{CO}_3$  additive can remove some disadvantages of the  $\text{NO}_x$ OUT process, *i.e.*  $\text{N}_2\text{O}$  and  $\text{CO}$  are eliminated diversely *via* the reactions  $\text{Na} + \text{N}_2\text{O} \rightarrow \text{NaO} + \text{N}_2$ ,  $\text{NaO} + \text{CO} \rightarrow \text{Na} + \text{CO}_2$  and  $\text{NaO}_2 + \text{CO} \rightarrow \text{NaO} + \text{CO}_2$ , in the promoted SNCR process.

## ACKNOWLEDGEMENTS

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## NOMENCLATURE

$A$	apparent frequency factor, $s^{-1}$
$E$	apparent activation, $J\cdot mol^{-1}$
$k$	reaction rate constant, $s^{-1}$
$M$	third body in some reactions
$N$	molar ratio of $NH_3$ to $NO$
$R$	gas constant ( $=8.314J\cdot mol^{-1}\cdot K^{-1}$ )
$T$	temperature, $K$
$t$	reaction time, $s$
$\alpha$	chain branching ratio
$\beta$	molar fraction of $Na_2CO_3$
$\tau_{NNH}$	lifetime of the $NNH$ radical, $s$
$\phi$	volume fraction

## Subscripts

inj	injection
0	initial value

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 ELEMENTS      ATOMIC  
 CONSIDERED    WEIGHT  
 -----

1. H            1.00797  
 2. O            15.9994  
 3. N            14.0067  
 4. C            12.0112  
 5. NA           22.9898  
 -----

C  
 P H  
 H A  
 A R

SPECIES CONSIDERED	S	G	MOLECULAR WEIGHT	TEMPERATURE		ELEMENT COUNT				
				LOW	HIGH	H	O	N	C	NA
1. H2	G	0	2.0159E+00	300	5000	2	0	0	0	0
2. H	G	0	1.0080E+00	300	5000	1	0	0	0	0
3. O2	G	0	3.1999E+01	300	5000	0	2	0	0	0
4. O	G	0	1.5999E+01	300	5000	0	1	0	0	0
5. OH	G	0	1.7007E+01	300	5000	1	1	0	0	0
6. H02	G	0	3.3007E+01	300	5000	1	2	0	0	0
7. H2O2	G	0	3.4015E+01	300	5000	2	2	0	0	0
8. H2O	G	0	1.8015E+01	300	5000	2	1	0	0	0
9. CO	G	0	2.8011E+01	300	5000	0	1	0	1	0
10. HCO	G	0	2.9019E+01	300	5000	1	1	0	1	0
11. CO2	G	0	4.4010E+01	300	5000	0	2	0	1	0
12. NO	G	0	3.0006E+01	300	5000	0	1	1	0	0
13. N	G	0	1.4007E+01	300	5000	0	0	1	0	0
14. NH	G	0	1.5015E+01	300	5000	1	0	1	0	0
15. NH2	G	0	1.6023E+01	300	5000	2	0	1	0	0
16. HNO	G	0	3.1014E+01	300	5000	1	1	1	0	0
17. N2O	G	0	4.4013E+01	300	5000	0	1	2	0	0
18. NNH	G	0	2.9021E+01	250	4000	1	0	2	0	0
19. N2H2	G	0	3.0029E+01	300	5000	2	0	2	0	0
20. HNOH	G	0	3.2022E+01	300	4000	2	1	1	0	0
21. NO2	G	0	4.6005E+01	300	5000	0	2	1	0	0
22. NH3	G	0	1.7031E+01	300	5000	3	0	1	0	0
23. H2NO	G	0	3.2022E+01	300	4000	2	1	1	0	0
24. HONO	G	0	4.7013E+01	300	5000	1	2	1	0	0
25. NO3	G	0	6.2005E+01	300	5000	0	3	1	0	0

26.	N2	G	0	2.8013E+01	300	5000	0	0	2	0	0
27.	N2H3	G	0	3.1037E+01	300	5000	3	0	2	0	0
28.	N2H4	G	0	3.2045E+01	300	5000	4	0	2	0	0
29.	NCO	G	0	4.2017E+01	300	5000	0	1	1	1	0
30.	HNCO	G	0	4.3025E+01	300	4000	1	1	1	1	0
31.	HNNO	G	0	4.5021E+01	300	4000	1	1	2	0	0
32.	NH2CONH2	G	0	6.0056E+01	300	5000	4	1	2	1	0
33.	NAO2	G	0	5.4989E+01	300	2000	0	2	0	0	1
34.	NAOH	G	0	3.9997E+01	300	2000	1	1	0	0	1
35.	NA	G	0	2.2990E+01	300	2000	0	0	0	0	1
36.	NAO	G	0	3.8989E+01	300	2000	0	1	0	0	1
37.	NA2CO3	G	0	1.0599E+02	300	2000	0	3	0	1	2
38.	NA2O	G	0	6.1979E+01	200	6000	0	1	0	0	2

(k = A T\*\*b exp(-E/RT))

REACTIONS CONSIDERED	A	b	E
1. OH+H2=H2O+H	2.14E+08	1.5	3449.0
2. O+OH=O2+H	2.02E+14	-0.4	0.0
3. O+H2=OH+H	5.06E+04	2.7	6290.0
4. H+O2+M=H2O+M	2.10E+18	-1.0	0.0
H2O	Enhanced by	1.000E+01	
CO2	Enhanced by	4.200E+00	
H2	Enhanced by	2.860E+00	
CO	Enhanced by	2.110E+00	
N2	Enhanced by	0.000E+00	
5. H+O2+N2=H2O+N2	6.70E+19	-1.4	0.0
6. OH+H2O=H2O+O2	1.90E+16	-1.0	0.0
7. H+H2O=2OH	1.69E+14	0.0	874.0
8. H+H2O=H2+O2	4.28E+13	0.0	1411.0
9. H+H2O=O+H2O	3.01E+13	0.0	1721.0
10. O+H2O=O2+OH	3.25E+13	0.0	0.0
11. 2OH=O+H2O	4.33E+03	2.7	-2485.7
12. H+H+M=H2+M	1.00E+18	-1.0	0.0
H2O	Enhanced by	0.000E+00	
H2	Enhanced by	0.000E+00	
CO2	Enhanced by	0.000E+00	
13. H+H+H2=H2+H2	9.20E+16	-0.6	0.0
14. H+H+H2O=H2+H2O	6.00E+19	-1.2	0.0
15. H+H+CO2=H2+CO2	5.49E+20	-2.0	0.0
16. H+OH+M=H2O+M	1.60E+22	-2.0	0.0

	H2O	Enhanced by	5.000E+00			
17.	H+O+M=OH+M			6.20E+16	-0.6	0.0
	H2O	Enhanced by	5.000E+00			
18.	O+O+M=O2+M			1.89E+13	0.0	-1788.0
	H2O	Enhanced by	5.000E+00			
	CO	Enhanced by	2.000E+00			
	CO2	Enhanced by	3.000E+00			
	H2	Enhanced by	2.000E+00			
19.	H02+H02=H202+02			4.20E+14	0.0	11982.0
	Declared duplicate reaction...					
20.	H02+H02=H202+02			1.30E+11	0.0	-1629.0
	Declared duplicate reaction...					
21.	H202+M=OH+OH+M			1.30E+17	0.0	45500.0
	H2O	Enhanced by	5.000E+00			
	CO	Enhanced by	2.000E+00			
	CO2	Enhanced by	3.000E+00			
	H2	Enhanced by	2.000E+00			
22.	H202+H=H02+H2			1.69E+12	0.0	3755.0
23.	H202+H=OH+H20			1.02E+13	0.0	3576.0
24.	H202+O=OH+H02			6.63E+11	0.0	3974.0
25.	H202+OH=H20+H02			7.83E+12	0.0	1331.0
	Declared duplicate reaction...					
26.	H02+N0=N02+OH			2.11E+12	0.0	-479.0
27.	N02+N02=N0+N0+02			1.63E+12	0.0	26123.0
28.	N02+H=N0+OH			8.40E+13	0.0	0.0
29.	N02+O=N0+02			3.90E+12	0.0	-238.0
30.	N0+O+M=N02+M			7.50E+19	-1.4	0.0
	N2	Enhanced by	1.700E+00			
	O2	Enhanced by	1.500E+00			
	H2O	Enhanced by	1.000E+01			
31.	N02+NH=N20+OH			1.00E+13	0.0	0.0
32.	N02+NH2=N20+H20			1.62E+16	-1.4	268.0
33.	NH2+N02=H2N0+N0			6.48E+16	-1.4	268.0
34.	N02+HNO=HONO+N0			6.00E+11	0.0	2000.0
35.	OH+N0+M=HONO+M			5.08E+23	-2.5	-67.6
	H2O	Enhanced by	5.000E+00			
36.	HONO+O=OH+N02			1.20E+13	0.0	5961.0
37.	HONO+OH=H20+N02			4.00E+12	0.0	0.0
38.	HONO+NH2=N02+NH3			7.11E+01	3.0	-4941.0
39.	HONO+H=H2+N02			1.20E+13	0.0	7352.0
40.	NH+02=HNO+O			4.61E+05	2.0	6500.0
41.	NH+02=N0+OH			1.28E+06	1.5	100.0
42.	NH+N0=N20+H			2.94E+14	-0.4	0.0
	Declared duplicate reaction...					

43.	$\text{NH}+\text{NO}=\text{N}_2+\text{H}$	*****	-0.2	0.0
	Declared duplicate reaction...			
44.	$\text{NH}+\text{NO}=\text{N}_2+\text{OH}$	2.16E+13	-0.2	0.0
45.	$\text{NH}+\text{OH}=\text{HNO}+\text{H}$	2.00E+13	0.0	0.0
46.	$\text{NH}+\text{OH}=\text{N}+\text{H}_2\text{O}$	5.00E+11	0.5	2000.0
47.	$\text{NH}+\text{N}=\text{N}_2+\text{H}$	3.00E+13	0.0	0.0
48.	$\text{NH}+\text{H}=\text{N}+\text{H}_2$	3.00E+13	0.0	0.0
49.	$\text{NH}+\text{O}=\text{NO}+\text{H}$	9.20E+13	0.0	0.0
50.	$\text{N}_2\text{O}+\text{OH}=\text{N}_2+\text{H}_2\text{O}$	1.29E-02	4.7	36561.0
51.	$\text{N}_2\text{O}+\text{OH}=\text{HNO}+\text{NO}$	1.18E-04	4.3	25081.0
52.	$\text{N}_2\text{O}+\text{NO}=\text{N}_2+\text{O}_2$	5.26E+05	2.2	46281.0
53.	$\text{N}_2\text{O}+\text{H}=\text{N}_2+\text{OH}$	3.31E+10	0.0	4729.0
	Declared duplicate reaction...			
54.	$\text{N}_2\text{O}+\text{H}=\text{N}_2+\text{OH}$	4.40E+14	0.0	19254.0
	Declared duplicate reaction...			
55.	$\text{N}_2\text{O}+\text{M}=\text{N}_2+\text{O}+\text{M}$	4.00E+14	0.0	56100.0
	N2	Enhanced by	1.700E+00	
	O2	Enhanced by	1.400E+00	
	H2O	Enhanced by	1.200E+01	
	CO	Enhanced by	1.500E+00	
	CO2	Enhanced by	3.000E+00	
56.	$\text{N}_2\text{O}+\text{O}=\text{N}_2+\text{O}_2$	1.00E+14	0.0	28000.0
57.	$\text{N}_2\text{O}+\text{O}=\text{NO}+\text{NO}$	6.60E+13	0.0	16630.0
58.	$\text{NH}_2+\text{O}=\text{HNO}+\text{H}$	6.63E+14	-0.5	0.0
59.	$\text{NH}_2+\text{O}=\text{NH}+\text{OH}$	6.75E+12	0.0	0.0
60.	$\text{NH}_2+\text{OH}=\text{NH}+\text{H}_2\text{O}$	4.00E+06	2.0	1000.0
61.	$\text{NH}_2+\text{H}=\text{NH}+\text{H}_2$	4.00E+13	0.0	3650.0
62.	$\text{NH}_2+\text{HO}_2=\text{NH}_3+\text{O}_2$	1.00E+13	0.0	0.0
63.	$\text{NH}_2+\text{HO}_2=\text{H}_2\text{NO}+\text{OH}$	5.00E+13	0.0	0.0
64.	$\text{NH}_2+\text{NH}_2=\text{N}_2\text{H}_2+\text{H}_2$	8.50E+11	0.0	0.0
65.	$\text{NH}_2+\text{NO}=\text{N}_2+\text{H}_2\text{O}$	2.77E+20	-2.7	1258.3
66.	$\text{NH}_2+\text{NO}=\text{NNH}+\text{OH}$	2.29E+10	0.4	-813.6
67.	$\text{NH}_3+\text{M}=\text{NH}_2+\text{H}+\text{M}$	2.20E+16	0.0	93470.0
	CO	Enhanced by	2.000E+00	
	H2	Enhanced by	2.000E+00	
	CO2	Enhanced by	3.000E+00	
	H2O	Enhanced by	5.000E+00	
68.	$\text{NH}_3+\text{OH}=\text{NH}_2+\text{H}_2\text{O}$	2.04E+06	2.0	566.0
69.	$\text{NH}_3+\text{H}=\text{NH}_2+\text{H}_2$	6.36E+05	2.4	10171.0
70.	$\text{NH}_3+\text{O}=\text{NH}_2+\text{OH}$	9.40E+06	1.9	6460.0
71.	$\text{NH}_3+\text{HO}_2=\text{NH}_2+\text{H}_2\text{O}_2$	3.00E+11	0.0	22000.0
72.	$\text{NNH}=\text{N}_2+\text{H}$	6.50E+07	0.0	0.0
73.	$\text{NNH}+\text{O}_2=\text{N}_2+\text{H}_2\text{O}_2$	2.00E+14	0.0	0.0
74.	$\text{NNH}+\text{O}_2=\text{N}_2+\text{O}_2+\text{H}$	5.00E+13	0.0	0.0

75.	$\text{NNH}+\text{NO}=\text{N}_2+\text{HNO}$		5.00E+13	0.0	0.0
76.	$\text{NNH}+\text{H}=\text{N}_2+\text{H}_2$		1.00E+14	0.0	0.0
77.	$\text{NNH}+\text{OH}=\text{N}_2+\text{H}_2\text{O}$		5.00E+13	0.0	0.0
78.	$\text{NNH}+\text{NH}_2=\text{N}_2+\text{NH}_3$		5.00E+13	0.0	0.0
79.	$\text{NNH}+\text{NH}=\text{N}_2+\text{NH}_2$		5.00E+13	0.0	0.0
80.	$\text{NNH}+\text{O}=\text{N}_2+\text{OH}$		8.00E+13	0.0	0.0
81.	$\text{NNH}+\text{O}=\text{N}_2\text{O}+\text{H}$		1.00E+14	0.0	0.0
82.	$\text{NNH}+\text{O}=\text{NH}+\text{NO}$		5.00E+13	0.0	0.0
83.	$\text{H}+\text{NO}+\text{M}=\text{HNO}+\text{M}$		4.00E+20	-1.8	0.0
	H2O	Enhanced by	1.000E+01		
	O2	Enhanced by	1.500E+00		
	H2	Enhanced by	2.000E+00		
	CO2	Enhanced by	3.000E+00		
	N2	Enhanced by	0.000E+00		
84.	$\text{H}+\text{NO}+\text{N}_2=\text{HNO}+\text{N}_2$		4.00E+20	-1.8	0.0
85.	$\text{HNO}+\text{OH}=\text{NO}+\text{H}_2\text{O}$		3.60E+13	0.0	0.0
86.	$\text{HNO}+\text{H}=\text{H}_2+\text{NO}$		4.46E+11	0.7	655.0
87.	$\text{HNO}+\text{O}=\text{OH}+\text{NO}$		1.00E+13	0.0	0.0
88.	$\text{HNO}+\text{NH}_2=\text{NH}_3+\text{NO}$		3.63E+06	1.6	-1252.0
89.	$\text{HNO}+\text{HNO}=\text{N}_2\text{O}+\text{H}_2\text{O}$		9.00E+08	0.0	3100.0
90.	$\text{HNO}+\text{O}_2=\text{HO}_2+\text{NO}$		2.00E+12	0.0	25000.0
91.	$\text{H}_2\text{NO}+\text{O}_2=\text{HNO}+\text{HO}_2$		3.00E+12	0.0	25000.0
92.	$\text{H}_2\text{NO}+\text{M}=\text{HNOH}+\text{M}$		1.10E+29	-4.0	43982.0
	H2O	Enhanced by	1.000E+01		
93.	$\text{H}_2\text{NO}+\text{M}=\text{HNO}+\text{H}+\text{M}$		2.80E+24	-2.8	64915.0
	H2O	Enhanced by	1.000E+01		
94.	$\text{H}_2\text{NO}+\text{NO}_2=\text{HNO}+\text{HONO}$		6.00E+11	0.0	2000.0
95.	$\text{H}_2\text{NO}+\text{H}=\text{HNO}+\text{H}_2$		3.00E+07	2.0	2000.0
96.	$\text{H}_2\text{NO}+\text{H}=\text{NH}_2+\text{OH}$		5.00E+13	0.0	0.0
97.	$\text{H}_2\text{NO}+\text{O}=\text{HNO}+\text{OH}$		3.00E+07	2.0	2000.0
98.	$\text{H}_2\text{NO}+\text{O}=\text{NH}_2+\text{O}_2$		2.50E+14	0.0	0.0
99.	$\text{H}_2\text{NO}+\text{OH}=\text{HNO}+\text{H}_2\text{O}$		2.00E+07	2.0	1000.0
100.	$\text{H}_2\text{NO}+\text{NO}=\text{HNO}+\text{HNO}$		2.00E+07	2.0	13000.0
101.	$\text{H}_2\text{NO}+\text{NH}_2=\text{NH}_3+\text{HNO}$		3.00E+12	0.0	1000.0
102.	$\text{H}_2\text{NO}+\text{HO}_2=\text{HNO}+\text{H}_2\text{O}_2$		2.90E+04	2.7	-1600.0
103.	$\text{HNOH}+\text{H}=\text{NH}_2+\text{OH}$		4.00E+13	0.0	0.0
104.	$\text{HNOH}+\text{H}=\text{HNO}+\text{H}_2$		4.80E+08	1.5	378.0
105.	$\text{HNOH}+\text{O}=\text{HNO}+\text{OH}$		7.00E+13	0.0	0.0
	Declared duplicate reaction...				
106.	$\text{HNOH}+\text{O}=\text{HNO}+\text{OH}$		3.30E+08	1.5	-358.0
	Declared duplicate reaction...				
107.	$\text{HNOH}+\text{OH}=\text{HNO}+\text{H}_2\text{O}$		2.40E+06	2.0	-1192.0
108.	$\text{HNOH}+\text{NH}_2=\text{NH}_3+\text{HNO}$		1.80E+06	1.9	-1152.0
109.	$\text{HNOH}+\text{HO}_2=\text{HNO}+\text{H}_2\text{O}_2$		2.90E+04	2.7	-1600.0

110.	$\text{HNOH}+\text{M}=\text{HNO}+\text{H}+\text{M}$	2.00E+24	-2.8	58934.0
	H2O	Enhanced by	1.000E+01	
111.	$\text{HNOH}+\text{O}_2=\text{HNO}+\text{HO}_2$	3.00E+12	0.0	25000.0
112.	$\text{HNOH}+\text{NO}_2=\text{HONO}+\text{HNO}$	6.00E+11	0.0	2000.0
113.	$\text{N}+\text{NO}=\text{N}_2+\text{O}$	3.27E+12	0.3	0.0
114.	$\text{N}+\text{O}_2=\text{NO}+\text{O}$	6.40E+09	1.0	6280.0
115.	$\text{N}+\text{OH}=\text{NO}+\text{H}$	3.80E+13	0.0	0.0
116.	$\text{NH}_2+\text{NH}=\text{N}_2\text{H}_2+\text{H}$	5.00E+13	0.0	0.0
117.	$\text{NH}+\text{NH}=\text{N}_2+\text{H}+\text{H}$	2.54E+13	0.0	0.0
118.	$\text{NH}_2+\text{N}=\text{N}_2+\text{H}+\text{H}$	7.20E+13	0.0	0.0
119.	$\text{N}_2\text{H}_2+\text{M}=\text{NNH}+\text{H}+\text{M}$	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	
120.	$\text{N}_2\text{H}_2+\text{H}=\text{NNH}+\text{H}_2$	5.00E+13	0.0	1000.0
121.	$\text{N}_2\text{H}_2+\text{O}=\text{NH}_2+\text{NO}$	1.00E+13	0.0	0.0
122.	$\text{N}_2\text{H}_2+\text{O}=\text{NNH}+\text{OH}$	2.00E+13	0.0	1000.0
123.	$\text{N}_2\text{H}_2+\text{OH}=\text{NNH}+\text{H}_2\text{O}$	1.00E+13	0.0	1000.0
124.	$\text{N}_2\text{H}_2+\text{NO}=\text{N}_2\text{O}+\text{NH}_2$	3.00E+12	0.0	0.0
125.	$\text{N}_2\text{H}_2+\text{NH}=\text{NNH}+\text{NH}_2$	1.00E+13	0.0	1000.0
126.	$\text{N}_2\text{H}_2+\text{NH}_2=\text{NH}_3+\text{NNH}$	1.00E+13	0.0	1000.0
127.	$\text{NO}_2+\text{O} (+\text{M})=\text{NO}_3 (+\text{M})$	1.30E+13	0.0	0.0
	Low pressure limit:	0.10000E+29	-0.40800E+01	0.24700E+04
	N2	Enhanced by	1.500E+00	
	O2	Enhanced by	1.500E+00	
	H2O	Enhanced by	1.860E+01	
128.	$\text{NO}_2+\text{NO}_2=\text{NO}_3+\text{NO}$	9.60E+09	0.7	20900.0
129.	$\text{NO}_3+\text{H}=\text{NO}_2+\text{OH}$	6.00E+13	0.0	0.0
130.	$\text{NO}_3+\text{O}=\text{NO}_2+\text{O}_2$	1.00E+13	0.0	0.0
131.	$\text{NO}_3+\text{OH}=\text{NO}_2+\text{HO}_2$	1.40E+13	0.0	0.0
132.	$\text{NO}_3+\text{HO}_2=\text{NO}_2+\text{O}_2+\text{OH}$	1.50E+12	0.0	0.0
133.	$\text{NO}_3+\text{NO}_2=\text{NO}+\text{NO}_2+\text{O}_2$	5.00E+10	0.0	2940.0
134.	$\text{H}_2+\text{O}_2=\text{OH}+\text{OH}$	1.70E+13	0.0	47780.0
135.	$\text{NH}_2+\text{NH}_2=\text{NH}_3+\text{NH}$	5.00E+13	0.0	10000.0
136.	$\text{NH}_2+\text{NH}_2 (+\text{M})=\text{N}_2\text{H}_4 (+\text{M})$	1.50E+13	0.0	0.0
	Low pressure limit:	0.10000E+19	0.00000E+00	0.00000E+00
	N2	Enhanced by	2.500E+00	
	H2O	Enhanced by	5.000E+00	
	NH3	Enhanced by	1.000E+01	
137.	$\text{N}_2\text{H}_4+\text{H}=\text{N}_2\text{H}_3+\text{H}_2$	1.30E+13	0.0	2500.0
138.	$\text{N}_2\text{H}_4+\text{O}=\text{N}_2\text{H}_2+\text{H}_2\text{O}$	8.50E+13	0.0	1200.0
139.	$\text{N}_2\text{H}_4+\text{OH}=\text{N}_2\text{H}_3+\text{H}_2\text{O}$	4.00E+13	0.0	0.0
140.	$\text{N}_2\text{H}_4+\text{NH}_2=\text{N}_2\text{H}_3+\text{NH}_3$	3.90E+12	0.0	1500.0

141.	$N_2H_3+M=N_2H_2+H+M$	3.50E+16	0.0	46000.0
142.	$N_2H_3+H=NH_2+NH_2$	1.60E+12	0.0	0.0
143.	$N_2H_3+O=N_2H_2+OH$	5.00E+12	0.0	5000.0
144.	$N_2H_3+O=NH_2+HNO$	1.00E+13	0.0	0.0
145.	$N_2H_3+OH=N_2H_2+H_2O$	1.00E+13	0.0	1000.0
146.	$N_2H_3+OH=NH_3+HNO$	1.00E+12	0.0	15000.0
147.	$N_2H_3+NH=N_2H_2+NH_2$	2.00E+13	0.0	0.0
148.	$HONO+HONO=NO+NO_2+H_2O$	2.30E+12	0.0	8400.0
149.	$NH+NO=N_2O+H$	*****	-0.2	0.0
	Declared duplicate reaction...			
150.	$H_2O_2+OH=H_2O+HO_2$	5.80E+14	0.0	9560.0
	Declared duplicate reaction...			
151.	$HNOH+NH_2=N_2H_3+OH$	1.00E+01	3.5	-467.0
152.	$CO+O+M=CO_2+M$	6.20E+14	0.0	3000.0
	H2O Enhanced by 1.860E+01			
153.	$CO+OH=CO_2+H$	1.50E+07	1.3	-765.0
154.	$CO+O_2=CO_2+O$	2.50E+12	0.0	47700.0
155.	$CO+HO_2=CO_2+OH$	1.50E+14	0.0	23650.0
156.	$HCO+H=CO+H_2$	1.20E+13	0.2	0.0
	Declared duplicate reaction...			
157.	$HCO+H=CO+H_2$	7.20E+13	0.0	0.0
	Declared duplicate reaction...			
158.	$HCO+O=CO+OH$	3.00E+13	0.0	0.0
159.	$HCO+O=CO_2+H$	3.00E+13	0.0	0.0
160.	$HCO+OH=CO+H_2O$	1.00E+14	0.0	0.0
161.	$HCO+O_2=CO+HO_2$	7.60E+12	0.0	400.0
162.	$HCO+M=H+CO+M$	1.90E+17	-1.0	17020.0
	N2 Enhanced by 1.500E+00			
	O2 Enhanced by 1.500E+00			
	H2O Enhanced by 5.000E+00			
163.	$HNCO+M=NH+CO+M$	1.10E+16	0.0	86000.0
	N2 Enhanced by 1.500E+00			
	O2 Enhanced by 1.500E+00			
	H2O Enhanced by 5.000E+00			
164.	$HNCO+H=NH_2+CO$	2.25E+07	1.7	3800.0
165.	$HNCO+O=NCO+OH$	2.20E+06	2.1	11430.0
166.	$HNCO+O=NH+CO_2$	9.60E+07	1.4	8520.0
167.	$HNCO+O=HNO+CO$	1.50E+08	1.6	44012.0
168.	$HNCO+OH=H_2O+NCO$	6.40E+05	2.0	2560.0
169.	$HNCO+HO_2=NCO+H_2O_2$	3.00E+11	0.0	29000.0
170.	$HNCO+O_2=HNO+CO_2$	1.00E+12	0.0	35000.0
171.	$HNCO+NH_2=NH_3+NCO$	5.00E+12	0.0	6200.0
172.	$HNCO+NH=NH_2+NCO$	3.00E+13	0.0	23700.0
173.	$HNCO+NO_2=HNNO+CO_2$	2.50E+12	0.0	26200.0

174.	$\text{NCO} + \text{M} = \text{N} + \text{CO} + \text{M}$			3.10E+16	-0.5	48000.0
	N2	Enhanced by	1.500E+00			
	O2	Enhanced by	1.500E+00			
	H2O	Enhanced by	5.000E+00			
175.	$\text{NCO} + \text{H} = \text{NH} + \text{CO}$			5.00E+13	0.0	0.0
176.	$\text{NCO} + \text{O} = \text{NO} + \text{CO}$			4.70E+13	0.0	0.0
177.	$\text{NCO} + \text{OH} = \text{NO} + \text{HCO}$			5.00E+12	0.0	15000.0
178.	$\text{NCO} + \text{H}_2 = \text{HNCO} + \text{H}$			7.60E+02	3.0	4000.0
179.	$\text{NCO} + \text{O}_2 = \text{NO} + \text{CO}_2$			2.00E+12	0.0	20000.0
180.	$\text{NCO} + \text{HCO} = \text{HNCO} + \text{CO}$			3.60E+13	0.0	0.0
181.	$\text{NCO} + \text{N} = \text{N}_2 + \text{CO}$			2.00E+13	0.0	0.0
182.	$\text{NCO} + \text{NO} = \text{N}_2\text{O} + \text{CO}$			6.20E+17	-1.7	763.0
183.	$\text{NCO} + \text{NO} = \text{N}_2 + \text{CO}_2$			7.80E+17	-1.7	763.0
184.	$\text{NCO} + \text{NO}_2 = 2\text{NO} + \text{CO}$			1.30E+13	0.0	0.0
	Declared duplicate reaction...					
185.	$\text{NCO} + \text{NO}_2 = 2\text{NO} + \text{CO}$			2.50E+11	0.0	-707.0
	Declared duplicate reaction...					
186.	$\text{NCO} + \text{NO}_2 = \text{N}_2\text{O} + \text{CO}_2$			5.40E+12	0.0	0.0
	Declared duplicate reaction...					
187.	$\text{NCO} + \text{NO}_2 = \text{CO}_2 + \text{N}_2\text{O}$			3.00E+12	0.0	-707.0
	Declared duplicate reaction...					
188.	$\text{NCO} + \text{HNO} = \text{HNCO} + \text{NO}$			1.80E+13	0.0	0.0
189.	$\text{NCO} + \text{HONO} = \text{HNCO} + \text{NO}_2$			3.60E+12	0.0	0.0
190.	$\text{NCO} + \text{NCO} = 2\text{CO} + \text{N}_2$			1.80E+13	0.0	0.0
191.	$\text{NO} + \text{HCO} = \text{CO} + \text{HNO}$			7.20E+12	0.0	0.0
192.	$\text{NO}_2 + \text{HCO} = \text{CO} + \text{HONO}$			2.10E+00	3.3	2350.0
193.	$\text{NO}_2 + \text{HCO} = \text{H} + \text{CO}_2 + \text{NO}$			8.40E+15	-0.8	1930.0
194.	$\text{NH}_2\text{CONH}_2 = \text{NH}_3 + \text{HNCO}$			1.27E+04	0.0	15540.0
195.	$\text{NH}_2\text{CONH}_2 + \text{H}_2\text{O} = 2\text{NH}_3 + \text{CO}_2$			6.13E+10	0.0	20980.0
196.	$\text{NA}_2\text{CO}_3 = \text{NA}_2\text{O} + \text{CO}_2$			2.54E+06	0.0	25820.0
197.	$\text{NA}_2\text{O} + \text{CO}_2 = \text{NA}_2\text{CO}_3$			1.11E+05	0.0	-15000.0
198.	$\text{NA}_2\text{O} + \text{H}_2\text{O} = 2\text{NAOH}$			9.18E+12	0.0	3120.0
199.	$\text{NA} + \text{N}_2\text{O} = \text{NAO} + \text{N}_2$			1.69E+14	0.0	3159.0
200.	$\text{NAO} + \text{H}_2\text{O} = \text{NAOH} + \text{OH}$			1.32E+13	0.0	0.0
201.	$\text{NAO} + \text{O} = \text{NA} + \text{O}_2$			2.23E+14	0.0	0.0
202.	$\text{NAO} + \text{NO} = \text{NA} + \text{NO}_2$			9.04E+13	0.0	0.0
203.	$\text{NAO} + \text{H}_2 = \text{NAOH} + \text{H}$			1.25E+13	0.0	0.0
204.	$\text{NA} + \text{O}_2 + \text{M} = \text{NAO}_2 + \text{M}$			1.74E+21	-1.3	0.0
	H2O	Enhanced by	5.000E+00			
	CO2	Enhanced by	3.000E+00			
	CO	Enhanced by	2.000E+00			
	H2	Enhanced by	2.000E+00			
205.	$\text{NA} + \text{OH} + \text{M} = \text{NAOH} + \text{M}$			1.82E+21	-1.0	0.0
206.	$\text{NAO} + \text{OH} = \text{NAOH} + \text{O}$			2.00E+13	0.0	0.0



207.	$\text{NAO} + \text{HO}_2 = \text{NAOH} + \text{O}_2$	5.00E+13	0.0	0.0
208.	$\text{NAO} + \text{H}_2 = \text{NA} + \text{H}_2\text{O}$	3.13E+12	0.0	0.0
209.	$\text{NAO} + \text{CO} = \text{NA} + \text{CO}_2$	1.00E+14	0.0	0.0
210.	$\text{H} + \text{NAO}_2 = \text{HO}_2 + \text{NA}$	2.00E+14	0.0	0.0
211.	$\text{NAO} + \text{H} = \text{NA} + \text{OH}$	2.00E+14	0.0	0.0
212.	$\text{NAO} + \text{OH} = \text{NA} + \text{HO}_2$	3.00E+13	0.0	0.0
213.	$\text{NA} + \text{HO}_2 = \text{NAOH} + \text{O}$	1.00E+14	0.0	0.0
214.	$\text{NAO}_2 + \text{H} = \text{NAO} + \text{OH}$	5.00E+13	0.0	0.0
215.	$\text{NAO} + \text{HO}_2 = \text{NAO}_2 + \text{OH}$	5.00E+13	0.0	0.0
216.	$\text{NAO}_2 + \text{H} = \text{NAOH} + \text{O}$	1.00E+14	0.0	0.0
217.	$\text{NAO}_2 + \text{CO} = \text{NAO} + \text{CO}_2$	1.00E+14	0.0	0.0
218.	$\text{NAO}_2 + \text{O} = \text{NAO} + \text{O}_2$	1.00E+14	0.0	0.0
219.	$\text{NAO} + \text{NH}_3 = \text{NAOH} + \text{NH}_2$	1.00E+13	0.0	0.0
220.	$\text{NAOH} + \text{H} = \text{NA} + \text{H}_2\text{O}$	1.07E+13	0.0	1967.0
221.	$\text{NAO}_2 + \text{OH} = \text{NAOH} + \text{O}_2$	8.00E+13	0.0	0.0

NOTE: A units mole-cm-sec-K, E units cal/mole

## THERMO

	300.000	1000.000	5000.000								
(CH2O)3	70590C	3H	60	3	G	0300.00	4000.00	1500.00			1
	0.01913678E+03	0.08578044E-01	-0.08882060E-05	-0.03574819E-08	0.06605142E-12						2
	-0.06560876E+06	-0.08432507E+03	-0.04662286E+02	0.06091547E+00	-0.04710536E-03						3
	0.01968843E-06	-0.03563271E-10	-0.05665403E+06	0.04525264E+03							4
AL	62987AL	1			G	0300.00	5000.00	0600.00			1
	0.02559589E+02	-0.10632239E-03	0.07202828E-06	-0.02121105E-09	0.02289429E-13						2
	0.03890214E+06	0.05234522E+02	0.02736825E+02	-0.05912374E-02	-0.04033937E-05						3
	0.02322343E-07	-0.01705599E-10	0.03886794E+06	0.04363879E+02							4
AL2H6	62987AL	2H	6		G	0300.00	1500.00	0600.00			1
	0.02634884E+02	0.02135952E+00	0.03154151E-05	-0.07684674E-07	0.02335831E-10						2
	0.08871346E+05	0.09827515E+02	-0.06800681E+02	0.05080744E+00	0.10397471E-04						3
	-0.11195819E-06	0.08459155E-09	0.10605371E+05	0.05554526E+03							4
AL2ME6	62987AL	2C	6H	18	G	0300.00	1500.00	0600.00			1
	0.01773147E+03	0.04935747E+00	0.11968535E-05	-0.16398263E-07	0.04890867E-10						2
	-0.03855560E+06	-0.05053298E+03	-0.07159750E+01	0.10671087E+00	0.02117604E-03						3
	-0.02193211E-05	0.16441438E-09	-0.03515546E+06	0.03890762E+03							4
ALAS	62987AL	1AS	1		G	0300.00	1500.00	0600.00			1
	0.04790026E+02	-0.01908225E-03	-0.01983390E-05	0.02239358E-08	-0.06904706E-12						2
	0.05259290E+06	0.03259703E+02	0.05047764E+02	-0.06419947E-02	-0.14320714E-05						3
	0.04754390E-07	-0.03297621E-10	0.05254264E+06	0.01985205E+02							4
ALH	62987AL	1H	1		G	0300.00	5000.00	1000.00			1
	0.03392644E+02	0.12153990E-02	-0.04676595E-05	0.08691624E-09	-0.06022668E-13						2
	0.03006845E+06	0.02758899E+02	0.03071503E+02	0.02165549E-01	-0.03275638E-04						3
	0.04136983E-07	-0.01877120E-10	0.03021221E+06	0.04548855E+02							4
ALH2	62987AL	1H	2		G	0300.00	1500.00	0600.00			1
	0.04486543E+02	0.03128831E-01	-0.01969438E-05	-0.10160304E-08	0.03497468E-11						2
	0.01960959E+06	0.08167897E+01	0.02442136E+02	0.09915913E-01	0.02471082E-05						3
	-0.02119583E-06	0.01710233E-09	0.01997587E+06	0.10652699E+02							4
ALH3	62987AL	1H	3		G	0300.00	1500.00	0600.00			1
	0.04186837E+02	0.06159249E-01	-0.03877593E-06	-0.02061928E-07	0.06600276E-11						2
	0.07908078E+05	0.05134396E+01	0.10083231E+01	0.16403245E-01	0.01976746E-04						3
	-0.03528558E-06	0.02753377E-09	0.08484656E+05	0.15858377E+02							4
ALME	62987AL	1C	1H	3	G	0300.00	1500.00	0600.00			1
	0.04662737E+02	0.07097939E-01	0.02520013E-05	-0.02114863E-07	0.06097489E-11						2
	0.08203227E+05	0.01769244E+02	0.02664176E+02	0.13249141E-01	0.02525847E-04						3
	-0.02394396E-06	0.01761854E-09	0.08574173E+05	0.11474494E+02							4
ALME2	62987AL	1C	2H	6	G	0300.00	1500.00	0600.00			1
	0.06481282E+02	0.14746049E-01	0.05816529E-05	-0.04621347E-07	0.13960405E-11						2
	0.03745072E+05	-0.02603325E+02	0.09494573E+01	0.03206353E+00	0.06134020E-04						3
	-0.06500042E-06	0.04911485E-09	0.04761408E+05	0.02419465E+03							4
ALME3	62987AL	1C	3H	9	G	0300.00	1500.00	0600.00			1
	0.06654948E+02	0.02455144E+00	0.11765745E-05	-0.07815023E-07	0.02255622E-10						2

-0.13409524E+05-0.03454481E+02-0.07027567E+01	0.04682764E+00	0.11499028E-04	3		
-0.09160441E-06	0.06687293E-09-0.12037989E+05	0.03232771E+03	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	0.04366000E+02	0.02500000E+02	0.00000000E+00	0.00000000E+00	3
0.00000000E+00	0.00000000E+00-0.07453750E+04	0.04366000E+02			4
AR+	121286AR	1E -1	G 0300.00 5000.00 1000.00	1	
0.02864864E+02-0.12035732E-03-0.10651992E-07	0.09074839E-10-0.09623876E-14			2	
0.01827230E+07	0.03543584E+02	0.02301341E+02	0.08035528E-02-0.01758805E-05	3	
-0.01781093E-08-0.08937268E-13	0.01829281E+07	0.06659358E+02		4	
AS	62987AS	1	G 0300.00 1500.00 0600.00	1	
0.02617010E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	2
0.03720454E+06	0.06995524E+02	0.02617010E+02	0.00000000E+00	0.00000000E+00	3
0.00000000E+00	0.00000000E+00	0.03720454E+06	0.06995524E+02		4
AS2	62987AS	2	G 0300.00 1500.00 0600.00	1	
0.04394201E+02	0.05389968E-02-0.02379401E-05-0.06541924E-09	0.05184186E-12		2	
0.02235093E+06	0.04897918E+02	0.03682891E+02	0.03121811E-01-0.10740519E-05	3	
-0.05629472E-07	0.05178811E-10	0.02247355E+06	0.08283423E+02	4	
AS3	62987AS	3	G 0300.00 1500.00 0600.00	1	
0.07404036E+02	0.07818425E-02-0.03918297E-05-0.05203629E-09	0.06291907E-12		2	
0.03063825E+06-0.03417323E+02	0.06403142E+02	0.04477098E-01-0.01866642E-04		3	
-0.07394750E-07	0.07012752E-10	0.03080965E+06	0.13371355E+01	4	
AS4	62987AS	4	G 0300.00 1500.00 0600.00	1	
0.09695766E+02	0.13062585E-02-0.05519564E-05-0.02150873E-08	0.14579349E-12		2	
0.15717321E+05-0.16188696E+02	0.07853760E+02	0.07916509E-01-0.02329820E-04		3	
-0.15263119E-07	0.13774348E-10	0.16036290E+05-0.07409755E+02		4	
ASALME	62987AS	1AL 1C 1H 3G	0300.00 1500.00 0600.00	1	
0.07127107E+02	0.07357863E-01	0.02300796E-06-0.02226398E-07	0.06927227E-11	2	
0.03273438E+06-0.01847179E+02	0.04053423E+02	0.01726125E+00	0.01833498E-04	3	
-0.03386952E-06	0.02626980E-09	0.03329309E+06	0.12996653E+02	4	
ASALME2	62987AS	1AL 1C 2H 6G	0300.00 1500.00 0600.00	1	
0.09909938E+02	0.14638499E-01	0.04118730E-05-0.04444657E-07	0.13295010E-11	2	
0.02815111E+06-0.15235312E+02	0.04808530E+02	0.03067687E+00	0.05048000E-04	3	
-0.05908099E-06	0.04462290E-09	0.02908816E+06	0.09471621E+02	4	
ASGAET	62987AS	1GA 1C 2H 5G	0300.00 1500.00 0600.00	1	
0.09081073E+02	0.16746316E-01	0.12831301E-06-0.05590435E-07	0.01781314E-10	2	
0.03807443E+06-0.09142782E+02	0.06364698E+01	0.04382467E+00	0.06144686E-04	3	
-0.09491641E-06	0.07374197E-09	0.03960893E+06	0.03164673E+03	4	
ASGAET2	62987AS	1GA 1C 4H 10G	0300.00 1500.00 0600.00	1	
0.10324288E+02	0.03073570E+00	0.10863354E-05-0.09971948E-07	0.02945979E-10	2	
0.03039490E+06-0.13164016E+02-0.03539248E+01	0.06369772E+00	0.13597417E-04		3	
-0.12861423E-06	0.09572181E-09	0.03236903E+06	0.03865086E+03	4	
ASGAME	62987AS	1GA 1C 1H 3G	0300.00 1500.00 0600.00	1	
0.07322183E+02	0.06995478E-01	0.10693509E-06-0.01995283E-07	0.06040446E-11	2	

0.03949448E+06-0.07416680E+01 0.04877266E+02 0.14825589E-01 0.16521240E-05	3
-0.02712058E-06 0.02080195E-09 0.03994071E+06 0.11076703E+02	4
ASGAME2 62987AS 1GA 1C 2H 6G 0300.00 1500.00 0600.00	1
0.09352436E+02 0.15048197E-01 0.05157975E-05-0.04553518E-07 0.13487630E-11	2
0.03735855E+06-0.12181144E+02 0.04382076E+02 0.03056344E+00 0.05477067E-04	3
-0.05834108E-06 0.04373509E-09 0.03827434E+06 0.11911109E+02	4
ASGAMEH 62987AS 1GA 1C 1H 4G 0300.00 1500.00 0600.00	1
0.07842794E+02 0.09682097E-01 0.10603061E-06-0.02991402E-07 0.09382673E-11	2
0.04435297E+06-0.05093455E+02 0.03585119E+02 0.02336317E+00 0.02873356E-04	3
-0.04737894E-06 0.03674461E-09 0.04512702E+06 0.15471604E+02	4
ASH 62987AS 1H 1 G 0300.00 1500.00 0600.00	1
0.03219848E+02 0.10012498E-02-0.04874997E-08-0.11076533E-09-0.09254321E-13	2
0.03008175E+06 0.06647311E+02 0.03865843E+02-0.11575710E-02-0.03494371E-05	3
0.07079686E-07-0.06014027E-10 0.02996829E+06 0.03549869E+02	4
ASH2 62987AS 1H 2 G 0300.00 1500.00 0600.00	1
0.03428307E+02 0.03181140E-01 0.14604843E-06-0.07937145E-08 0.01694413E-11	2
0.02010282E+06 0.02904703E+02 0.03778945E+02 0.01759233E-01 0.08070806E-05	3
0.02358763E-07-0.03043521E-10 0.02004861E+06 0.12729740E+01	4
ASH3 62987AS 1H 3 G 0300.00 1500.00 0600.00	1
0.04172022E+02 0.04371322E-01 0.02177574E-05-0.11832641E-08 0.04536373E-11	2
0.06882915E+05 0.02803476E+02 0.09446356E+01 0.15084686E-01 0.12016960E-05	3
-0.03397465E-06 0.02767656E-09 0.07459168E+05 0.01832267E+03	4
ASME 62987AS 1C 1H 3 G 0300.00 1500.00 0600.00	1
0.04657260E+02 0.06976297E-01 0.02147556E-05-0.02101159E-07 0.06082149E-11	2
0.02806422E+06 0.03409834E+02 0.02625270E+02 0.13252423E-01 0.02441628E-04	3
-0.02419566E-06 0.01786943E-09 0.02844080E+06 0.13273359E+02	4
ASME2 62987AS 1C 2H 6 G 0300.00 1500.00 0600.00	1
0.05981395E+02 0.15212837E-01 0.06993355E-05-0.04721619E-07 0.13699115E-11	2
0.14679847E+05 0.11927411E+01 0.13903998E+01 0.02923331E+00 0.06598870E-04	3
-0.05620559E-06 0.04130367E-09 0.15533022E+05 0.02349980E+03	4
ASME3 62987AS 1C 3H 9 G 0300.00 1500.00 0600.00	1
0.06347764E+02 0.02466454E+00 0.11546286E-05-0.07877435E-07 0.02202225E-10	2
-0.16173225E+04-0.06316786E+01 0.02667388E+01 0.04253171E+00 0.11651064E-04	3
-0.07914706E-06 0.05603126E-09-0.04685539E+04 0.02904590E+03	4
C 121086C 1 G 0300.00 5000.00 1000.00	1
0.02602087E+02-0.01787081E-02 0.09087041E-06-0.11499333E-10 0.03310844E-14	2
0.08542154E+06 0.04195177E+02 0.02498584E+02 0.08085776E-03-0.02697697E-05	3
0.03040729E-08-0.11066518E-12 0.08545878E+06 0.04753459E+02	4
C(S) 121286C 1 S 0300.00 5000.00 1000.00	1
0.14901664E+01 0.16621256E-02-0.06687204E-05 0.12908796E-09-0.09205334E-13	2
-0.07074018E+04-0.08717785E+02-0.06705661E+01 0.07181499E-01-0.05632921E-04	3
0.02142298E-07-0.04168562E-11-0.07339498E+03 0.02601595E+02	4
C+ 120186C 1E -1 G 0300.00 5000.00 1000.00	1
0.02511827E+02-0.01735978E-03 0.09504267E-07-0.02218851E-10 0.01862189E-14	2

0.02166772E+07	0.04286130E+02	0.02595384E+02	-0.04068664E-02	0.06892366E-05	3
-0.05266488E-08	0.15083378E-12	0.02166628E+07	0.03895729E+02		4
C-	121686C	1E 1	G	0300.00 5000.00 1000.00	1
0.02990221E+02	-0.09184596E-02	0.05055560E-05	-0.07703410E-09	0.03163271E-13	2
0.06983931E+06	0.12594533E+01	0.02783902E+02	-0.01774287E-01	0.03696760E-04	3
-0.03066693E-07	0.08637622E-11	0.06998511E+06	0.02726281E+02		4
C2	121286C	2	G	0300.00 5000.00 1000.00	1
0.04135978E+02	0.06531618E-03	0.01837099E-05	-0.05295085E-09	0.04712137E-13	2
0.09967272E+06	0.07472923E+01	0.06996045E+02	-0.07400601E-01	0.03234703E-04	3
0.04802535E-07	-0.03295917E-10	0.09897487E+06	-0.13862268E+02		4
C2-	121286C	2E 1	G	0300.00 5000.00 1000.00	1
0.03796891E+02	0.02530049E-02	0.09709118E-06	-0.16148038E-10	-0.03212893E-15	2
0.05207981E+06	0.16581468E+01	0.03468011E+02	-0.02352874E-02	0.12439123E-05	3
0.04705960E-08	-0.08164274E-11	0.05231215E+06	0.03886699E+02		4
C2CL3	53090C	2CL 3	G	0300.00 5000.00 1500.00	1
0.11931098E+02	0.08300908E-02	-0.02468074E-05	0.03291583E-09	-0.15435010E-14	2
0.02307865E+06	-0.02946919E+03	0.04781562E+02	0.02228654E+00	-0.02579608E-03	3
0.13963552E-07	-0.02878611E-10	0.02514597E+06	0.07344525E+02		4
C2CL5	53090C	2CL 5	G	0300.00 5000.00 1500.00	1
0.01769161E+03	0.09089599E-02	-0.04077701E-05	0.08191884E-09	-0.06083311E-13	2
-0.02347038E+05	-0.05499588E+03	0.06466099E+02	0.03836376E+00	-0.04796191E-03	3
0.02685202E-06	-0.05597977E-10	0.04647776E+04	0.13758384E+01		4
C2CL6	53090C	2CL 6	G	0300.00 5000.00 1500.00	1
0.02031376E+03	0.16109885E-02	-0.05122820E-05	0.06369724E-09	-0.02637223E-13	2
-0.02345211E+06	-0.07153936E+03	0.07476241E+02	0.04328185E+00	-0.05294544E-03	3
0.02962827E-06	-0.06219843E-10	-0.02006351E+06	-0.06566180E+02		4
C2F6	82489C	2F 6	G	0300.00 5000.00 1000.00	1
0.16020573E+02	0.06273007E-01	-0.02797778E-04	0.05517547E-08	-0.04004651E-12	2
-0.16756543E+06	-0.05519459E+03	0.03577448E+02	0.03913670E+00	-0.02714862E-03	3
0.04348459E-08	0.04007135E-10	-0.16421741E+06	0.09098384E+02		4
C2H	20387C	2H 1	G	0300.00 5000.00 1000.00	1
0.04427688E+02	0.02216268E-01	-0.06048952E-05	0.09882517E-09	-0.07351179E-13	2
0.06590415E+06	-0.11994418E+01	0.03050667E+02	0.06051674E-01	-0.04956634E-04	3
0.02804159E-07	-0.08193332E-11	0.06630011E+06	0.05954361E+02		4
C2H2	121386C	2H 2	G	0300.00 5000.00 1000.00	1
0.04436770E+02	0.05376039E-01	-0.01912816E-04	0.03286379E-08	-0.02156709E-12	2
0.02566766E+06	-0.02800338E+02	0.02013562E+02	0.15190446E-01	-0.16163189E-04	3
0.09078992E-07	-0.01912746E-10	0.02612444E+06	0.08805378E+02		4
C2H3	12787C	2H 3	G	0300.00 5000.00 1000.00	1
0.05933468E+02	0.04017745E-01	-0.03966739E-05	-0.14412666E-09	0.02378643E-12	2
0.03185434E+06	-0.08530313E+02	0.02459276E+02	0.07371476E-01	0.02109872E-04	3
-0.13216421E-08	-0.11847838E-11	0.03335225E+06	0.11556202E+02		4
C2H4	121286C	2H 4	G	0300.00 5000.00 1000.00	1
0.03528418E+02	0.11485185E-01	-0.04418385E-04	0.07844600E-08	-0.05266848E-12	2

	0.04428288E+05	0.02230389E+02	-0.08614880E+01	0.02796162E+00	-0.03388677E-03	3	
	0.02785152E-06	-0.09737879E-10	0.05573046E+05	0.02421148E+03		4	
C2H5	12387C	2H	5	G	0300.00 5000.00 1000.00	1	
	0.07190480E+02	0.06484077E-01	-0.06428064E-05	-0.02347879E-08	0.03880877E-12	2	
	0.10674549E+05	-0.14780892E+02	0.02690701E+02	0.08719133E-01	0.04419838E-04	3	
	0.09338703E-08	-0.03927773E-10	0.12870404E+05	0.12138195E+02		4	
C2H6	121686C	2H	6	G	0300.00 4000.00 1000.00	1	
	0.04825938E+02	0.13840429E-01	-0.04557258E-04	0.06724967E-08	-0.03598161E-12	2	
	-0.12717793E+05	-0.05239506E+02	0.14625388E+01	0.15494667E-01	0.05780507E-04	3	
	-0.12578319E-07	0.04586267E-10	-0.11239176E+05	0.14432295E+02		4	
C2HCL	112989C	2H	1CL	1	G	0300.00 5000.00 1000.00	1
	0.06295372E+02	0.03883113E-01	-0.15060494E-05	0.02700003E-08	-0.01830213E-12	2	
	0.02357278E+06	-0.08137063E+02	0.03618443E+02	0.13319791E-01	-0.13218222E-04	3	
	0.06092023E-07	-0.08879026E-11	0.02415385E+06	0.05050645E+02		4	
C2N	121286C	2N	1	G	0300.00 5000.00 1000.00	1	
	0.06151561E+02	0.15116498E-02	-0.06629362E-05	0.12861485E-09	-0.09160830E-13	2	
	0.06484318E+06	-0.08177850E+02	0.03498544E+02	0.08554433E-01	-0.06288697E-04	3	
	0.08638478E-08	0.04915996E-11	0.06556611E+06	0.05548374E+02		4	
C2N2	121286C	2N	2	G	0300.00 5000.00 1000.00	1	
	0.06548002E+02	0.03984707E-01	-0.16342164E-05	0.03038596E-08	-0.02111069E-12	2	
	0.03490716E+06	-0.09735790E+02	0.04265459E+02	0.11922569E-01	-0.13420142E-04	3	
	0.09192297E-07	-0.02778941E-10	0.03547887E+06	0.01713212E+02		4	
C2O	121286C	2O	1	G	0300.00 5000.00 1000.00	1	
	0.04849809E+02	0.02947585E-01	-0.10907286E-05	0.01792562E-08	-0.11157585E-13	2	
	0.03282055E+06	-0.06453225E+01	0.03368850E+02	0.08241803E-01	-0.08765145E-04	3	
	0.05569262E-07	-0.15400086E-11	0.03317081E+06	0.06713314E+02		4	
C3	121286C	3		G	0300.00 5000.00 1000.00	1	
	0.03803709E+02	0.02253566E-01	-0.07704534E-05	0.13162939E-09	-0.08694264E-13	2	
	0.09736135E+06	0.06128062E+02	0.04345527E+02	0.12644661E-02	-0.04652557E-04	3	
	0.08695855E-07	-0.04243535E-10	0.09731403E+06	0.03519437E+02		4	
C3H2	121686C	3H	2	G	0300.00 5000.00 1000.00	1	
	0.06530853E+02	0.05870316E-01	-0.01720776E-04	0.02127498E-08	-0.08291910E-13	2	
	0.05115213E+06	-0.11227278E+02	0.02691077E+02	0.14803664E-01	-0.03250551E-04	3	
	-0.08644363E-07	0.05284877E-10	0.05219072E+06	0.08757391E+02		4	
C3H4	40687C	3H	4	G	0300.00 5000.00 1000.00	1	
	0.05729144E+02	0.12368045E-01	-0.04805626E-04	0.08601364E-08	-0.05812802E-12	2	
	0.02012984E+06	-0.09448668E+02	-0.02131968E+01	0.03358713E+00	-0.03804870E-03	3	
	0.02745838E-06	-0.08690044E-10	0.02162048E+06	0.02029392E+03		4	
C3H4C	121686C	3H	4	G	0300.00 5000.00 1000.00	1	
	0.06699993E+02	0.10357372E-01	-0.03455116E-04	0.05065295E-08	-0.02668227E-12	2	
	0.03019905E+06	-0.13391933E+02	-0.02462104E+00	0.02319721E+00	-0.01847435E-04	3	
	-0.15927594E-07	0.08684615E-10	0.03233413E+06	0.02271659E+03		4	
C3H4P	40687C	3H	4	G	0300.00 5000.00 1000.00	1	
	0.05511034E+02	0.12469562E-01	-0.04814164E-04	0.08573770E-08	-0.05771561E-12	2	

	0.01961967E+06-0.10794748E+02	0.06271447E+01	0.03116179E+00-0.03747663E-03	3
	0.02964117E-06-0.09987381E-10	0.02083492E+06	0.13468796E+02	4
C3H6	120186C	3H 6	G 0300.00 5000.00 1000.00	1
	0.06732257E+02	0.14908336E-01-0.04949899E-04	0.07212022E-08-0.03766204E-12	2
	-0.09235703E+04-0.13313348E+02	0.14933071E+01	0.02092517E+00 0.04486794E-04	3
	-0.16689121E-07	0.07158146E-10	0.10748264E+04 0.16145340E+02	4
C3H8	120186C	3H 8	G 0300.00 5000.00 1000.00	1
	0.07525217E+02	0.01889034E+00-0.06283924E-04	0.09179373E-08-0.04812410E-12	2
	-0.16464548E+05-0.01784390E+03	0.08969208E+01	0.02668986E+00 0.05431425E-04	3
	-0.02126000E-06	0.09243330E-10-0.13954918E+05	0.01935533E+03	4
C3O2	121286C	3O 2	G 0300.00 5000.00 1000.00	1
	0.08098897E+02	0.05560039E-01-0.02312264E-04	0.04340709E-08-0.03036387E-12	2
	-0.14214353E+05-0.15219745E+02	0.04018127E+02	0.01836660E+00-0.01907148E-03	3
	0.11855871E-07-0.03418747E-10-0.13128236E+05	0.05582083E+02		4
C4	121286C	4	G 0300.00 5000.00 1000.00	1
	0.06500180E+02	0.04228632E-01-0.01790717E-04	0.03404812E-08-0.02403978E-12	2
	0.11434008E+06-0.11488894E+02	0.02343028E+02	0.16429811E-01-0.15279858E-04	3
	0.07343826E-07-0.15822743E-11	0.11545384E+06	0.09826204E+02	4
C4H	121686C	4H 1	G 0300.00 5000.00 1000.00	1
	0.06242882E+02	0.06193682E-01-0.02085931E-04	0.03082203E-08-0.16364826E-13	2
	0.07568019E+06-0.07210806E+02	0.05023247E+02	0.07092375E-01-0.06073762E-07	3
	-0.02275752E-07	0.08086994E-11	0.07623812E+06-0.06942594E+00	4
C4H3	62592C	4H 3	G 0300.00 5000.00 1000.00	1
	0.84874201E+01	0.86908937E-02-0.28544437E-05	0.41200798E-09-0.21301093E-13	2
	0.47970555E+05-0.19018509E+02	0.35539713E+01	0.19461986E-01-0.48102484E-05	3
	-0.97301225E-08	0.62390535E-11	0.49453863E+05 0.70829868E+01	4
C4H10	62090C	4H 10	G 0300.00 4000.00 1500.00	1
	0.01998784E+03	0.10372807E-01-0.09610818E-05-0.04623017E-08	0.08202828E-12	2
	-0.02625571E+06-0.08837907E+03-0.02256618E+02	0.05881732E+00-0.04525782E-03		3
	0.02037115E-06-0.04079458E-10-0.01760233E+06	0.03329595E+03		4
C4H2	121686C	4H 2	G 0300.00 5000.00 1000.00	1
	0.09031407E+02	0.06047252E-01-0.01948788E-04	0.02754863E-08-0.13856080E-13	2
	0.05294735E+06-0.02385067E+03	0.04005191E+02	0.01981000E+00-0.09865877E-04	3
	-0.06635158E-07	0.06077413E-10	0.05424065E+06 0.01845736E+02	4
C4H6	120186C	4H 6	G 0300.00 5000.00 1000.00	1
	0.08046583E+02	0.16485251E-01-0.05522227E-04	0.08123593E-08-0.04295078E-12	2
	0.13701305E+05-0.01800457E+03	0.03197108E+02	0.02025591E+00 0.06510192E-04	3
	-0.16584423E-07	0.06400282E-10	0.15715203E+05 0.09895660E+02	4
C4H8	120386C	4H 8	G 0300.00 5000.00 1000.00	1
	0.02053584E+02	0.03435050E+00-0.15883196E-04	0.03308966E-07-0.02536104E-11	2
	-0.02139723E+05	0.15543201E+02	0.11811380E+01 0.03085338E+00 0.05086524E-04	3
	-0.02465488E-06	0.11110192E-10-0.01790400E+05	0.02106247E+03	4
C5	121286C	5	G 0300.00 5000.00 1000.00	1
	0.08078081E+02	0.05743464E-01-0.02436405E-04	0.04638916E-08-0.03278909E-12	2

0.11470216E+06-0.01953023E+03 0.02115273E+02 0.02326331E+00-0.02109499E-03	3
0.09072734E-07-0.15400926E-11 0.11627381E+06 0.10976027E+02	4
C5H                    20387C    5H   1            G 0300.00   5000.00   1000.00	1
0.08695749E+02 0.06054301E-01-0.02016010E-04 0.02892892E-08-0.14700996E-13	2
0.09031069E+06-0.02101594E+03 0.16348248E+01 0.02509538E+00-0.12066364E-04	3
-0.10465110E-07 0.08809988E-10 0.09212488E+06 0.15121937E+02	4
C5H12                  20387C    5H   12            G 0300.00   4000.00   1000.00	1
0.16677979E+02 0.02114483E+00-0.03533321E-04-0.05742202E-08 0.15159483E-12	2
-0.02553670E+06-0.06372940E+03 0.01877907E+02 0.04121645E+00 0.12532337E-04	3
-0.03701536E-06 0.15255685E-10-0.02003815E+06 0.01877256E+03	4
C5H2                    20587C    5H   2            G 0300.00   5000.00   1000.00	1
0.11329175E+02 0.07424056E-01-0.02628188E-04 0.04082541E-08-0.02301332E-12	2
0.07878706E+06-0.03617117E+03 0.03062321E+02 0.02709998E+00-0.10091697E-04	3
-0.12727451E-07 0.09167219E-10 0.08114969E+06 0.07071078E+02	4
C5H3                    20387C    5H   3            G 0300.00   5000.00   1000.00	1
0.10787622E+02 0.09539619E-01-0.03206744E-04 0.04733323E-08-0.02512135E-12	2
0.06392904E+06-0.03005444E+03 0.04328720E+02 0.02352480E+00-0.05856723E-04	3
-0.12154494E-07 0.07726478E-10 0.06588531E+06 0.04173258E+02	4
C5H6                    20387C    5H   6            G 0300.00   5000.00   1000.00	1
0.09689815E+02 0.01838262E+00-0.06264884E-04 0.09393377E-08-0.05087708E-12	2
0.11021242E+05-0.03122908E+03-0.03196739E+02 0.04081361E+00 0.06816505E-05	3
-0.03137459E-06 0.15772230E-10 0.15290676E+05 0.03869938E+03	4
C6H                    121686C    6H   1            G 0300.00   5000.00   1000.00	1
0.11587352E+02 0.07295362E-01-0.02466008E-04 0.03407045E-08-0.14981855E-13	2
0.10314481E+06-0.03172578E+03 0.04769848E+02 0.02457279E+00-0.07561252E-04	3
-0.14806908E-07 0.09768053E-10 0.10485231E+06 0.03241530E+02	4
C6H10                  20387C    6H   10            G 0300.00   5000.00   1000.00	1
0.15927771E+02 0.02374412E+00-0.06908672E-04 0.08109777E-08-0.02683122E-12	2
-0.08642656E+05-0.06525186E+03-0.13942280E+01 0.04720693E+00 0.11960419E-04	3
-0.04162895E-06 0.01740335E-09-0.02217790E+05 0.03129603E+03	4
C6H14                  20387C    6H   14            G 0300.00   4000.00   1000.00	1
0.02280471E+03 0.02097989E+00-0.03530674E-04-0.05466245E-08 0.14789499E-12	2
-0.03073756E+06-0.09583162E+03 0.01836174E+02 0.05098461E+00 0.12595857E-04	3
-0.04428362E-06 0.01872237E-09-0.02292749E+06 0.02088145E+03	4
C6H2                    121686C    6H   2            G 0300.00   5000.00   1000.00	1
0.12756519E+02 0.08034381E-01-0.02618215E-04 0.03725060E-08-0.01878850E-12	2
0.08075469E+06-0.04041262E+03 0.05751085E+02 0.02636719E+00-0.11667596E-04	3
-0.10714498E-07 0.08790297E-10 0.08262012E+06-0.04335532E+02	4
C6H3                    20387C    6H   3            G 0300.00   5000.00   1000.00	1
0.12761181E+02 0.10385573E-01-0.03479192E-04 0.05109733E-08-0.02690965E-12	2
0.07477706E+06-0.03891745E+03 0.05007089E+02 0.02692851E+00-0.05919865E-04	3
-0.15272335E-07 0.09408310E-10 0.07713200E+06 0.02225621E+02	4
C6H4                    20387C    6H   4            G 0300.00   5000.00   1000.00	1
0.10062741E+02 0.01690304E+00-0.06473045E-04 0.11240806E-08-0.07307566E-12	2



0.05645373E+06-0.02969310E+03-0.13004846E+01	0.03866476E+00-0.03643944E-04	3							
-0.02668580E-06	0.14509357E-10	0.06002907E+06	0.03124939E+03	4					
C6H5	82489C	6H	5	G	0300.00	4000.00	1000.00	1	
0.15775887E+02	0.09651109E-01-0.09429416E-05-0.05469111E-08	0.10265216E-12	2						
0.03302698E+06-0.06176280E+03	0.11435567E+00	0.03627324E+00	0.11582856E-05	3					
-0.02196964E-06	0.08463556E-10	0.03836054E+06	0.02380117E+03	4					
C6H5(L)	82489C	6H	5	G	0300.00	4000.00	1000.00	1	
0.01721540E+03	0.08621068E-01-0.08221340E-05-0.04752164E-08	0.08844086E-12	2						
0.06385819E+06-0.06139128E+03	0.04854268E+02	0.03031659E+00	0.01742892E-05	3					
-0.01811010E-06	0.07392511E-10	0.06798733E+06	0.05854934E+02	4					
C6H5O	82489C	6H	50	1	G	0300.00	4000.00	1000.00	1
0.01822638E+03	0.10039851E-01-0.09915668E-05-0.05672804E-08	0.10683716E-12	2						
-0.02620846E+05-0.07361390E+03	0.11074965E+01	0.03956945E+00	0.08497295E-05	3					
-0.02436311E-06	0.09650659E-10	0.03159672E+05	0.01973496E+03	4					
C6H5OH	82489C	6H	60	1	G	0300.00	4000.00	1000.00	1
0.01821632E+03	0.11424269E-01-0.10966843E-05-0.06427442E-08	0.11988930E-12	2						
-0.02053664E+06-0.07304233E+03	0.13914556E+01	0.03931957E+00	0.01777096E-04	3					
-0.02277673E-06	0.08309659E-10-0.14721809E+05	0.01917813E+03	4						
C6H6	20387C	6H	6	G	0300.00	5000.00	1000.00	1	
0.12910740E+02	0.01723296E+00-0.05024210E-04	0.05893497E-08-0.01947521E-12	2						
0.03664511E+05-0.05002699E+03-0.03138012E+02	0.04723103E+00-0.02962207E-04	3							
-0.03262819E-06	0.01718691E-09	0.08890031E+05	0.03657573E+03	4					
C6H7	82489C	6H	7	G	0300.00	4000.00	1000.00	1	
0.01755221E+03	0.12270795E-01-0.11857424E-05-0.06959661E-08	0.13013259E-12	2						
0.16245813E+05-0.07166588E+03	0.04639166E+01	0.03975928E+00	0.02529095E-04	3					
-0.02223792E-06	0.07557053E-10	0.02225169E+06	0.02235387E+03	4					
C8H	121686C	8H	1	G	0300.00	5000.00	1000.00	1	
0.14749907E+02	0.09931501E-01-0.03374841E-04	0.04687592E-08-0.02073536E-12	2						
0.13994481E+06-0.04892689E+03	0.04489507E+02	0.03521521E+00-0.10193898E-04	3						
-0.02197024E-06	0.14214164E-10	0.14259919E+06	0.03996225E+02	4					
C8H2	121686C	8H	2	G	0300.00	5000.00	1000.00	1	
0.15680213E+02	0.11154614E-01-0.03724372E-04	0.05197891E-08-0.02375550E-12	2						
0.10811225E+06-0.05571437E+03	0.04630427E+02	0.03937080E+00-0.11480348E-04	3						
-0.02562213E-06	0.16707913E-10	0.11082850E+06	0.08077425E+01	4					
CCL	112989C	1CL	1	G	0300.00	5000.00	1000.00	1	
0.04072804E+02	0.05508787E-02-0.02319334E-05	0.04669038E-09-0.03236856E-13	2						
0.05909198E+06	0.03481073E+02	0.03188782E+02	0.02965197E-01-0.02305370E-04	3					
0.04866913E-08	0.09990141E-12	0.05932937E+06	0.08037628E+02	4					
CCL2	112989C	1CL	2	G	0300.00	5000.00	1000.00	1	
0.03501741E+02	0.05749397E-01-0.02589721E-04	0.04783950E-08-0.03188271E-12	2						
0.02763633E+06	0.10829469E+02	0.02651916E+02	0.15169552E-01-0.02230162E-03	3					
0.15041039E-07-0.03452951E-10	0.02739027E+06	0.13136703E+02	4						
CCL2CCLO	53090C	20	1CL	3	G	0300.00	5000.00	1500.00	1
0.15141676E+02	0.06977550E-02-0.02990825E-05	0.04990197E-09-0.02906948E-13	2						

-0.01791145E+06-0.04609734E+03 0.05021425E+02 0.02873361E+00-0.03166389E-03	3
0.16482881E-07-0.03326171E-10-0.14736788E+05 0.06864806E+02	4
CCL2CCL0H 53090C 2H 10 1CL 3G 0300.00 5000.00 1500.00	1
0.15672590E+02 0.02218766E-01-0.04425239E-05 0.06261725E-10 0.03673506E-13	2
-0.02855361E+06-0.05085224E+03 0.04602117E+02 0.03408841E+00-0.03836908E-03	3
0.02120271E-06-0.04527143E-10-0.02507945E+06 0.06859776E+02	4
CCL2CH 53090C 2H 1CL 2 G 0300.00 5000.00 1500.00	1
0.11285897E+02 0.10882791E-02-0.02970597E-05 0.02568798E-09 0.07721928E-15	2
0.02690442E+06-0.03051886E+03 0.02864643E+02 0.02486908E+00-0.02845679E-03	3
0.15845013E-07-0.03413406E-10 0.02962549E+06 0.13599581E+02	4
CCL2H00 53090C 1H 10 2CL 2G 0300.00 5000.00 1500.00	1
0.12739674E+02 0.16717894E-02-0.03280073E-05 0.09239023E-10 0.02183938E-13	2
-0.05665040E+05-0.03552584E+03 0.03425417E+02 0.02745544E+00-0.02973832E-03	3
0.15883908E-07-0.03309427E-10-0.02675528E+05 0.13334742E+02	4
CCL20HCH2 53090C 2H 30 1CL 2G 0300.00 5000.00 1500.00	1
0.16063548E+02 0.02856411E-01-0.05564238E-05 0.02056416E-09 0.02871365E-13	2
-0.01756114E+06-0.05438455E+03 0.02870958E+02 0.04462273E+00-0.05377945E-03	3
0.03093185E-06-0.06719238E-10-0.13796362E+05 0.13054657E+02	4
CCL20HCHCL 53090C 2H 20 1CL 3G 0300.00 5000.00 1500.00	1
0.01681474E+03 0.02433420E-01-0.04717311E-05 0.15953268E-10 0.02647196E-13	2
-0.02217114E+06-0.05406904E+03 0.05487264E+02 0.03719540E+00-0.04391385E-03	3
0.02501465E-06-0.05417859E-10-0.01882134E+06 0.04237537E+02	4
CCL3 112989C 1CL 3 G 0300.00 5000.00 1000.00	1
0.08639372E+02 0.15880909E-02-0.07176410E-05 0.14271238E-09-0.10407368E-13	2
0.06701065E+05-0.14518221E+02 0.04866162E+02 0.11903691E-01-0.07849049E-04	3
-0.14484371E-08 0.02169760E-10 0.07655364E+05 0.04781636E+02	4
CCL3CCLH2 53090C 2H 2CL 4 G 0300.00 5000.00 1500.00	1
0.01788619E+03 0.02281235E-01-0.04746597E-05 0.01962666E-09 0.02451768E-13	2
-0.02496335E+06-0.06312882E+03 0.03463508E+02 0.04144805E+00-0.04421052E-03	3
0.02320524E-06-0.04772524E-10-0.02028144E+06 0.12759561E+02	4
CCL3CCLO 53090C 20 1CL 4 G 0300.00 5000.00 1500.00	1
0.01695666E+03 0.12164193E-02-0.03883945E-05 0.05659408E-09-0.03108071E-13	2
-0.03446237E+06-0.05335311E+03 0.06322721E+02 0.03467971E+00-0.04187452E-03	3
0.02335691E-06-0.04912887E-10-0.03151848E+06 0.08933105E+01	4
CCL3CH2 53090C 2H 2CL 3 G 0300.00 5000.00 1500.00	1
0.14682432E+02 0.02202648E-01-0.03960690E-05 0.02319279E-10 0.03655521E-13	2
0.03875530E+05-0.04495230E+03 0.05008132E+02 0.03031102E+00-0.03453619E-03	3
0.01951049E-06-0.04245839E-10 0.06936588E+05 0.05474640E+02	4
CCL3CHCL 53090C 2H 1CL 4 G 0300.00 5000.00 1500.00	1
0.16101979E+02 0.15972234E-02-0.04069891E-05 0.04158082E-09-0.11056349E-14	2
-0.02318813E+04-0.04936573E+03 0.05761929E+02 0.03433482E+00-0.04163980E-03	3
0.02362341E-06-0.05054182E-10 0.02663919E+05 0.03399587E+02	4
CCL3CHO 53090C 2H 10 1CL 3G 0300.00 5000.00 1500.00	1
0.15321347E+02 0.01914228E-01-0.03622777E-05 0.05526563E-10 0.03016202E-13	2

-0.02886498E+06-0.04774515E+03 0.05016866E+02 0.02961902E+00-0.03140320E-03	3
0.16666434E-07-0.03481661E-10-0.02544921E+06 0.06644421E+02	4
CCL300 53090C 10 2CL 3 G 0300.00 5000.00 1500.00	1
0.14732491E+02 0.08345102E-02-0.03627944E-05 0.07101158E-09-0.05165897E-13	2
-0.05526644E+05-0.04381960E+03 0.04317420E+02 0.03486414E+00-0.04287094E-03	3
0.02371950E-06-0.04903871E-10-0.02855911E+05 0.08720693E+02	4
CCL4 112989C 1CL 4 G 0300.00 5000.00 1000.00	1
0.11369968E+02 0.01933276E-01-0.08832003E-05 0.01770067E-08-0.12982896E-13	2
-0.15283466E+05-0.02874324E+03 0.06286815E+02 0.15997799E-01-0.10203526E-04	3
-0.03043311E-07 0.03546287E-10-0.14032573E+05-0.02850812E+02	4
CCLH200 53090C 1H 20 2CL 1G 0300.00 5000.00 1500.00	1
0.11313508E+02 0.02330645E-01-0.03546376E-05-0.02064087E-09 0.06154082E-13	2
-0.04225590E+05-0.03183829E+03 0.15835406E+01 0.02745395E+00-0.02803155E-03	3
0.14915985E-07-0.03172719E-10-0.08340802E+04 0.01999022E+03	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 0.02072875E-01-0.05134431E-04	3
0.05733890E-07-0.01955533E-10 0.07045259E+06 0.03331587E+02	4
CH+ 121286C 1H 1E -1 G 0300.00 5000.00 1000.00	1
0.02753358E+02 0.15528998E-02-0.05368453E-05 0.08921772E-09-0.05416801E-13	2
0.01948467E+07 0.04654892E+02 0.03327207E+02 0.13470505E-02-0.03895861E-04	3
0.05129390E-07-0.02054575E-10 0.01946452E+07 0.14084738E+01	4
CH2 120186C 1H 2 G 0250.00 4000.00 1000.00	1
0.03636407E+02 0.01933056E-01-0.01687016E-05-0.10098994E-09 0.01808255E-12	2
0.04534134E+06 0.02156560E+02 0.03762237E+02 0.11598191E-02 0.02489585E-05	3
0.08800836E-08-0.07332435E-11 0.04536790E+06 0.01712577E+02	4
CH2(S) 31287C 1H 2 G 0300.00 4000.00 1000.00	1
0.03552888E+02 0.02066788E-01-0.01914116E-05-0.11046733E-09 0.02021349E-12	2
0.04984975E+06 0.01686570E+02 0.03971265E+02-0.01699088E-02 0.10253689E-05	3
0.02492550E-07-0.01981266E-10 0.04989367E+06 0.05753207E+00	4
CH2CCL 53090C 2H 2CL 1 G 0300.00 5000.00 1500.00	1
0.09117805E+02 0.02336015E-01-0.03466389E-05-0.03584809E-09 0.08154328E-13	2
0.02697366E+06-0.02251741E+03 0.15531771E+01 0.02243158E+00-0.02366950E-03	3
0.13232700E-07-0.02931822E-10 0.02962338E+06 0.01769303E+03	4
CH2CCL2 53090C 2H 2CL 2 G 0300.00 5000.00 1500.00	1
0.11694514E+02 0.02435982E-01-0.03733045E-05-0.14194121E-10 0.05199337E-13	2
-0.04601974E+05-0.03547414E+03 0.15271658E+01 0.02983780E+00-0.03171097E-03	3
0.01728379E-06-0.03709638E-10-0.11739856E+04 0.01827540E+03	4
CH2CCL0H 53090C 2H 30 1CL 1G 0300.00 5000.00 1500.00	1
0.12676007E+02 0.03201391E-01-0.04788878E-05-0.02136104E-09 0.07030796E-13	2
-0.02402379E+06-0.04128497E+03 0.06647839E+01 0.03723168E+00-0.04115205E-03	3
0.02307135E-06-0.05021609E-10-0.02012318E+06 0.02165269E+03	4
CH2CHCCH 82489C 4H 4 G 0300.00 4000.00 1000.00	1
0.10697773E+02 0.06982014E-01-0.06567747E-05-0.03884517E-08 0.07200946E-12	2

0.03034803E+06-0.03128430E+03 0.03233893E+02 0.01865634E+00 0.12703205E-05	3
-0.09410096E-07 0.02956110E-10 0.03301097E+06 0.09922676E+02	4
CH2CHCCH2 82489C 4H 5 G 0300.00 4000.00 1000.00	1
0.11997762E+02 0.07990580E-01-0.08098172E-05-0.04568733E-08 0.08636911E-12	2
0.03228493E+06-0.03528494E+03 0.03879443E+02 0.01997663E+00 0.01872777E-04	3
-0.09306953E-07 0.02386116E-10 0.03526859E+06 0.09842152E+02	4
CH2CHCH2 82489C 3H 5 G 0300.00 4000.00 1000.00	1
0.09651539E+02 0.08075596E-01-0.07965424E-05-0.04650696E-08 0.08603281E-12	2
0.15300955E+05-0.02686773E+03 0.02276486E+02 0.01985564E+00 0.11238421E-05	3
-0.10145757E-07 0.03441342E-10 0.01789496E+06 0.13725151E+02	4
CH2CHCHCH 82489C 4H 5 G 0300.00 4000.00 1000.00	1
0.12865971E+02 0.07943369E-01-0.08626466E-05-0.04655635E-08 0.08951131E-12	2
0.03783552E+06-0.04182502E+03 0.02995240E+02 0.02288456E+00 0.01975471E-04	3
-0.11482454E-07 0.03197823E-10 0.04142218E+06 0.12894539E+02	4
CH2CHCHCH2 120189C 4H 6 G 0300.00 4000.00 1000.00	1
0.12544366E+02 0.09596525E-01-0.09187012E-05-0.05429640E-08 0.10053636E-12	2
0.08597330E+05-0.04217450E+03 0.01931624E+02 0.02479030E+00 0.03018071E-04	3
-0.11546856E-07 0.02586623E-10 0.12554682E+05 0.01701999E+03	4
CH2CHCL 53090C 2H 3CL 1 G 0300.00 5000.00 1500.00	1
0.10298199E+02 0.03042925E-01-0.03881390E-05-0.04925564E-09 0.10050715E-13	2
-0.02492899E+05-0.03108614E+03 0.11180263E+00 0.02796358E+00-0.02726558E-03	3
0.14632574E-07-0.03204074E-10 0.12878441E+04 0.02381617E+03	4
CH2CL 53090C 1H 2CL 1 G 0300.00 5000.00 1500.00	1
0.06822514E+02 0.16597443E-02-0.02075515E-05-0.02793518E-09 0.05509086E-13	2
0.10804545E+05-0.10905042E+02 0.02419924E+02 0.13033171E-01-0.13565594E-04	3
0.07836107E-07-0.01800534E-10 0.12431121E+05 0.12698449E+02	4
CH2CL2 112989C 1H 2CL 2 G 0300.00 5000.00 1000.00	1
0.05917327E+02 0.06762395E-01-0.02676163E-04 0.04856687E-08-0.03316973E-12	2
-0.13859256E+05-0.03877739E+02 0.14232844E+01 0.02116658E+00-0.02178088E-03	3
0.13458726E-07-0.03811649E-10-0.12686636E+05 0.01893445E+03	4
CH2CLCCL2 53090C 2H 2CL 3 G 0300.00 5000.00 1500.00	1
0.14381561E+02 0.02379634E-01-0.04167425E-05-0.02445116E-10 0.04499574E-13	2
-0.02746720E+05-0.04351762E+03 0.03351194E+02 0.03297632E+00-0.03604138E-03	3
0.01977452E-06-0.04233823E-10 0.08620011E+04 0.14447600E+02	4
CH2CLCCL0 53090C 2H 20 1CL 2G 0300.00 5000.00 1500.00	1
0.13920275E+02 0.02589602E-01-0.04141891E-05-0.16431689E-10 0.06237174E-13	2
-0.03517256E+06-0.04389502E+03 0.02705994E+02 0.03210128E+00-0.03357727E-03	3
0.01814310E-06-0.03890009E-10-0.03130905E+06 0.15660126E+02	4
CH2CLCH2 53090C 2H 4CL 1 G 0300.00 5000.00 1500.00	1
0.11670112E+02 0.03554721E-01-0.04124240E-05-0.07276109E-09 0.13167557E-13	2
0.06201629E+05-0.03604549E+03 0.16358643E+01 0.02680201E+00-0.02491421E-03	3
0.13492354E-07-0.03046571E-10 0.10142940E+05 0.01864247E+03	4
CH2CLCH2CL 53090C 2H 4CL 2 G 0300.00 5000.00 1500.00	1
0.14431431E+02 0.03836770E-01-0.05299122E-05-0.05165412E-09 0.11776360E-13	2

-0.02296285E+06-0.05130124E+03-0.02436500E+01	0.04032574E+00-0.03956993E-03	3
0.02074244E-06-0.04412604E-10-0.01767830E+06	0.02741366E+03	4
CH2CLCHCL	53090C 2H 3CL 2 G 0300.00 5000.00 1500.00	1
0.12955933E+02 0.03001688E-01-0.04165161E-05-0.03909055E-09	0.09041090E-13	2
0.09932077E+04-0.03925386E+03 0.02276185E+02	0.03011400E+00-0.03047664E-03	3
0.16548801E-07-0.03613198E-10 0.04836340E+05	0.01792166E+03	4
CH2CLCHCL2	53090C 2H 3CL 3 G 0300.00 5000.00 1500.00	1
0.16187391E+02 0.03047680E-01-0.05011496E-05-0.15967010E-10	0.07107547E-13	2
-0.02474417E+06-0.05695454E+03 0.12390108E+01	0.04148443E+00-0.04188653E-03	3
0.02163214E-06-0.04467363E-10-0.01960717E+06	0.02257855E+03	4
CH2CLCHO	53090C 2H 30 1CL 1G 0300.00 5000.00 1500.00	1
0.12279553E+02 0.03320979E-01-0.04106709E-05-0.06199826E-09	0.11905937E-13	2
-0.02678416E+06-0.03762355E+03 0.06553003E+01	0.02959045E+00-0.02635055E-03	3
0.13275453E-07-0.02838288E-10-0.02227004E+06	0.02576796E+03	4
CH2CO	121686C 2H 20 1 G 0300.00 5000.00 1000.00	1
0.06038817E+02 0.05804840E-01-0.01920953E-04	0.02794484E-08-0.14588676E-13	2
-0.08583402E+05-0.07657581E+02 0.02974970E+02	0.12118712E-01-0.02345045E-04	3
-0.06466685E-07 0.03905649E-10-0.07632636E+05	0.08673553E+02	4
CH2F2	82489C 1H 2F 2 G 0300.00 5000.00 1000.00	1
0.04730052E+02 0.07997300E-01-0.03186045E-04	0.05801159E-08-0.03967925E-12	2
-0.05637288E+06-0.04954843E+01 0.03669433E+01	0.02168917E+00-0.02441912E-03	3
0.01942310E-06-0.06978343E-10-0.05510102E+06	0.02202214E+03	4
CH2HCO	1201860 1H 3C 2 G 0300.00 5000.00 1000.00	1
0.05975670E+02 0.08130591E-01-0.02743624E-04	0.04070304E-08-0.02176017E-12	2
0.04903218E+04-0.05045251E+02 0.03409062E+02	0.10738574E-01 0.01891492E-04	3
-0.07158583E-07 0.02867385E-10 0.15214766E+04	0.09558290E+02	4
CH2O	121286C 1H 20 1 G 0300.00 5000.00 1000.00	1
0.02995606E+02 0.06681321E-01-0.02628954E-04	0.04737153E-08-0.03212517E-12	2
-0.15320369E+05 0.06912572E+02 0.16527311E+01	0.12631439E-01-0.01888168E-03	3
0.02050031E-06-0.08413237E-10-0.14865404E+05	0.13784820E+02	4
CH2OH	120186H 3C 10 1 G 0250.00 4000.00 1000.00	1
0.06327520E+02 0.03608270E-01-0.03201547E-05-0.01938750E-08	0.03509704E-12	2
-0.04474509E+05-0.08329365E+02 0.02862628E+02	0.10015273E-01-0.05285435E-05	3
-0.05138539E-07 0.02246041E-10-0.03349678E+05	0.10397938E+02	4
CH2OHCCL2	53090C 2H 30 1CL 2G 0300.00 5000.00 1500.00	1
0.16021814E+02 0.02846351E-01-0.04974217E-05-0.02167449E-10	0.05246046E-13	2
-0.01829578E+06-0.05402134E+03 0.01922939E+02	0.04158207E+00-0.04427504E-03	3
0.02343015E-06-0.04851867E-10-0.13755118E+05	0.02001901E+03	4
CH2OHCCL	53090C 2H 40 1CL 1G 0300.00 5000.00 1500.00	1
0.14462976E+02 0.03569514E-01-0.05419118E-05-0.02862176E-09	0.08920560E-13	2
-0.14755591E+05-0.04942815E+03 0.03505696E+01	0.04212748E+00-0.04493839E-03	3
0.02448187E-06-0.05236589E-10-0.10073139E+05	0.02495260E+03	4
CH3	121286C 1H 3 G 0300.00 5000.00 1000.00	1
0.02844051E+02 0.06137974E-01-0.02230345E-04	0.03785161E-08-0.02452159E-12	2

0.16437809E+05	0.05452697E+02	0.02430442E+02	0.11124099E-01	-0.01680220E-03	3
0.16218288E-07	-0.05864952E-10	0.16423781E+05	0.06789794E+02		4
CH3C(O)CL	53090C	2H 30	1CL 1G	0300.00 5000.00 1500.00	1
0.12405677E+02	0.03210496E-01	-0.03737156E-05	-0.06739591E-09	0.12191219E-13	2
-0.03432420E+06	-0.03909195E+03	0.02275117E+02	0.02518533E+00	-0.02152419E-03	3
0.10840052E-07	-0.02369191E-10	-0.03024375E+06	0.16570161E+02		4
CH3CC	82489C	3H 3	G	0300.00 4000.00 1000.00	1
0.07640221E+02	0.05233556E-01	-0.05053635E-05	-0.02919772E-08	0.05445700E-12	2
0.05909763E+06	-0.16295735E+02	0.03798751E+02	0.08749062E-01	0.02523014E-04	3
-0.15293730E-08	-0.14105619E-11	0.06077425E+06	0.05989223E+02		4
CH3CCCH2	82489C	4H 5	G	0300.00 4000.00 1000.00	1
0.11565059E+02	0.08030297E-01	-0.07649450E-05	-0.04476533E-08	0.08313260E-12	2
0.03256813E+06	-0.03014066E+03	0.05068450E+02	0.15717475E-01	0.02968975E-04	3
-0.04990586E-07	-0.02984224E-11	0.03518855E+06	0.06791893E+02		4
CH3CCCH3	120189C	4H 6	G	0300.00 4000.00 1000.00	1
0.11336582E+02	0.10057637E-01	-0.09511323E-05	-0.05660496E-08	0.10494509E-12	2
0.15476594E+05	-0.03350866E+03	0.04077105E+02	0.01703158E+00	0.04707490E-04	3
-0.03767239E-07	-0.02066962E-10	0.01859756E+06	0.08444801E+02		4
CH3CCH2	82489C	3H 5	G	0300.00 4000.00 1000.00	1
0.09101018E+02	0.07964167E-01	-0.07884945E-05	-0.04562036E-08	0.08529212E-12	2
0.02670680E+06	-0.02150559E+03	0.03385811E+02	0.14045337E-01	0.03204127E-04	3
-0.03824120E-07	-0.09053742E-11	0.02909066E+06	0.11266487E+02		4
CH3CCL	53090C	2H 3CL 1	G	0300.00 5000.00 1500.00	1
0.10239621E+02	0.02767116E-01	-0.03228852E-05	-0.05752548E-09	0.10434300E-13	2
0.02633606E+06	-0.02806184E+03	0.01687397E+02	0.02164346E+00	-0.01891465E-03	3
0.09699015E-07	-0.02134580E-10	0.02975387E+06	0.01882235E+03		4
CH3CCL2	53090C	2H 3CL 2	G	0300.00 5000.00 1500.00	1
0.13000347E+02	0.02940484E-01	-0.03746456E-05	-0.05040643E-09	0.10063317E-13	2
-0.04228816E+04	-0.03979862E+03	0.03213472E+02	0.02587378E+00	-0.02419993E-03	3
0.12738171E-07	-0.02788481E-10	0.03325662E+05	0.13333204E+02		4
CH3CCL3	53090C	2H 3CL 3	G	0300.00 5000.00 1500.00	1
0.16371605E+02	0.02935021E-01	-0.04836108E-05	-0.14547226E-10	0.06731690E-13	2
-0.02378095E+06	-0.05941863E+03	0.02484363E+02	0.03909474E+00	-0.04013637E-03	3
0.02110179E-06	-0.04418213E-10	0.01902539E+06	0.14356027E+02		4
CH3CCLO	53090C	2H 30	1CL 1G	0300.00 5000.00 1500.00	1
0.12405953E+02	0.03210266E-01	-0.03736396E-05	-0.06740236E-09	0.12190806E-13	2
-0.03432283E+06	-0.03909604E+03	0.02277402E+02	0.02517912E+00	-0.02151631E-03	3
0.10835236E-07	-0.02368078E-10	-0.03024307E+06	0.16555561E+02		4
CH3CH2CCH	120189C	4H 6	G	0300.00 4000.00 1000.00	1
0.12006946E+02	0.09576069E-01	-0.08995018E-05	-0.05369808E-08	0.09934174E-12	2
0.01729419E+06	-0.03802692E+03	0.03726043E+02	0.02053492E+00	0.03021439E-04	3
-0.08131812E-07	0.10952799E-11	0.02048821E+06	0.08538826E+02		4
CH3CH2CH2C	62090C	4H 10	G	0300.00 4000.00 1500.00	1
0.02032597E+03	0.10251895E-01	-0.09348665E-05	-0.04706743E-08	0.08327282E-12	2

-0.02590868E+06-0.08998431E+03-0.02544545E+02	0.05770712E+00-0.04104932E-03	3
0.01684742E-06-0.03176652E-10-0.01682846E+06	0.03586176E+03	4
CH3CH2CL	53090C 2H 5CL 1 G 0300.00 5000.00 1500.00	1
0.13011182E+02 0.04448941E-01-0.05200473E-05-0.09119710E-09	0.16588421E-13	2
-0.02013502E+06-0.04677847E+03-0.06981899E+01	0.03567705E+00-0.03230260E-03	3
0.01689621E-06-0.03727523E-10-0.14760543E+05	0.02802218E+03	4
CH3CH2O	103190C 2H 5O 1 G 0300.00 4000.00 1500.00	1
0.11871147E+02 0.05390415E-01-0.04990159E-05-0.02399584E-08	0.04255456E-12	2
-0.05950457E+05-0.03996584E+03 0.06904570E+01	0.02951397E+00-0.02245116E-03	3
0.10116003E-07-0.02044100E-10-0.15599183E+04	0.02130229E+03	4
CH3CHCH	82489C 3H 5 G 0300.00 4000.00 1000.00	1
0.09209764E+02 0.07871412E-01-0.07724522E-05-0.04497357E-08	0.08377272E-12	2
0.02853967E+06-0.02232369E+03 0.03161863E+02	0.15180997E-01 0.02722659E-04	3
-0.05177112E-07 0.05435286E-12 0.03095547E+06	0.11979733E+02	4
CH3CHCL	53090C 2H 4CL 1 G 0300.00 5000.00 1500.00	1
0.11662910E+02 0.03539284E-01-0.03858423E-05-0.08186870E-09	0.14075489E-13	2
0.03696641E+05-0.03616107E+03 0.01903574E+02	0.02438192E+00-0.02062778E-03	3
0.10683821E-07-0.02414460E-10 0.07722870E+05	0.01768152E+03	4
CH3CHCL2	53090C 2H 4CL 2 G 0300.00 5000.00 1500.00	1
0.14543108E+02 0.03772378E-01-0.05189301E-05-0.05141063E-09	0.11630760E-13	2
-0.02277045E+06-0.05147426E+03 0.04510763E+01	0.03884900E+00-0.03832912E-03	3
0.02029502E-06-0.04357591E-10-0.01767233E+06	0.02414545E+03	4
CH3CHOH	103190C 2H 4O 1 G 0300.00 4000.00 1500.00	1
0.11611482E+02 0.05173117E-01-0.04856684E-05-0.02202894E-08	0.03913721E-12	2
-0.12488109E+05-0.03688212E+03 0.14159398E+01	0.02870648E+00-0.02373820E-03	3
0.11488865E-07-0.02391420E-10-0.08638718E+05	0.01844256E+03	4
CH3CL	112989C 1H 3CL 1 G 0300.00 5000.00 1000.00	1
0.03633875E+02 0.08664625E-01-0.03343871E-04	0.05950130E-08-0.04001401E-12	2
-0.11776588E+05 0.04430651E+02 0.04621901E+01	0.02068247E+00-0.02553133E-03	3
0.02160310E-06-0.07706816E-10-0.10936672E+05	0.02032976E+03	4
CH3CO	120186C 2H 3O 1 G 0300.00 5000.00 1000.00	1
0.05612279E+02 0.08449886E-01-0.02854147E-04	0.04238376E-08-0.02268403E-12	2
-0.05187863E+05-0.03274949E+02 0.03125278E+02	0.09778220E-01 0.04521448E-04	3
-0.09009462E-07 0.03193717E-10-0.04108507E+05	0.11228854E+02	4
CH3F	82489C 1H 3F 1 G 0300.00 5000.00 1000.00	1
0.03014978E+02 0.09314397E-01-0.03611697E-04	0.06443728E-08-0.04339594E-12	2
-0.02977838E+06 0.06323815E+02 0.02600910E+01	0.02000787E+00-0.02662584E-03	3
0.02561176E-06-0.09935237E-10-0.02896232E+06	0.02031799E+03	4
CH3HCO	120186C 2O 1H 4 G 0300.00 5000.00 1000.00	1
0.05868650E+02 0.10794241E-01-0.03645530E-04	0.05412912E-08-0.02896844E-12	2
-0.02264568E+06-0.06012946E+02 0.02505695E+02	0.13369907E-01 0.04671953E-04	3
-0.11281401E-07 0.04263566E-10-0.02124588E+06	0.13350887E+02	4
C2H4O	61192C 2H 4O 1 G 0300.00 5000.00 1000.00	1
0.59249249E+01 0.11120714E-01-0.37434083E-05	0.55413918E-09-0.29549886E-13	2

-0.93028008E+04-0.93792849E+01-0.24173594E+00	0.20761095E-01	0.21481201E-05	3		
-0.16948157E-07	0.81075771E-11-0.71720117E+04	0.24432190E+02	4		
CH3NO	103190C	1H 3N 10 1G	0300.00 4000.00 1500.00	1	
0.08820547E+02	0.03706233E-01-0.02894740E-05-0.01897910E-08	0.03237544E-12	2		
0.05362862E+05-0.02213220E+03	0.02109955E+02	0.15178216E-01-0.07071789E-04	3		
0.15106108E-08-0.16042035E-12	0.08293612E+05	0.15697023E+02	4		
CH3NO2	103190C	1H 3N 10 2G	0300.00 4000.00 1500.00	1	
0.10901579E+02	0.04326381E-01-0.04203547E-05-0.01893070E-08	0.03417444E-12	2		
-0.13708618E+05-0.03073183E+03	0.03224716E+01	0.02665146E+00-0.01930573E-03	3		
0.07762620E-07-0.13987461E-11-0.09597527E+05	0.02726156E+03		4		
CH3O	121686C	1H 3O 1 G	0300.00 3000.00 1000.00	1	
0.03770799E+02	0.07871497E-01-0.02656384E-04	0.03944431E-08-0.02112616E-12	2		
0.12783252E+03	0.02929575E+02	0.02106204E+02	0.07216595E-01	0.05338472E-04	3
-0.07377636E-07	0.02075610E-10	0.09786011E+04	0.13152177E+02	4	
CH3OCH3	103190C	1H 6O 1 G	0300.00 4000.00 1500.00	1	
0.12280999E+02	0.06711031E-01-0.04726871E-05-0.03636408E-08	0.06084545E-12	2		
-0.02839742E+06-0.04434692E+03	0.12452464E+01	0.02381198E+00-0.08266949E-04	3		
0.03068452E-08	0.01909247E-11-0.02335996E+06	0.01855817E+03	4		
CH3OCL	53090C	1H 3O 1CL 1G	0300.00 5000.00 1500.00	1	
0.10225182E+02	0.02780046E-01-0.03331582E-05-0.05437857E-09	0.10127989E-13	2		
-0.11728864E+05-0.02912014E+03	0.15753918E+01	0.02255641E+00-0.02052644E-03	3		
0.10753116E-07-0.02371139E-10-0.08346834E+05	0.01804592E+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	0.02378195E+02	0.02660115E+02	0.07341508E-01	0.07170050E-04	3
-0.08793194E-07	0.02390570E-10-0.02535348E+06	0.11232631E+02	4		
CH3ONO	103190C	1H 3N 1O 2G	0300.00 4000.00 1500.00	1	
0.11361289E+02	0.04159349E-01-0.04145670E-05-0.01695140E-08	0.03028732E-12	2		
-0.12814815E+05-0.03545434E+03	0.14903451E+01	0.02645433E+00-0.02112331E-03	3		
0.09414399E-07-0.01811204E-10-0.09125782E+05	0.01813766E+03		4		
CH3ONO2	103190C	1H 3N 1O 3G	0300.00 4000.00 1500.00	1	
0.14361885E+02	0.04112243E-01-0.05113052E-05-0.14964364E-09	0.03012156E-12	2		
-0.01972440E+06-0.05131841E+03	0.07803354E+01	0.03454203E+00-0.02822327E-03	3		
0.12323244E-07-0.02302164E-10-0.14653465E+05	0.02245751E+03		4		
CH3SICL3	112989C	1H 3CL 3SI 1G	0300.00 1500.00 1000.00	1	
0.11803988E+02	0.07642902E-01-0.09493348E-06-0.01852654E-07	0.05302190E-11	2		
-0.06773651E+06-0.02794492E+03	0.04637712E+02	0.03733016E+00-0.04798528E-03	3		
0.03353132E-06-0.09484405E-10-0.06629348E+06	0.06524867E+02		4		
CH4	121286C	1H 4 C	0300.00 5000.00 1000.00	1	
0.01683478E+02	0.10237236E-01-0.03875128E-04	0.06785585E-08-0.04503423E-12	2		
-0.10080787E+05	0.09623395E+02	0.07787415E+01	0.01747668E+00-0.02783409E-03	3	
0.03049708E-06-0.12239307E-10-0.09825229E+05	0.13722195E+02		4		
CHCL	112989C	1H 1CL 1 C	0300.00 5000.00 1200.00	1	
0.03216518E+02	0.05976969E-01-0.02918238E-04	0.05912801E-08-0.04297945E-12	2		



0.03879839E+06	0.07793842E+02	0.02781262E+02	0.07805384E-01	-0.10637111E-04	3	
0.10654407E-07	-0.03916796E-10	0.03916144E+06	0.10455153E+02		4	
CHCL2	53090C	1H	1CL	2 G	0300.00 5000.00 1500.00	1
0.08032398E+02	0.11531976E-02	-0.02169291E-05	0.04339871E-10	0.16242214E-14	2	
0.07172277E+05	-0.13608548E+02	0.02605184E+02	0.01704116E+00	-0.01946890E-03	3	
0.10921945E-07	-0.02355848E-10	0.08860428E+05	0.14609755E+02		4	
CHCL2CCL2	53090C	2H	1CL	4 G	0300.00 5000.00 1500.00	1
0.15608872E+02	0.01838544E-01	-0.04072595E-05	0.02565420E-09	0.09429433E-14	2	
-0.01711874E+05	-0.04532078E+03	0.04093589E+02	0.03504542E+00	-0.03934971E-03	3	
0.02132083E-06	-0.04452537E-10	0.01825593E+05	0.14572336E+02		4	
CHCL2CCLO	53090C	2H	10	1CL 3G	0300.00 5000.00 1500.00	1
0.15320352E+02	0.01958823E-01	-0.04029279E-05	0.01718038E-09	0.01947391E-13	2	
-0.03512710E+06	-0.04770829E+03	0.04171598E+02	0.03364874E+00	-0.03751009E-03	3	
0.02045352E-06	-0.04317592E-10	-0.03161401E+06	0.10511701E+02		4	
CHCL2CH2	53090C	2H	3CL	2 G	0300.00 5000.00 1500.00	1
0.13066320E+02	0.02964322E-01	-0.04303601E-05	-0.03173130E-09	0.08244908E-13	2	
0.04594697E+05	-0.03814765E+03	0.02234888E+02	0.03152885E+00	-0.03307989E-03	3	
0.01825220E-06	-0.03994163E-10	0.08375531E+05	0.01944506E+03		4	
CHCL2CHCL	53090C	2H	2CL	3 G	0300.00 5000.00 1500.00	1
0.14450509E+02	0.02336553E-01	-0.04132107E-05	-0.05243785E-11	0.04204775E-13	2	
-0.05183249E+04	-0.04362698E+03	0.03789098E+02	0.03243338E+00	-0.03598338E-03	3	
0.01993302E-06	-0.04287482E-10	0.02920910E+05	0.12219906E+02		4	
CHCL2CHCL2	53090C	2H	2CL	4 G	0300.00 5000.00 1500.00	1
0.01745859E+03	0.02484178E-01	-0.05127802E-05	0.02266908E-09	0.02371932E-13	2	
-0.02510698E+06	-0.06065212E+03	0.02711746E+02	0.04441279E+00	-0.04905961E-03	3	
0.02632472E-06	-0.05466292E-10	-0.02052420E+06	0.16248570E+02		4	
CHCL3	112989C	1H	1CL	3 G	0300.00 5000.00 1000.00	1
0.08523544E+02	0.04480142E-01	-0.01837282E-04	0.03424891E-08	-0.02387283E-12	2	
-0.15461167E+05	-0.15056193E+02	0.03437633E+02	0.01941496E+00	-0.16494730E-04	3	
0.05196545E-07	-0.06939614E-12	-0.14161262E+05	0.10863299E+02		4	
CHCLCCL	53090C	2H	1CL	2 G	0300.00 5000.00 1500.00	1
0.10529550E+02	0.14895809E-02	-0.02819799E-05	0.10881009E-10	0.12974696E-14	2	
0.02402717E+06	-0.02591375E+03	0.02527849E+02	0.02424350E+00	-0.02697107E-03	3	
0.14741279E-07	-0.03118468E-10	0.02655177E+06	0.15875552E+02		4	
CHCLCLOH	53090C	2H	20	1CL 2G	0300.00 5000.00 1500.00	1
0.14122059E+02	0.02583764E-01	-0.04576900E-05	0.05215675E-10	0.03521299E-13	2	
-0.02752481E+06	-0.04544297E+03	0.02020546E+02	0.03810981E+00	-0.04280146E-03	3	
0.02343806E-06	-0.04934735E-10	-0.02385981E+06	0.01729375E+03		4	
CHCLCH	53090C	2H	2CL	1 G	0300.00 5000.00 1500.00	1
0.09924881E+02	0.16181081E-02	-0.02995767E-05	-0.09718418E-11	0.03296694E-13	2	
0.02834311E+06	-0.02704592E+03	0.11901221E+01	0.02432799E+00	-0.02555964E-03	3	
0.13751585E-07	-0.02941848E-10	0.03138156E+06	0.01944186E+03		4	
CHCLCHCL	53090C	2H	2CL	2 G	0300.00 5000.00 1500.00	1
0.11636478E+02	0.02461980E-01	-0.03900519E-05	-0.15216774E-10	0.05853766E-13	2	

-0.05593248E+05-0.03507354E+03 0.10543396E+01 0.03076644E+00-0.03252548E-03	3
0.01763454E-06-0.03774444E-10-0.02006846E+05 0.02094010E+03	4
CHCLCHOH 53090C 2H 30 1CL 1G 0300.00 5000.00 1500.00	1
0.12854640E+02 0.03107712E-01-0.04837734E-05-0.02088656E-09 0.07393125E-13	2
-0.02505588E+06-0.04274804E+03-0.02073396E+01 0.03868021E+00-0.04104567E-03	3
0.02211251E-06-0.04680556E-10-0.02074261E+06 0.02608356E+03	4
CHCLOH 53090C 1H 20 1CL 1G 0300.00 5000.00 1500.00	1
0.09427376E+02 0.01722642E-01-0.02912706E-05-0.03765844E-10 0.03354461E-13	2
-0.12245752E+05-0.02330123E+03 0.13193716E+01 0.02406118E+00-0.02560105E-03	3
0.13567377E-07-0.02812530E-10-0.09640457E+05 0.01925639E+03	4
CHCLOHCH2 53090C 2H 40 1CL 1G 0300.00 5000.00 1500.00	1
0.14384355E+02 0.03552541E-01-0.05033147E-05-0.04051247E-09 0.10011716E-13	2
-0.13838992E+05-0.04819745E+03 0.14737570E+01 0.03764187E+00-0.03898775E-03	3
0.02112109E-06-0.04543829E-10-0.09395106E+05 0.02033823E+03	4
CHCLOHCHCL 53090C 2H 30 1CL 2G 0300.00 5000.00 1500.00	1
0.15672403E+02 0.02970040E-01-0.04827588E-05-0.13665995E-10 0.06500296E-13	2
-0.01896002E+06-0.05132922E+03 0.02626025E+02 0.03856174E+00-0.04091474E-03	3
0.02190241E-06-0.04603079E-10-0.14681885E+05 0.01735864E+03	4
CHF 82489C 1H 1F 1 G 0300.00 5000.00 1000.00	1
0.04242812E+02 0.02066316E-01-0.06527951E-05 0.13887000E-09-0.12133360E-13	2
0.13559817E+05 0.01680196E+02 0.03029060E+02 0.04850873E-01-0.04971678E-04	3
0.05277968E-07-0.02403154E-10 0.14014348E+05 0.08324101E+02	4
CHF3 82489C 1H 1F 3 G 0300.00 5000.00 1000.00	1
0.06834333E+02 0.06248730E-01-0.02575750E-04 0.04809112E-08-0.03352074E-12	2
-0.08663771E+06-0.10627405E+02 0.08725142E+01 0.02308431E+00-0.02123718E-03	3
0.11144284E-07-0.02909229E-10-0.08496391E+06 0.02021498E+03	4
CHOHCLCL2 53090C 2H 20 1CL 3G 0300.00 5000.00 1500.00	1
0.01681824E+03 0.02450153E-01-0.04706624E-05 0.13132630E-10 0.03046283E-13	2
-0.02253367E+06-0.05396958E+03 0.04216443E+02 0.03898553E+00-0.04360467E-03	3
0.02374677E-06-0.04984764E-10-0.01867017E+06 0.11525205E+02	4
CL 42189CL 1 G 0300.00 5000.00 1000.00	1
0.02920236E+02-0.03597985E-02 0.12942943E-06-0.02162776E-09 0.13765171E-14	2
0.13713381E+05 0.03262690E+02 0.02381576E+02 0.08891079E-02 0.04070475E-05	3
-0.02168943E-07 0.11608274E-11 0.13839987E+05 0.06021817E+02	4
CL2 42189CL 2 G 0300.00 5000.00 1000.00	1
0.04274586E+02 0.03717336E-02-0.01893489E-05 0.05337465E-09-0.05057602E-13	2
-0.13311486E+04 0.02256946E+02 0.03439587E+02 0.02870774E-01-0.02385870E-04	3
0.02892918E-08 0.02915057E-11-0.11317875E+04 0.06471359E+02	4
CL2CCCL2 53090C 2CL 4 G 0300.00 5000.00 1500.00	1
0.14457529E+02 0.11829323E-02-0.03070696E-05 0.03493311E-09-0.15665261E-14	2
-0.08068503E+05-0.04355548E+03 0.05551468E+02 0.02782136E+00-0.03184817E-03	3
0.01712716E-06-0.03511767E-10-0.05495138E+05 0.02316436E+02	4
CL2CCHCL 53090C 2H 1CL 3 G 0300.00 5000.00 1500.00	1
0.13049359E+02 0.01810829E-01-0.03396077E-05 0.10752700E-10 0.01767918E-13	2

-0.07104110E+05-0.03819015E+03	0.03355271E+02	0.02909211E+00-0.03190027E-03	3
0.01720590E-06-0.03603159E-10-0.04036294E+05	0.12506626E+02		4
CL2CCHO	53090C	2H 10 1CL 2G 0300.00 5000.00 1500.00	1
0.13459408E+02	0.01684243E-01-0.03667104E-05	0.06998698E-10 0.03279151E-13	2
-0.11766869E+05-0.04096513E+03	0.03200431E+02	0.02879558E+00-0.03079282E-03	3
0.16585494E-07-0.03532857E-10-0.08260927E+05	0.13448008E+02		4
CL2CH0H	53090C	1H 20 1CL 2G 0300.00 5000.00 1500.00	1
0.11291137E+02	0.02286704E-01-0.03461512E-05-0.01814479E-09	0.05661342E-13	2
-0.03803060E+06-0.03079830E+03	0.02619078E+02	0.02601285E+00-0.02784252E-03	3
0.15286815E-07-0.03294007E-10-0.03513998E+06	0.14924622E+02		4
CL2C0	53090C	10 1CL 2 G 0300.00 5000.00 1500.00	1
0.08882827E+02	0.07655041E-02-0.01920555E-05	0.01770151E-09-0.02378096E-14	2
-0.02980404E+06-0.01803109E+03	0.03419655E+02	0.16562349E-01-0.01875560E-03	3
0.10181519E-07-0.02127050E-10-0.02813022E+06	0.10368457E+02		4
CL2COH	53090C	10 1H 1CL 2G 0300.00 5000.00 1500.00	1
0.10262146E+02	0.13167960E-02-0.02754008E-05	0.16307709E-10 0.06472563E-14	2
-0.15116554E+05-0.02298314E+03	0.03800719E+02	0.02204678E+00-0.02673857E-03	3
0.15318545E-07-0.03305322E-10-0.13320531E+05	0.09915879E+02		4
CL2HCO	53090C	1H 10 1CL 2G 0300.00 5000.00 1500.00	1
0.10518375E+02	0.14993163E-02-0.02927670E-05	0.07898750E-10 0.01988433E-13	2
-0.06272394E+05-0.02634097E+03	0.02241202E+02	0.02456990E+00-0.02682371E-03	3
0.14431699E-07-0.03023080E-10-0.03624525E+05	0.01703507E+03		4
CL3C0	53090C	10 1CL 3 G 0300.00 5000.00 1500.00	1
0.12085258E+02	0.07759038E-02-0.02700075E-05	0.04346263E-09-0.02671642E-13	2
-0.06464078E+05-0.03099432E+03	0.04548646E+02	0.02463303E+00-0.02974898E-03	3
0.16471538E-07-0.03433021E-10-0.04416522E+05	0.07360693E+02		4
CL3COH	53090C	10 1H 1CL 3G 0300.00 5000.00 1500.00	1
0.12859853E+02	0.15880835E-02-0.03377500E-05	0.02031362E-09 0.08017922E-14	2
-0.03807818E+06-0.03561944E+03	0.04269172E+02	0.02791722E+00-0.03272753E-03	3
0.01828271E-06-0.03882978E-10-0.03558879E+06	0.08521096E+02		4
CLCC0	53090C	20 1CL 1 G 0300.00 5000.00 1500.00	1
0.09368609E+02	0.03733935E-02-0.12869813E-06	0.12064694E-10 0.09220282E-15	2
0.01762807E+06-0.02046751E+03	0.04417443E+02	0.11293645E-01-0.10134881E-04	3
0.04661357E-07-0.09098661E-11	0.01952423E+06	0.06539246E+02	4
CLCH20H	53090C	1H 30 1CL 1G 0300.00 5000.00 1500.00	1
0.09750194E+02	0.02974385E-01-0.03450482E-05-0.06010047E-09	0.10897835E-13	2
-0.03248678E+06-0.02345467E+03	0.08330909E+01	0.02358999E+00-0.02137296E-03	3
0.11058075E-07-0.02402401E-10-0.02905350E+06	0.02503745E+03		4
CLC0	53090C	10 1CL 1 G 0300.00 5000.00 1500.00	1
0.06256075E+02	0.04221480E-02-0.06162585E-06-0.05242782E-10	0.12984405E-14	2
-0.05440142E+05-0.03936950E+02	0.04743091E+02	0.03444522E-01-0.02651746E-04	3
0.12115870E-08-0.02554134E-11-0.04807119E+05	0.04464128E+02		4
CLCOH	53090C	1H 10 1CL 1G 0300.00 5000.00 1500.00	1
0.07642907E+02	0.15078143E-02-0.02651580E-05-0.14667845E-10	0.04797316E-13	2

-0.02511908E+05-0.14050463E+02	0.02037662E+02	0.01733328E+00-0.01936442E-03	3
0.10993657E-07-0.02427340E-10-0.06596141E+04	0.15384218E+02		4
CLH2CO	53090C	1H 20 1CL 1G 0300.00 5000.00 1500.00	1
0.09104530E+02	0.02130628E-01-0.02994563E-05-0.02733652E-09	0.06437596E-13	2
-0.05255641E+05-0.02258799E+03	0.08437505E+01	0.02258902E+00-0.02217447E-03	3
0.11652041E-07-0.02487574E-10-0.02264707E+05	0.02176388E+03		4
CLHCO	53090C	1H 10 1CL 1G 0300.00 5000.00 1500.00	1
0.07478598E+02	0.13790644E-02-0.01882603E-05-0.02004445E-09	0.04421104E-13	2
-0.02544646E+06-0.13621474E+02	0.02232024E+02	0.13655028E-01-0.12657141E-04	3
0.06455344E-07-0.13717423E-11-0.02346492E+06	0.14818314E+02		4
CLO	530900	1CL 1 G 0300.00 5000.00 1500.00	1
0.04329087E+02	0.15411786E-03-0.05723158E-06	0.09837751E-10-0.06441328E-14	2
0.13283263E+05	0.01718692E+02	0.02919247E+02	3
0.03120682E-07-0.06485608E-11	0.13659815E+05	0.08874760E+02	4
CLOCL	530900	1CL 2 G 0300.00 5000.00 1500.00	1
0.06635185E+02	0.03284434E-02-0.12253275E-06	0.02123621E-09-0.14043771E-14	2
0.07672351E+05-0.06410996E+02	0.03397879E+02	0.10801274E-01-0.13246551E-04	3
0.07392960E-07-0.15465835E-11	0.08527797E+05	0.09981834E+02	4
CN	121286C	1N 1 G 0300.00 5000.00 1000.00	1
0.03720119E+02	0.15183506E-03	0.01987381E-05-0.03798371E-09	2
0.05111626E+06	0.02888597E+02	0.03663204E+02-0.11565290E-02	3
0.01854208E-08-0.08214695E-11	0.05128118E+06	0.03739015E+02	4
CN+	121286C	1N 1E -1 G 0300.00 5000.00 1000.00	1
0.03701463E+02	0.07482931E-02-0.01790173E-05	0.02366368E-09-0.14370368E-14	2
0.02155966E+07	0.04108678E+02	0.03118657E+02	3
0.14795005E-08-0.09096763E-11	0.02158512E+07	0.07456254E+02	4
CN-	121286C	1N 1E 1 G 0300.00 5000.00 1000.00	1
0.02981276E+02	0.14647728E-02-0.05672737E-05	0.10176226E-09-0.06870930E-13	2
0.06346098E+05	0.06171693E+02	0.03278995E+02	3
0.05629874E-07-0.02473496E-10	0.06279509E+05	0.04568972E+02	4
CN2	121686C	1N 2 G 0300.00 5000.00 1000.00	1
0.05567064E+02	0.02100501E-01-0.09010517E-05	0.01718571E-08-0.12062552E-13	2
0.05489968E+06-0.05630054E+02	0.03039963E+02	0.08812105E-01-0.07605508E-04	3
0.03554357E-07-0.08746100E-11	0.05563268E+06	0.07555298E+02	4
CNN	121286C	1N 2 G 0300.00 5000.00 1000.00	1
0.04785930E+02	0.02559553E-01-0.10031326E-05	0.01807148E-08-0.12273827E-13	2
0.06870411E+06-0.02953957E+01	0.03524436E+02	0.07271923E-01-0.08272698E-04	3
0.05628704E-07-0.16415759E-11	0.06899647E+06	0.05932444E+02	4
CNO	103190C	1N 10 1 G 0300.00 4000.00 1500.00	1
0.06328598E+02	0.07390401E-02-0.11107610E-06-0.01846497E-09	0.04400816E-13	2
0.04683386E+06-0.09091839E+02	0.03819863E+02	0.06416254E-01-0.05303312E-04	3
0.02308211E-07-0.04256413E-11	0.04775979E+06	0.04507300E+02	4
CO	121286C	10 1 G 0300.00 5000.00 1000.00	1
0.03025078E+02	0.14426885E-02-0.05630827E-05	0.10185813E-09-0.06910951E-13	2

-0.14268350E+05	0.06108217E+02	0.03262451E+02	0.15119409E-02	-0.03881755E-04						3
0.05581944E-07	-0.02474951E-10	-0.14310539E+05	0.04848897E+02							4
C02	121286C	10	2		G	0300.00	5000.00	1000.00		1
0.04453623E+02	0.03140168E-01	-0.12784105E-05	0.02393996E-08	-0.16690333E-13						2
-0.04896696E+06	-0.09553959E+01	0.02275724E+02	0.09922072E-01	-0.10409113E-04						3
0.06866686E-07	-0.02117280E-10	-0.04837314E+06	0.10188488E+02							4
C02-	121286C	10	2E	1	G	0300.00	5000.00	1000.00		1
0.04610574E+02	0.02532962E-01	-0.10701653E-05	0.02026770E-08	-0.14249581E-13						2
-0.05479881E+06	0.14496295E+01	0.02637077E+02	0.07803230E-01	-0.08196187E-04						3
0.06537897E-07	-0.02520220E-10	-0.05416772E+06	0.11889549E+02							4
COS	121286C	10	1S	1	G	0300.00	5000.00	1000.00		1
0.05191924E+02	0.02506123E-01	-0.10243963E-05	0.01943914E-08	-0.13707999E-13						2
-0.01846210E+06	-0.02825755E+02	0.02858530E+02	0.09515458E-01	-0.08884915E-04						3
0.04220994E-07	-0.08557340E-11	-0.01785144E+06	0.09081989E+02							4
CS	121686C	1S	1		G	0300.00	5000.00	1000.00		1
0.03737430E+02	0.08180451E-02	-0.03178918E-05	0.05356801E-09	-0.02886194E-13						2
0.03247725E+06	0.03576556E+02	0.02938623E+02	0.02724351E-01	-0.02397706E-04						3
0.01689500E-07	-0.06665050E-11	0.03273992E+06	0.07848720E+02							4
CS2	121286C	1S	2		G	0300.00	5000.00	1000.00		1
0.05930515E+02	0.01813645E-01	-0.07492172E-05	0.14458920E-09	-0.10326380E-13						2
0.12051166E+05	-0.06093909E+02	0.03566139E+02	0.08374927E-01	-0.06835704E-04						3
0.02091214E-07	-0.06737193E-12	0.12688482E+05	0.06085967E+02							4
DIOXANE	103190C	4H	80	2	G	0300.00	4000.00	1500.00		1
0.02168169E+03	0.10496442E-01	-0.10538776E-05	-0.04473944E-08	0.08168288E-12						2
-0.04922004E+06	-0.09955139E+03	-0.05862900E+02	0.07081444E+00	-0.05458695E-03						3
0.02315148E-06	-0.04289513E-10	-0.03876476E+06	0.05061959E+03							4
E	120186E	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
-0.07453749E+04	-0.11734026E+02	0.02500000E+02	0.00000000E+00	0.00000000E+00						3
0.00000000E+00	0.00000000E+00	-0.07453750E+04	-0.11734026E+02							4
F	121286F	1			G	0300.00	5000.00	1000.00		1
0.02687459E+02	-0.02010358E-02	0.08597957E-06	-0.16449738E-10	0.11661605E-14						2
0.08722883E+05	0.03882212E+02	0.02913904E+02	-0.07336339E-02	0.05571015E-05						3
-0.02666871E-08	0.08643255E-12	0.08651201E+05	0.02677115E+02							4
F2	121286F	2			G	0300.00	5000.00	1000.00		1
0.04018308E+02	0.06221479E-02	-0.02420845E-05	0.04742076E-09	-0.03418141E-13						2
-0.13007128E+04	0.11263273E+01	0.02940287E+02	0.03491491E-01	-0.02458207E-04						3
0.01837073E-08	0.02850916E-11	-0.10104296E+04	0.06694194E+02							4
F2SINH	42489SI	1N	1F	2H	1G	0300.00	3000.00	1000.00		1
0.10048301E+02	0.01983144E-01	-0.02703168E-05	-0.01767852E-08	0.04444367E-12						2
-0.07739741E+06	-0.02303888E+03	0.04951547E+02	0.13296361E-01	-0.02098648E-04						3
-0.10072757E-07	0.05552285E-10	-0.07597540E+06	0.03690891E+02							4
F3SIN	22790F	3SI	1N	1	G	0300.00	4000.00	1000.00		1
0.11512423E+02	0.11150295E-02	-0.16054655E-06	-0.05271933E-09	0.11608998E-13						2

-0.10459191E+06-0.02981224E+03 0.06028419E+02 0.12786807E-01-0.01878856E-04	3
-0.09695426E-07 0.05184847E-10-0.10299499E+06-0.08217830E+01	4
FNNF 42489F 2N 2 G 0300.00 3000.00 1000.00	1
0.07255211E+02 0.02274409E-01-0.02793346E-05-0.02203843E-08 0.05359234E-12	2
0.06360352E+05-0.10942477E+02 0.03127143E+02 0.10571342E-01-0.09746113E-05	3
-0.07208357E-07 0.03567978E-10 0.07615830E+05 0.11074648E+02	4
FN03 121286F 1N 10 3 G 0300.00 5000.00 1000.00	1
0.09176275E+02 0.04219072E-01-0.01835575E-04 0.03553717E-08-0.02541078E-12	2
-0.02118638E+05-0.01934397E+03 0.02985786E+02 0.02094642E+00-0.16527329E-04	3
0.04318770E-07 0.16607836E-12-0.04237215E+04 0.12667929E+02	4
FO 121286F 10 1 G 0300.00 5000.00 1000.00	1
0.03913735E+02 0.07210714E-02-0.02796614E-05 0.05337821E-09-0.03720183E-13	2
0.11801406E+05 0.03346367E+02 0.02879578E+02 0.03399121E-01-0.02572854E-04	3
0.07422381E-08-0.04328053E-12 0.12096633E+05 0.08738887E+02	4
F02 121286F 10 2 G 0300.00 5000.00 1000.00	1
0.05678971E+02 0.14424551E-02-0.06229546E-05 0.11996118E-09-0.08543416E-13	2
-0.03861836E+04-0.01941811E+02 0.03872542E+02 0.06409974E-01-0.05517784E-04	3
0.02232770E-07-0.03876157E-11 0.11570760E+03 0.07406949E+02	4
FSIN 42489SI 1N 1F 1 G 0300.00 3000.00 1000.00	1
0.06269572E+02 0.06747867E-02-0.12419759E-06-0.04970158E-09 0.14244521E-13	2
0.02533350E+06-0.04201141E+02 0.04269969E+02 0.05298358E-01-0.11038015E-05	3
-0.03962805E-07 0.02282982E-10 0.02587238E+06 0.06215038E+02	4
GA 62987GA 1 G 0300.00 1500.00 0600.00	1
0.02679919E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00	2
0.03368804E+06 0.06788109E+02 0.02679919E+02 0.00000000E+00 0.00000000E+00	3
0.00000000E+00 0.00000000E+00 0.03368803E+06 0.06788109E+02	4
GA2H6 62987GA 2H 6 G 0300.00 1500.00 0600.00	1
0.06016247E+02 0.01788370E+00-0.12042288E-06-0.06487881E-07 0.02075367E-10	2
0.13125479E+05-0.05228029E+02-0.03914560E+02 0.04965434E+00 0.07401903E-04	3
-0.11241373E-06 0.08726339E-09 0.14930795E+05 0.04274882E+03	4
GAAS 62987GA 1AS 1 G 0300.00 1500.00 0600.00	1
0.04471149E+02 0.04238449E-02-0.02279404E-05-0.04441172E-10 0.02618952E-12	2
0.04313359E+06 0.06212470E+02 0.03967473E+02 0.02318966E-01-0.11454521E-05	3
-0.03411430E-07 0.03365821E-10 0.04321919E+06 0.08599628E+02	4
GAAS(3,C) 62987GA 3AS 3 G 0300.00 1500.00 0600.00	1
0.14852467E+02 0.02959435E-01-0.07124246E-05-0.05316048E-08 0.12873211E-12	2
0.11912617E+06-0.03514144E+03 0.14701892E+02 0.03827728E-01-0.02945747E-04	3
0.02465370E-07-0.15205979E-11 0.11914958E+06-0.03445955E+03	4
GAAS(3,L) 62987GA 3AS 3 G 0300.00 1500.00 0600.00	1
0.13568498E+02 0.02802435E-01-0.07969918E-05-0.06437098E-08 0.15602546E-12	2
0.12480055E+06-0.13810628E+02 0.13412763E+02 0.03617689E-01-0.02726208E-04	3
0.01877183E-07-0.12591780E-11 0.12482649E+06-0.13091947E+02	4
GAAS(5,C) 62987GA 5AS 5 G 0300.00 1500.00 0600.00	1
0.02573672E+03 0.05523956E-01-0.12034680E-05-0.10437431E-08 0.02528930E-11	2

	0.01721381E+07-0.08254488E+03	0.02546511E+03	0.07014337E-01-0.04881356E-04	3		
	0.03825484E-07-0.02450420E-10	0.01721819E+07-0.08130267E+03		4		
GAAS (5, L)	62987GA	5AS 5	G 0300.00 1500.00 0600.00	1		
	0.03045793E+03	0.05403151E-01-0.16494765E-05-0.09968843E-08	0.02413154E-11	2		
	0.02020691E+07-0.07768010E+03	0.03015255E+03	0.07234394E-01-0.06497993E-04	3		
	0.05559584E-07-0.03339653E-10	0.02021150E+07-0.07630866E+03		4		
GAET	62987GA	1C 2H 5	G 0300.00 1500.00 0600.00	1		
	0.05932970E+02	0.13424544E-01	0.04110518E-05-0.04286069E-07	0.12387095E-11	2	
	0.06504863E+05	0.03090838E+02	0.01846399E+02	0.02592050E+00	0.05522393E-04	3
	-0.04977960E-06	0.03654361E-09	0.07264445E+05	0.02294638E+03		4
GAET2	62987GA	1C 4H 10	G 0300.00 1500.00 0600.00	1		
	0.07213832E+02	0.03055227E+00	0.12494508E-05-0.09990274E-07	0.02881965E-10	2	
	-0.13921194E+04-0.07795098E+00-0.02162930E+02	0.05892512E+00	0.14471449E-04		3	
	-0.11686023E-06	0.08526654E-09	0.03561840E+04	0.04552626E+03		4
GAET3	62987GA	1C 6H 15	G 0300.00 1500.00 0600.00	1		
	0.08436453E+02	0.04804950E+00	0.02119157E-04-0.15816849E-07	0.04571178E-10	2	
	-0.13469963E+05-0.06196490E+02-0.06544288E+02	0.09332246E+00	0.02364121E-03		3	
	-0.01874104E-05	0.13677210E-09-0.10676594E+05	0.06666796E+03		4	
GAH	62987GA	1H 1	G 0300.00 1500.00 0600.00	1		
	0.03232142E+02	0.13432469E-02-0.04325498E-06-0.02791841E-08	0.04973590E-12		2	
	0.02656059E+06	0.05947896E+02	0.03524579E+02	0.03386213E-02-0.02064013E-05	3	
	0.03220998E-07-0.02936132E-10	0.02651074E+06	0.04554066E+02		4	
GAH2	62987GA	1H 2	G 0300.00 1500.00 0600.00	1		
	0.03762384E+02	0.03210792E-01	0.02180096E-06-0.08908394E-08	0.02219062E-11	2	
	0.01936646E+06	0.05783398E+02	0.03559710E+02	0.03676741E-01	0.06484499E-05	3
	-0.03109349E-07	0.15854136E-11	0.01940976E+06	0.06803081E+02		4
GAH3	62987GA	1H 3	G 0300.00 1500.00 0600.00	1		
	0.03345475E+02	0.06399313E-01	0.11229964E-06-0.02065899E-07	0.05780202E-11	2	
	0.12281851E+05	0.06394841E+02	0.01726153E+02	0.11247386E-01	0.02447526E-04	3
	-0.02026314E-06	0.14470000E-10	0.12586196E+05	0.14284450E+02		4
GAME	62987GA	1C 1H 3	G 0300.00 1500.00 0600.00	1		
	0.04809857E+02	0.06824206E-01	0.02258235E-05-0.02018341E-07	0.05736453E-11	2	
	0.07558677E+05	0.02595904E+02	0.03054536E+02	0.12186402E-01	0.02332213E-04	3
	-0.02121866E-06	0.15442261E-10	0.07885868E+05	0.11128781E+02		4
GAME2	62987GA	1C 2H 6	G 0300.00 1500.00 0600.00	1		
	0.07068372E+02	0.14216021E-01	0.05120694E-05-0.04421986E-07	0.13096413E-11	2	
	0.05453790E+05-0.04173960E+02	0.02257655E+02	0.02916445E+00	0.05669861E-04		3
	-0.05709755E-06	0.04268905E-09	0.06341297E+05	0.01915435E+03		4
GAME3	62987GA	1C 3H 9	G 0300.00 1500.00 0600.00	1		
	0.08410636E+02	0.02262803E+00	0.10430190E-05-0.07049610E-07	0.02015307E-10	2	
	-0.09087271E+05-0.10722496E+02	0.02120238E+02	0.04161029E+00	0.09959505E-04		3
	-0.07846792E-06	0.05693396E-09-0.07911968E+05	0.01988516E+03		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

	0.02547162E+06-0.04601176E+01	0.02500000E+02	0.00000000E+00	0.00000000E+00	3
	0.00000000E+00	0.00000000E+00	0.02547162E+06-0.04601176E+01		4
Hnr	120186H	1	G	0300.00 5000.00 1000.00	1
	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	2
	0.02547162E+06-0.04601176E+01	0.02500000E+02	0.00000000E+00	0.00000000E+00	3
	0.00000000E+00	0.00000000E+00	0.02547162E+06-0.04601176E+01		4
H+	120186H	1E -1	G	0300.00 5000.00 1000.00	1
	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	2
	0.01840334E+07-0.11538620E+01	0.02500000E+02	0.00000000E+00	0.00000000E+00	3
	0.00000000E+00	0.00000000E+00	0.01840334E+07-0.11538621E+01		4
H-	120186H	1E 1	G	0300.00 5000.00 1000.00	1
	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	2
	0.15961045E+05-0.11524488E+01	0.02500000E+02	0.00000000E+00	0.00000000E+00	3
	0.00000000E+00	0.00000000E+00	0.15961045E+05-0.11524486E+01		4
H2	121286H	2	G	0300.00 5000.00 1000.00	1
	0.02991423E+02	0.07000644E-02-0.05633828E-06-0.09231578E-10	0.15827519E-14		2
	-0.08350340E+04-0.13551101E+01	0.03298124E+02	0.08249441E-02-0.08143015E-05		3
	-0.09475434E-09	0.04134872E-11-0.10125209E+04-0.03294094E+02			4
H2ALME	62987AL	1C 1H 5	G	0300.00 1500.00 0600.00	1
	0.04898410E+02	0.13582233E-01	0.02611458E-05-0.04575170E-07	0.13848023E-11	2
	0.08743072E+04-0.11131169E+01-0.06283259E+01	0.03089530E+00	0.05774090E-04		3
	-0.06488033E-06	0.04907111E-09	0.01889333E+05	0.02565779E+03	4
H2ASME	62987AS	1C 1H 5	G	0300.00 1500.00 0600.00	1
	0.05686213E+02	0.02154421E+00	0.08185247E-05-0.07069951E-07	0.02101522E-10	2
	0.09331084E+05-0.06513957E+02-0.02113506E+02	0.04564229E+00	0.09983227E-04		3
	-0.09399697E-06	0.07014021E-09	0.10771701E+05	0.03132610E+03	4
H2C40	120189H	2C 40 1	G	0300.00 4000.00 1000.00	1
	0.10268878E+02	0.04896164E-01-0.04885080E-05-0.02708566E-08	0.05107013E-12		2
	0.02346902E+06-0.02815985E+03	0.04810971E+02	0.13139988E-01	0.09865073E-05	3
	-0.06120720E-07	0.16400028E-11	0.02545803E+06	0.02113424E+02	4
H2CCCCH	82489C	4H 3	G	0300.00 4000.00 1000.00	1
	0.11314095E+02	0.05014414E-01-0.05350444E-05-0.02825309E-08	0.05403279E-12		2
	0.05181211E+06-0.03062434E+03	0.06545799E+02	0.12424768E-01	0.05603226E-05	3
	-0.05631141E-07	0.16652183E-11	0.05352502E+06-0.04264082E+02		4
H2CCCCH2	82489C	4H 4	G	0300.00 4000.00 1000.00	1
	0.10620828E+02	0.07199370E-01-0.06806234E-05-0.04021185E-08	0.07378498E-12		2
	0.03358797E+06-0.03193583E+03	0.03849007E+02	0.01713169E+00	0.16442703E-05	3
	-0.07761590E-07	0.01947859E-10	0.03608372E+06	0.05732120E+02	4
H2CCCH	82489C	3H 3	G	0300.00 4000.00 1000.00	1
	0.08831047E+02	0.04357194E-01-0.04109066E-05-0.02368723E-08	0.04376520E-12		2
	0.03847419E+06-0.02177919E+03	0.04754199E+02	0.11080277E-01	0.02793323E-05	3
	-0.05479212E-07	0.01949629E-10	0.03988883E+06	0.05854549E+01	4
H2CCCL0	53090C	2H 20 1CL 1G	G	0300.00 5000.00 1500.00	1
	0.12404621E+02	0.02067657E-01-0.03889951E-05-0.03138120E-10	0.04625008E-13		2



-0.11145027E+05-0.03928723E+03 0.01680421E+02 0.03020641E+00-0.03234256E-03	3
0.01779343E-06-0.03877220E-10-0.07395297E+05 0.01777265E+03	4
H2CCH20H 103190C 2H 50 1 G 0300.00 4000.00 1500.00	1
0.11449565E+02 0.05249185E-01-0.04887850E-05-0.02243250E-08 0.03973359E-12	2
-0.07554972E+05-0.03426082E+03 0.13044058E+01 0.02873214E+00-0.02387448E-03	3
0.11669883E-07-0.02450026E-10-0.03718933E+05 0.02078756E+03	4
H2CCHO 103190C 2H 30 1 G 0300.00 4000.00 1500.00	1
0.09710060E+02 0.03854965E-01-0.04677824E-05-0.15051791E-09 0.02941428E-12	2
-0.02692491E+05-0.02810566E+03 0.02802205E+01 0.02740310E+00-0.02554683E-03	3
0.13066794E-07-0.02750425E-10 0.06682647E+04 0.02239731E+03	4
H2CN 41687H 2C 1N 1 G 0300.00 4000.00 1000.00	1
0.05209703E+02 0.02969291E-01-0.02855589E-05-0.16355504E-09 0.03043259E-12	2
0.02767711E+06-0.04444478E+02 0.02851661E+02 0.05695233E-01 0.10711403E-05	3
-0.16226120E-08-0.02351108E-11 0.02863782E+06 0.08992751E+02	4
H2CNCH2 103190C 2H 4N 1 G 0300.00 4000.00 1500.00	1
0.10653852E+02 0.05191287E-01-0.05816522E-05-0.02206912E-08 0.04101340E-12	2
0.02345063E+06-0.03469894E+03-0.12030756E+00 0.03225369E+00-0.02968722E-03	3
0.15272903E-07-0.03242499E-10 0.02728820E+06 0.02297042E+03	4
H2CNCH2O 103190C 2H 4N 10 1G 0300.00 4000.00 1500.00	1
0.13276525E+02 0.04830938E-01-0.04858949E-05-0.02009495E-08 0.03640181E-12	2
0.16249619E+05-0.04713093E+03-0.01978522E+01 0.03341279E+00-0.02432022E-03	3
0.09438643E-07-0.16040495E-11 0.02141154E+06 0.02658264E+03	4
H2CNCHO 103190C 2H 3N 10 1G 0300.00 4000.00 1500.00	1
0.11967920E+02 0.03915427E-01-0.03860933E-05-0.01696876E-08 0.03041049E-12	2
-0.05902236E+05-0.03958544E+03 0.10960659E+01 0.02577215E+00-0.01711629E-03	3
0.05880104E-07-0.08956774E-11-0.16120634E+04 0.02032528E+03	4
H2CNH 41687C 1H 3N 1 G 0300.00 4000.00 1000.00	1
0.05221589E+02 0.04748525E-01-0.04179158E-05-0.02606612E-08 0.04703140E-12	2
0.08657219E+05-0.04500776E+02 0.02365878E+02 0.06780570E-01 0.02422999E-04	3
-0.06157824E-08-0.16150971E-11 0.09971141E+05 0.12307176E+02	4
H2CNNHO 103190C 1H 3N 20 1G 0300.00 4000.00 1500.00	1
0.11577543E+02 0.04489179E-01-0.05033233E-05-0.16510659E-09 0.03069138E-12	2
0.01986782E+06-0.03656957E+03 0.05954945E+01 0.03239559E+00-0.02993965E-03	3
0.14890538E-07-0.03022863E-10 0.02364485E+06 0.02192790E+03	4
H2CNNO 103190C 1H 2N 20 1G 0300.00 4000.00 1500.00	1
0.10162339E+02 0.03065936E-01-0.03082820E-05-0.11944245E-09 0.02169866E-12	2
0.02494088E+06-0.02762274E+03 0.02498334E+02 0.01993008E+00-0.15578788E-04	3
0.06838955E-07-0.13132504E-11 0.02786476E+06 0.14170250E+02	4
H2CNN02 41687H 2C 1N 20 2G 0300.00 4000.00 1000.00	1
0.11407942E+02 0.04564542E-01-0.04600304E-05-0.02513538E-08 0.04782211E-12	2
0.12421422E+05-0.03165237E+03 0.03534316E+02 0.01811271E+00 0.02394017E-05	3
-0.10800240E-07 0.04222725E-10 0.15090057E+05 0.11311378E+02	4
H2CNO 103190C 1H 2N 10 1G 0300.00 4000.00 1500.00	1
0.08485639E+02 0.02633277E-01-0.03017498E-05-0.08341916E-09 0.15939773E-13	2

	0.01716434E+06-0.02052156E+03	0.10458559E+01	0.02126493E+00-0.01962753E-03	3
	0.09659592E-07-0.01941068E-10	0.01974611E+06	0.01919718E+03	4
H2CN02	103190C	1H 2N 10 2G	0300.00 4000.00 1500.00	1
	0.11274813E+02	0.02584711E-01-0.03934330E-05-0.05614969E-09	0.13924004E-13	2
	0.13604697E+05-0.03461951E+03	0.11656956E+01	0.02890489E+00-0.02817662E-03	3
	0.13875688E-07-0.02727594E-10	0.01694545E+06	0.01888293E+03	4
H2CONO	103190C	1H 2N 10 2G	0300.00 4000.00 1500.00	1
	0.10757541E+02	0.02983288E-01-0.04123563E-05-0.08096724E-09	0.01720194E-12	2
	0.12302534E+05-0.02976009E+03	0.02120026E+02	0.02709056E+00-0.02799615E-03	3
	0.14791451E-07-0.03074996E-10	0.15043271E+05	0.15460916E+02	4
NH2CONH2	dummy*H	4N 20 1C 1G	0300.00 5000.00 1000.00	1
	0.03615144E+02	0.03212486E-01-0.01260337E-04	0.02267298E-08-0.01536236E-12	2
	0.11769108E+05	0.04810264E+02	0.02784403E+02	3
	0.09437980E-07-0.03753146E-10	0.12025976E+05	0.09035629E+02	4
HNC	L11/92H	1N 1C 1 G	200.000 6000.000 1000.00	1
	4.22248103E+00	2.59458278E-03-8.58480969E-07	1.30745002E-10-7.50339765E-15	2
	2.20127593E+04-7.79447358E-02	2.30186735E+00	1.54157529E-02-3.13262156E-05	3
	3.08816551E-08-1.11912353E-11	2.22277183E+04	8.14751135E+00	4
H2GAET	62987GA	1C 2H 7 G	0300.00 1500.00 0600.00	1
	0.07187273E+02	0.01867211E+00	0.06156157E-05-0.06027763E-07	2
	-0.04232757E+05-0.04686699E+02	0.04124020E+01	0.03972971E+00	3
	-0.08059233E-06	0.06040387E-09-0.02983932E+05	0.02816147E+03	4
H2GAME	62987GA	1C 1H 5 G	0300.00 1500.00 0600.00	1
	0.05831604E+02	0.12228715E-01	0.03033669E-05-0.03956941E-07	2
	0.05189255E+05-0.04446614E+02	0.05251130E+01	0.02904695E+00	3
	-0.06097646E-06	0.04672763E-09	0.06158712E+05	4
H2NF	42489H	2N 1F 1 G	0300.00 3000.00 1000.00	1
	0.04143658E+02	0.03805135E-01-0.02771153E-05-0.03589717E-08	0.07589549E-12	2
	-0.04891486E+05	0.02309362E+02	0.02597862E+02	3
	-0.01948600E-07	0.03634002E-11-0.04301253E+05	0.10982895E+02	4
H2NNO	103190H	2N 20 1 G	0300.00 4000.00 1500.00	1
	0.07759736E+02	0.03025701E-01-0.02888915E-05-0.12629896E-09	0.02195026E-12	2
	0.05894193E+05-0.16477133E+02	0.02088915E+02	0.01684997E+00-0.14289772E-04	3
	0.06830146E-07-0.13689850E-11	0.07907340E+05	0.13943810E+02	4
H2NO	102290H	2N 10 1 G	0300.00 4000.00 1500.00	1
	0.05673346E+02	0.02298836E-01-0.01774445E-05-0.11034818E-09	0.01859762E-12	2
	0.05569325E+05-0.06153540E+02	0.02530589E+02	0.08596035E-01-0.05471030E-04	3
	0.02276249E-07-0.04648073E-11	0.06868030E+05	0.11266506E+02	4
H2NOH	103190H	3N 10 1 G	0300.00 4000.00 1500.00	1
	0.06764632E+02	0.03047035E-01-0.02777797E-05-0.12504874E-09	0.02191094E-12	2
	-0.09026701E+05-0.12698452E+02	0.14070026E+01	0.16584981E-01-0.14635943E-04	3
	0.07318354E-07-0.15118974E-11-0.07158595E+05	0.15896491E+02		4
H2O	20387H	20 1 G	0300.00 5000.00 1000.00	1
	0.02672145E+02	0.03056293E-01-0.08730260E-05	0.12009964E-09-0.06391618E-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	0.02590232E+02		4		
H2O(L)	120186H	20	1	L	0273.15 1000.00 1000.00	1	
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2	
0.00000000E+00	0.00000000E+00	0.12712782E+02	-0.01766279E+00	-0.02255666E-03		3	
0.02082090E-05	-0.02407861E-08	-0.03748320E+06	-0.05911534E+03			4	
H2O(S)	120186H	20	1	S	0200.00 0273.15 1000.00	1	
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2	
0.00000000E+00	0.00000000E+00	-0.03926933E+00	0.01692042E+00	0.00000000E+00		3	
0.00000000E+00	0.00000000E+00	-0.03594958E+06	0.05693378E+01			4	
H2O2	120186H	20	2	G	0300.00 5000.00 1000.00	1	
0.04573167E+02	0.04336136E-01	-0.14746888E-05	0.02348903E-08	-0.14316536E-13		2	
-0.01800696E+06	0.05011369E+01	0.03388753E+02	0.06569226E-01	-0.14850125E-06		3	
-0.04625805E-07	0.02471514E-10	-0.01766314E+06	0.06785363E+02			4	
H2S	121286H	2S	1	G	0300.00 5000.00 1000.00	1	
0.02883147E+02	0.03827835E-01	-0.14233978E-05	0.02497998E-08	-0.16602733E-13		2	
-0.03480742E+05	0.07258161E+02	0.03071029E+02	0.05578261E-01	-0.10309669E-04		3	
0.12019529E-07	-0.04838369E-10	-0.03559826E+05	0.05935226E+02			4	
H2SI(NH2)2	22790SI	1H	6N	2	G	0300.00 4000.00 1000.00	1
0.13021791E+02	0.06465444E-01	-0.05816746E-05	-0.03484493E-08	0.06340675E-12		2	
-0.02357070E+06	-0.04132569E+03	0.05615307E+02	0.02079854E+00	-0.09999531E-05		3	
-0.12885246E-07	0.06091865E-10	-0.02126283E+06	-0.16156578E+01			4	
H2SIN	22790H	2SI	1N	1	G	0300.00 4000.00 1000.00	1
0.06826533E+02	0.02125460E-01	-0.02343131E-05	-0.11663394E-09	0.02277273E-12		2	
0.07253672E+06	-0.10521624E+02	0.03549344E+02	0.07311004E-01	0.03249025E-05		3	
-0.03682945E-07	0.11215113E-11	0.07370656E+06	0.07565328E+02			4	
H2SINH	42489SI	1N	1H	3	G	0300.00 3000.00 1000.00	1
0.06588295E+02	0.04903194E-01	-0.04944719E-05	-0.05014630E-08	0.11394698E-12		2	
0.01809794E+06	-0.09522970E+02	0.02822195E+02	0.12455182E-01	-0.08350819E-05		3	
-0.07411813E-07	0.03579019E-10	0.01923616E+06	0.10547831E+02			4	
H2SINH2	42489SI	1N	1H	4	G	0300.00 3000.00 1000.00	1
0.07392047E+02	0.05476841E-01	-0.04453276E-05	-0.05236661E-08	0.11383899E-12		2	
0.11368581E+05	-0.11380495E+02	0.04053222E+02	0.11822311E-01	-0.04348128E-05		3	
-0.06225818E-07	0.02798829E-10	0.12419705E+05	0.06562032E+02			4	
H2SINH3	121386SI	1H	5N	1	G	0300.00 4000.00 1000.00	1
0.08711392E+02	0.05909106E-01	-0.05436615E-05	-0.03248350E-08	0.05960257E-12		2	
0.08441694E+05	-0.01933470E+03	0.04269729E+02	0.11252245E-01	0.01951721E-04		3	
-0.03578372E-07	-0.08372202E-12	0.10222041E+05	0.05876735E+02			4	
H2SISIH2	42489SI	2H	4	G	0300.00 3000.00 1000.00	1	
0.08986817E+02	0.05405047E-01	-0.05214021E-05	-0.05313742E-08	0.11887266E-12		2	
0.02832747E+06	-0.02004478E+03	0.05133186E+02	0.12528548E-01	-0.04620421E-05		3	
-0.06606075E-07	0.02864344E-10	0.02956915E+06	0.07605133E+01			4	
H3ASGAET3	62987AS	1GA	1C	6H	18G	0300.00 1500.00 0600.00	1
0.08508501E+02	0.05632369E+00	0.02524140E-04	-0.01861451E-06	0.05372402E-10		2	

-0.10855169E+05-0.03399857E+02-0.08974745E+02	0.10905161E+00	0.02811457E-03	3		
-0.02195513E-05	0.15997339E-09-0.07592761E+05	0.08165459E+03	4		
H3ASGAME3	62987AS	1GA 1C 3H 12G	0300.00 1500.00 0600.00	1	
0.11254990E+02	0.03159752E+00	0.11779036E-05-0.10133524E-07	0.02947355E-10	2	
-0.07280344E+05-0.02238729E+03	0.12671606E+01	0.06214586E+00	0.13856307E-04	3	
-0.12200444E-06	0.08982019E-09-0.05425619E+05	0.02613306E+03		4	
H3CONHO	103190C	1H 4N 10 2G	0300.00 4000.00 1500.00	1	
0.12492702E+02	0.04773900E-01-0.04717255E-05-0.01987934E-08	0.03599460E-12		2	
-0.02354754E+05-0.03945441E+03	0.01930733E+02	0.02865910E+00-0.02313062E-03		3	
0.10684024E-07-0.02139376E-10	0.16388909E+04	0.01796108E+03		4	
H3SIN	22790H	3SI 1N 1 G	0300.00 4000.00 1000.00	1	
0.07964213E+02	0.03355633E-01-0.03579695E-05-0.01889818E-08	0.03650912E-12		2	
0.11486972E+06-0.01924110E+03	0.02790628E+02	0.11345662E-01	0.08321879E-05	3	
-0.05845045E-07	0.01685969E-10	0.11673571E+06	0.09384630E+02	4	
H3SINH	42489SI	1N 1H 4 G	0300.00 3000.00 1000.00	1	
0.07697340E+02	0.05657943E-01-0.05209306E-05-0.05617966E-08	0.12635020E-12		2	
0.02282005E+06-0.13303793E+02	0.02778390E+02	0.15107111E-01-0.06734260E-05		3	
-0.08928515E-07	0.04115347E-10	0.02435913E+06	0.13093859E+02	4	
H3SISIH	90589SI	2H 4 G	0300.00 2000.00 1000.00	1	
0.07778291E+02	0.07255418E-01-0.08123265E-05-0.11682818E-08	0.03425139E-11		2	
0.03742600E+06-0.13484629E+02	0.02774192E+02	0.02555302E+00-0.02883836E-03		3	
0.02000737E-06-0.06100616E-10	0.03861801E+06	0.11350098E+02		4	
H3SISIH3	42489SI	2H 6 G	0300.00 3000.00 1000.00	1	
0.10682729E+02	0.08221416E-01-0.08096035E-05-0.08337975E-08	0.01908205E-11		2	
0.05316920E+05-0.03082188E+03	0.03898289E+02	0.01977415E+00	0.01791014E-05	3	
-0.10331682E-07	0.03931698E-10	0.07621719E+05	0.06227022E+02	4	
HALME	62987AL	1C 1H 4 G	0300.00 1500.00 0600.00	1	
0.04812273E+02	0.10296448E-01	0.02582807E-05-0.03323596E-07	0.09884584E-11	2	
0.11766730E+05	0.09557062E+01	0.11187894E+01	0.02180038E+00	0.04120785E-04	3
-0.04366690E-06	0.03273825E-09	0.12447363E+05	0.01886107E+03		4
HALME2	62987AL	1C 2H 7 G	0300.00 1500.00 0600.00	1	
0.05705171E+02	0.01924317E+00	0.06377855E-05-0.06346800E-07	0.01896799E-10		2
-0.06049864E+05-0.06331378E+01-0.14942614E+01	0.04158567E+00	0.08686772E-04		3	
-0.08604142E-06	0.06447652E-09-0.04722516E+05	0.03427724E+03		4	
HASALME	62987AS	1AL 1C 1H 4G	0300.00 1500.00 0600.00	1	
0.06956538E+02	0.10612781E-01	0.02440153E-05-0.03297737E-07	0.10200039E-11		2
0.02582505E+06-0.08625792E+01	0.02544858E+02	0.02465794E+00	0.03677807E-04		3
-0.05008893E-06	0.03848383E-09	0.02663010E+06	0.02046858E+03		4
HASGAET	62987AS	1GA 1C 2H 6G	0300.00 1500.00 0600.00	1	
0.06336445E+02	0.02340603E+00	0.09066638E-05-0.07519059E-07	0.01828115E-10		2
0.03184605E+06	0.05812180E+02	0.05642723E+02	0.02296738E+00	0.10948674E-04	3
-0.02449038E-06	0.09602700E-10	0.03204717E+06	0.09675533E+02		4
HASGAME	62987AS	1GA 1C 1H 4G	0300.00 1500.00 0600.00	1	
0.07507970E+02	0.09277900E-01	0.01891931E-05-0.02769886E-07	0.07996069E-11		2

0.03253907E+06-0.14226081E+01	0.04859126E+02	0.01750423E+00	0.02831995E-04	3					
-0.03107936E-06	0.02299468E-09	0.03302941E+06	0.11429521E+02	4					
HASME	62987AS	1C	1H	4	G	0300.00	1500.00	0600.00	1
0.05753261E+02	0.01841813E+00	0.07493312E-05	-0.05919916E-07	0.01726246E-10	2				
0.01880057E+06-0.05360325E+02	-0.15750948E+00	0.03649094E+00	0.08332939E-04	3					
-0.07234666E-06	0.05330928E-09	0.01989791E+06	0.02335316E+03	4					
HASME2	62987AS	1C	2H	7	G	0300.00	1500.00	0600.00	1
0.05850436E+02	0.01841765E+00	0.08066844E-05	-0.05868715E-07	0.01726428E-10	2				
0.06450535E+05	0.03909152E+01	-0.02908405E+01	0.03729576E+00	0.08335854E-04	3				
-0.07455611E-06	0.05527881E-09	0.07587765E+05	0.03020451E+03	4					
HCCHCCH	82489C	4H	3		G	0300.00	4000.00	1000.00	1
0.10752738E+02	0.05381153E-01	-0.05549637E-05	-0.03052266E-08	0.05761740E-12	2				
0.06121419E+06-0.02973025E+03	0.04153881E+02	0.01726287E+00	-0.02389374E-05	3					
-0.10187000E-07	0.04340504E-10	0.06338070E+06	0.06036506E+02	4					
HCCO	32387H	1C	20	1	G	0300.00	4000.00	1000.00	1
0.06758073E+02	0.02000400E-01	-0.02027607E-05	-0.10411318E-09	0.01965164E-12	2				
0.01901513E+06-0.09071262E+02	0.05047965E+02	0.04453478E-01	0.02268282E-05	3					
-0.14820945E-08	0.02250741E-11	0.01965891E+06	0.04818439E+01	4					
HCCOH	32387H	2C	20	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+05-0.14012140E+02	0.03899465E+02	0.09701075E-01	-0.03119309E-05	3					
-0.05537732E-07	0.02465732E-10	0.08701190E+05	0.04491874E+02	4					
HCL	42189CL	1H	1		G	0300.00	5000.00	1000.00	1
0.02755335E+02	0.14735811E-02	-0.04971254E-05	0.08108658E-09	0.05072063E-13	2				
-0.11918058E+05	0.06515116E+02	0.03338534E+02	0.12682066E-02	-0.03666916E-04	3				
0.04703992E-07	-0.01836011E-10	-0.12131511E+05	0.03193555E+02	4					
HCLCCLO	53090C	2H	10	1CL	2G	0300.00	5000.00	1500.00	1
0.13498820E+02	0.16663118E-02	-0.03827891E-05	0.14597646E-10	0.02459497E-13	2				
-0.15679374E+05-0.04104068E+03	0.03080147E+02	0.03035742E+00	-0.03373486E-03	3					
0.01857727E-06	-0.03992575E-10	-0.12233708E+05	0.13810983E+02	4					
HCLCCHO	53090C	2H	20	1CL	1G	0300.00	5000.00	1500.00	1
0.12281935E+02	0.02136310E-01	-0.03756941E-05	-0.13473743E-10	0.05834907E-13	2				
-0.08447210E+05-0.03860056E+03	0.15446619E+01	0.02882430E+00	-0.02921313E-03	3					
0.15578111E-07	-0.03358527E-10	-0.04546644E+05	0.01905110E+03	4					
HCN	121286H	1C	1N	1	G	0300.00	5000.00	1000.00	1
0.03650077E+02	0.03460998E-01	-0.12742788E-05	0.02217655E-08	-0.14771774E-13	2				
0.14983916E+05	0.02393220E+02	0.02490462E+02	0.08611280E-01	-0.10310342E-04	3				
0.07481498E-07	-0.02229109E-10	0.15208344E+05	0.07904981E+02	4					
HCNH	41687C	1H	2N	1	G	0300.00	4000.00	1000.00	1
0.04923292E+02	0.03332897E-01	-0.03370896E-05	-0.01901619E-08	0.03531825E-12	2				
0.03132669E+06-0.16325088E+01	0.02759456E+02	0.06103386E-01	0.07713149E-05	3					
-0.02063093E-07	0.01931919E-11	0.03217247E+06	0.10574895E+02	4					
HCNO	120186H	1C	1N	10	1G	0250.00	4000.00	1000.00	1
0.06692412E+02	0.02368360E-01	-0.02371510E-05	-0.12755033E-09	0.02407137E-12	2				

0.01694736E+06-0.12454345E+02 0.03184858E+02 0.09752316E-01-0.12802028E-05	3	
-0.06163104E-07 0.03226275E-10 0.01797907E+06 0.06123843E+02	4	
HCO	121286H 1C 10 1 G 0300.00 5000.00 1000.00	1
0.03557271E+02 0.03345572E-01-0.13350060E-05 0.02470572E-08-0.01713850E-12	2	
0.03916324E+05 0.05552299E+02 0.02898329E+02 0.06199146E-01-0.09623084E-04	3	
0.10898249E-07-0.04574885E-10 0.04159922E+05 0.08983614E+02	4	
HCO+	121286H 1C 10 1E -1G 0300.00 5000.00 1000.00	1
0.03692074E+02 0.03454732E-01-0.13165244E-05 0.02323551E-08-0.15541321E-13	2	
0.09890941E+06 0.02330722E+02 0.02496483E+02 0.08690658E-01-0.10604453E-04	3	
0.07882791E-07-0.02418385E-10 0.09915097E+06 0.08048177E+02	4	
HCOOH	103190C 1H 20 2 G 0300.00 4000.00 1500.00	1
0.07959697E+02 0.03024532E-01-0.03434242E-05-0.13267675E-09 0.02520240E-12	2	
-0.05027445E+06-0.01872208E+03 0.09326031E+01 0.01891001E+00-0.15549638E-04	3	
0.07290030E-07-0.14836946E-11-0.04760071E+06 0.01950653E+03	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	
HE+	120186HE 1E -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	
0.02853426E+07 0.16084045E+01 0.02500000E+02 0.00000000E+00 0.00000000E+00	3	
0.00000000E+00 0.00000000E+00 0.02853426E+07 0.16084046E+01	4	
HF	121286H 1F 1 G 0300.00 5000.00 1000.00	1
0.02956767E+02 0.07721015E-02-0.09899834E-06-0.04993520E-10 0.14293306E-14	2	
-0.03361061E+06 0.04011673E+02 0.03431841E+02 0.04404165E-02-0.08828452E-05	3	
0.06574516E-08-0.02055909E-12-0.03381977E+06 0.12382699E+01	4	
HGAET	62987GA 1C 2H 6 G 0300.00 1500.00 0600.00	1
0.06580151E+02 0.16101323E-01 0.05009545E-05-0.05185148E-07 0.15240853E-11	2	
0.08765131E+05-0.04046067E+01 0.11632838E+01 0.03282212E+00 0.06765717E-04	3	
-0.06509541E-06 0.04835806E-09 0.09767174E+05 0.02588269E+03	4	
HGAET2	62987GA 1C 4H 11 G 0300.00 1500.00 0600.00	1
0.06511306E+02 0.02819753E+00 0.14187506E-05-0.09000947E-07 0.02572894E-10	2	
-0.04482180E+05 0.04709021E+02-0.14865759E+01 0.05217640E+00 0.13563420E-04	3	
-0.10119820E-06 0.07319853E-09-0.02985242E+05 0.04364749E+03	4	
HGAME	62987GA 1C 1H 4 G 0300.00 1500.00 0600.00	1
0.05318279E+02 0.09490931E-01 0.02277164E-05-0.03005070E-07 0.09037830E-11	2	
0.12535338E+05-0.10657105E+00 0.01784749E+02 0.02058861E+00 0.03548509E-04	3	
-0.04111927E-06 0.03108978E-09 0.13184225E+05 0.01700701E+03	4	
HGAME2	62987GA 1C 2H 7 G 0300.00 1500.00 0600.00	1
0.06759397E+02 0.14261030E-01-0.11740239E-06-0.05001401E-07 0.15027851E-11	2	
-0.14732646E+04-0.02967135E+02 0.09039155E+01 0.03264779E+00 0.05389243E-04	3	
-0.06814504E-06 0.05150323E-09-0.03978242E+04 0.02539304E+03	4	
HMEGAET	62987GA 1C 3H 9 G 0300.00 1500.00 0600.00	1
0.07025463E+02 0.02564787E+00 0.09619100E-05-0.08403699E-07 0.02488960E-10	2	

-0.13613768E+04-0.03319484E+02-0.02079142E+02	0.05373076E+00	0.11810364E-04	3						
-0.10998548E-06	0.08189554E-09	0.03216961E+04	0.04086070E+03	4					
HN(OH)2	103190H	3N	10	2	G	0300.00	4000.00	1500.00	1
0.09963640E+02	0.02864736E-01-0.03812929E-05-0.07443355E-09	0.16101241E-13	2						
-0.16621838E+05-0.02871769E+03	0.03244199E+01	0.02850544E+00-0.02753933E-03	3						
0.13372943E-07-0.02571777E-10-0.13544987E+05	0.02201479E+03		4						
HN3	82687H	1N	3		G	0300.00	4000.00	1000.00	1
0.06023015E+02	0.02454362E-01-0.02404279E-05-0.13229726E-09	0.02474146E-12	2						
0.03394051E+06-0.07015537E+02	0.03621003E+02	0.06030785E-01	0.04054460E-05	3					
-0.02545270E-07	0.06174280E-11	0.03482373E+06	0.06333769E+02	4					
HNCN	62790C	1H	1N	2	G	0300.00	4000.00	1500.00	1
0.07251951E+02	0.15873633E-02-0.01995579E-05-0.04841944E-09	0.09908280E-13	2						
0.03563666E+06-0.13120801E+02	0.02951908E+02	0.12450280E-01-0.11616110E-04	3						
0.05786107E-07-0.11750035E-11	0.03712483E+06	0.09811426E+02	4						
HNCNH	62790C	1H	2N	2	G	0300.00	4000.00	1500.00	1
0.08374142E+02	0.02366143E-01-0.03502324E-05-0.04391102E-09	0.10968595E-13	2						
0.14610875E+05-0.02107393E+03	0.10019852E+01	0.02464016E+00-0.02759770E-03	3						
0.15324719E-07-0.03268279E-10	0.01679368E+06	0.01694325E+03	4						
HNCO	31287H	1N	1C	10	1G	0300.00	4000.00	1000.00	1
0.06211867E+02	0.02297137E-01-0.02216128E-05-0.12220438E-09	0.02272406E-12	2						
-0.14770725E+05-0.08016633E+02	0.03694059E+02	0.06657236E-01-0.05054468E-06	3						
-0.03473411E-07	0.13605694E-11-0.13919758E+05	0.05712742E+02	4						
HNF	42489H	1N	1F	1	G	0300.00	3000.00	1000.00	1
0.04133219E+02	0.01912056E-01-0.16253301E-06-0.01726461E-08	0.03743691E-12	2						
0.14670521E+05	0.03292122E+02	0.03249760E+02	0.03261817E-01	0.04355642E-06	3				
-0.11002765E-08	0.02926757E-11	0.14991264E+05	0.08187434E+02	4					
HNF2	42489H	1N	1F	2	G	0300.00	3000.00	1000.00	1
0.05704866E+02	0.03049897E-01-0.02826802E-05-0.02923184E-08	0.06551055E-12	2						
-0.09107488E+05-0.03941331E+02	0.02572812E+02	0.08762144E-01-0.02326921E-05	3						
-0.05000826E-07	0.02143837E-10-0.08086760E+05	0.13006810E+02	4						
HNNHO	103190H	2N	2O	1	G	0300.00	4000.00	1500.00	1
0.07462348E+02	0.03113521E-01-0.02614534E-05-0.13946008E-09	0.02363351E-12	2						
0.07517607E+05-0.16192929E+02	0.07974964E+01	0.01693170E+00-0.11410855E-04	3						
0.04201242E-07-0.06926417E-11	0.10106646E+05	0.02038764E+03	4						
HNNO	103190H	1N	2O	1	G	0300.00	4000.00	1500.00	1
0.06991217E+02	0.01875970E-01-0.02124584E-05-0.06710472E-09	0.12305080E-13	2						
0.02497566E+06-0.11235229E+02	0.02238298E+02	0.13591997E-01-0.11798728E-04	3						
0.05392970E-07-0.10108589E-11	0.02660258E+06	0.14136789E+02	4						
HNO	121286H	1N	1O	1	G	0300.00	5000.00	1000.00	1
0.03615144E+02	0.03212485E-01-0.12603370E-05	0.02267297E-08-0.15362358E-13	2						
0.10661911E+05	0.04810263E+02	0.02784402E+02	0.06609646E-01-0.09300223E-04	3					
0.09437980E-07-0.03753146E-10	0.10918779E+05	0.09035629E+02	4						
HN02	103190H	1N	1O	2	G	0300.00	4000.00	1500.00	1
0.06479629E+02	0.01995274E-01-0.01740386E-05-0.09695872E-09	0.01701479E-12	2						

-0.09999271E+05-0.10672857E+02 0.01934838E+02 0.10100361E-01-0.04964616E-04	3
0.08701121E-08-0.02324135E-13-0.08105484E+05 0.14732500E+02	4
HN03 121286H 1N 10 3 G 0300.00 5000.00 1000.00	1
0.07003844E+02 0.05811493E-01-0.02333788E-04 0.04288814E-08-0.02959385E-12	2
-0.01889952E+06-0.10478628E+02 0.13531850E+01 0.02220024E+00-0.01978811E-03	3
0.08773908E-07-0.16583844E-11-0.01738562E+06 0.01851868E+03	4
HNOH 102290H 2N 10 1 G 0300.00 4000.00 1500.00	1
0.06396134E+02 0.01821067E-01-0.01870891E-05-0.07844471E-09 0.14448555E-13	2
0.07859615E+05-0.10404785E+02 0.02125274E+02 0.10662818E-01-0.07602588E-04	3
0.03081641E-07-0.05726498E-11 0.09553544E+05 0.13096718E+02	4
H02 20387H 10 2 G 0300.00 5000.00 1000.00	1
0.04072191E+02 0.02131296E-01-0.05308145E-05 0.06112269E-09-0.02841164E-13	2
-0.15797270E+03 0.03476029E+02 0.02979963E+02 0.04996697E-01-0.03790997E-04	3
0.02354192E-07-0.08089024E-11 0.01762273E+04 0.09222724E+02	4
HOCH2OH 103190C 1H 40 2 G 0300.00 4000.00 1500.00	1
0.10890480E+02 0.04000443E-01-0.04729597E-05-0.12959699E-09 0.02552658E-12	2
-0.05347440E+06-0.03540622E+03-0.06548874E+01 0.03377715E+00-0.03157595E-03	3
0.15322165E-07-0.02994258E-10-0.04963411E+06 0.02579207E+03	4
HOCL 53090H 10 1CL 1 G 0300.00 5000.00 1500.00	1
0.05125698E+02 0.09494990E-02-0.12088029E-06-0.13583997E-10 0.02818422E-13	2
-0.11259688E+05-0.01742146E+02 0.02788194E+02 0.07568178E-01-0.08171332E-04	3
0.04665821E-07-0.10381677E-11-0.10484059E+05 0.10534440E+02	4
HOCN 120186H 10 1C 1N 1G 0250.00 4000.00 1000.00	1
0.05645607E+02 0.02298206E-01-0.02162629E-05-0.12148014E-09 0.02238636E-12	2
-0.03178109E+05-0.03590263E+02 0.03628292E+02 0.05664184E-01-0.11702056E-06	3
-0.02348638E-07 0.08016402E-11-0.02475925E+05 0.07476825E+02	4
HOCO 103190C 1H 10 2 G 0300.00 4000.00 1500.00	1
0.07517634E+02 0.12590288E-02-0.01910900E-05-0.03136391E-09 0.07547673E-13	2
-0.02634121E+06-0.14483918E+02 0.02285122E+02 0.13514351E-01-0.11604072E-04	3
0.05047011E-07-0.09032231E-11-0.02448416E+06 0.13678737E+02	4
HONO 31787H 1N 10 2 G 0300.00 5000.00 1000.00	1
0.05486892E+02 0.04218064E-01-0.16491426E-05 0.02971876E-08-0.02021148E-12	2
-0.11268646E+05-0.02997002E+02 0.02290413E+02 0.14099223E-01-0.13678717E-04	3
0.07498780E-07-0.01876905E-10-0.10431945E+05 0.13280769E+02	4
HON02 103190H 1N 10 3 G 0300.00 4000.00 1500.00	1
0.09756148E+02 0.01900947E-01-0.03240019E-05-0.03976638E-09 0.11003341E-13	2
-0.01942244E+06-0.02690023E+03 0.07877667E+01 0.02382329E+00-0.02205964E-03	3
0.10340485E-07-0.01972856E-10-0.16304425E+05 0.02108964E+03	4
HSI(NH2)2 22790SI 1H 5N 2 G 0300.00 4000.00 1000.00	1
0.11716773E+02 0.05339021E-01-0.04667823E-05-0.02824087E-08 0.05080915E-12	2
-0.12641686E+04-0.03245117E+03 0.06289698E+02 0.16750596E-01-0.15208775E-05	3
-0.10700650E-07 0.05538640E-10 0.03154770E+04-0.03746008E+02	4
HSI(NH2)3 22790SI 1H 7N 3 G 0300.00 4000.00 1000.00	1
0.16614058E+02 0.07395874E-01-0.06440009E-05-0.03918887E-08 0.07045959E-12	2



-0.03859547E+06-0.05865317E+03 0.07070983E+02 0.02754435E+00-0.02603669E-04	3
-0.01874567E-06 0.09778511E-10-0.03582658E+06-0.08209675E+02	4
HSICL 121986SI 1H 1CL 1 G 0300.00 2000.00 1000.00	1
0.04900627E+02 0.01981752E-01-0.03634646E-05-0.02285211E-08 0.07633527E-12	2
0.06914634E+05 0.13770041E+01 0.03072747E+02 0.09057843E-01-0.11591338E-04	3
0.08310476E-07-0.02482999E-10 0.07324210E+05 0.10334904E+02	4
HSIN 22790H 1SI 1N 1 G 0300.00 4000.00 1000.00	1
0.05746590E+02 0.11671186E-02-0.13607424E-06-0.05908616E-09 0.11746961E-13	2
0.04484671E+06-0.05931788E+02 0.04865176E+02 0.01775119E-01 0.04890869E-05	3
0.03922382E-08-0.07913276E-11 0.04526352E+06-0.07134509E+01	4
HSINH 42489SI 1H 2N 1 G 0300.00 3000.00 1000.00	1
0.06493435E+02 0.02567980E-01-0.03126526E-05-0.02577467E-08 0.06216479E-12	2
0.04035934E+06-0.07830112E+02 0.03566343E+02 0.08446736E-01-0.07699952E-05	3
-0.05270970E-07 0.02581065E-10 0.04124903E+06 0.07780791E+02	4
HSINH2 42489SI 1N 1H 3 G 0300.00 3000.00 1000.00	1
0.06177894E+02 0.04689964E-01-0.03583293E-05-0.04457980E-08 0.09379187E-12	2
0.10912773E+05-0.07006672E+02 0.02716144E+02 0.12042781E-01-0.09827195E-05	3
-0.07408477E-07 0.03789792E-10 0.11907715E+05 0.11262523E+02	4
I*C3H7 120186C 3H 7 G 0300.00 5000.00 1000.00	1
0.08063369E+02 0.15744876E-01-0.05182391E-04 0.07477245E-08-0.03854422E-12	2
0.05313871E+05-0.02192646E+03 0.01713299E+02 0.02542616E+00 0.15808083E-05	3
-0.01821286E-06 0.08827710E-10 0.07535808E+05 0.12979008E+02	4
ME2GAET 62987GA 1C 4H 11 G 0300.00 1500.00 0600.00	1
0.07174541E+02 0.03235532E+00 0.14951986E-05-0.10482260E-07 0.03053961E-10	2
-0.06383914E+05-0.02026765E+02-0.03218207E+02 0.06398884E+00 0.15545521E-04	3
-0.12847095E-06 0.09441259E-09-0.04451897E+05 0.04848091E+03	4
MEGAET 62987GA 1C 3H 8 G 0300.00 1500.00 0600.00	1
0.06600990E+02 0.02284791E+00 0.10133754E-05-0.07318045E-07 0.02140196E-10	2
0.04071592E+05 0.05239051E+01-0.08169937E+01 0.04554296E+00 0.10531326E-04	3
-0.09079987E-06 0.06700563E-09 0.05448005E+05 0.03655501E+03	4
MEGAET2 62987GA 1C 5H 13 G 0300.00 1500.00 0600.00	1
0.08123155E+02 0.03978908E+00 0.01690979E-04-0.13084149E-07 0.03852598E-10	2
-0.08091056E+05-0.05039992E+02-0.05607498E+02 0.08187357E+00 0.01920530E-03	3
-0.01678978E-05 0.12433538E-09-0.05546687E+05 0.06163371E+03	4
N 120186N 1 G 0300.00 5000.00 1000.00	1
0.02450268E+02 0.10661458E-03-0.07465337E-06 0.01879652E-09-0.10259839E-14	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
N*C3H7 120186C 3H 7 G 0300.00 5000.00 1000.00	1
0.07978290E+02 0.15761134E-01-0.05173243E-04 0.07443892E-08-0.03824978E-12	2
0.07579402E+05-0.01935611E+03 0.01922536E+02 0.02478927E+00 0.01810249E-04	3
-0.01783265E-06 0.08582996E-10 0.09713281E+05 0.13992715E+02	4
N2 121286N 2 G 0300.00 5000.00 1000.00	1
0.02926640E+02 0.14879768E-02-0.05684760E-05 0.10097038E-09-0.06753351E-13	2

-0.09227977E+04	0.05980528E+02	0.03298677E+02	0.14082404E-02	-0.03963222E-04	3
0.05641515E-07	-0.02444854E-10	-0.10208999E+04	0.03950372E+02		4
N2H2	121286N	2H 2	G	0300.00 5000.00 1000.00	1
0.03371185E+02	0.06039968E-01	-0.02303853E-04	0.04062789E-08	-0.02713144E-12	2
0.02418172E+06	0.04980585E+02	0.16179994E+01	0.13063122E-01	-0.01715711E-03	3
0.16056079E-07	-0.06093638E-10	0.02467526E+06	0.13794670E+02		4
N2H3	120186N	2H 3	G	0300.00 5000.00 1000.00	1
0.04441846E+02	0.07214270E-01	-0.02495684E-04	0.03920564E-08	-0.02298949E-12	2
0.16642211E+05	-0.04275204E+01	0.03174203E+02	0.04715907E-01	0.13348671E-04	3
-0.01919684E-06	0.07487563E-10	0.01727269E+06	0.07557224E+02		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	-0.02962989E+02	0.06442605E+00	0.02749729E+00	-0.02899451E-03	3
0.01745239E-06	-0.04422282E-10	0.10451917E+05	0.02127789E+03		4
N2H4(L)	90589H	4N 2	L	0300.00 0600.00 0450.00	1
0.08890683E+02	0.08330343E-01	0.04945549E-04	-0.04909251E-08	-0.03355824E-10	2
0.03032250E+05	-0.03871433E+03	0.09047444E+02	0.09241592E-01	0.02263547E-04	3
-0.08952247E-07	0.14868629E-10	0.02970392E+05	-0.03974033E+03		4
N2O	121286N	2O 1	G	0300.00 5000.00 1000.00	1
0.04718977E+02	0.02873713E-01	-0.11974958E-05	0.02250551E-08	-0.15753370E-13	2
0.08165811E+05	-0.16572504E+01	0.02543057E+02	0.09492193E-01	-0.09792775E-04	3
0.06263844E-07	-0.01901825E-10	0.08765100E+05	0.09511222E+02		4
N2O+	121286N	2O 1E -1	G	0300.00 5000.00 1000.00	1
0.05398516E+02	0.02249478E-01	-0.09577056E-05	0.01823192E-08	-0.12844222E-13	2
0.15848513E+06	-0.03733146E+02	0.03187228E+02	0.08350714E-01	-0.07894548E-04	3
0.04597444E-07	-0.13810748E-11	0.15912794E+06	0.07779425E+02		4
N2O4	121286N	2O 4	G	0300.00 5000.00 1000.00	1
0.10482201E+02	0.05972272E-01	-0.02564043E-04	0.04916885E-08	-0.03490969E-12	2
-0.02849988E+05	-0.02612289E+03	0.03624592E+02	0.02474708E+00	-0.02172874E-03	3
0.09927103E-07	-0.02222817E-10	-0.09128241E+04	0.09457174E+02		4
N3	121286N	3	G	0300.00 5000.00 1000.00	1
0.05208505E+02	0.02444507E-01	-0.10389415E-05	0.01977416E-08	-0.13956436E-13	2
0.04796178E+06	-0.03612755E+02	0.02882218E+02	0.08930338E-01	-0.08539038E-04	3
0.05045585E-07	-0.15212480E-11	0.04863468E+06	0.08481757E+02		4
NCN	103190C	1N 2	G	0300.00 4000.00 1500.00	1
0.06652120E+02	0.06108034E-02	-0.13897266E-06	0.02695549E-10	0.16699439E-14	2
0.05172403E+06	-0.11385166E+02	0.03101270E+02	0.09981674E-01	-0.09920701E-04	3
0.04758919E-07	-0.08968626E-11	0.05285757E+06	0.07317579E+02		4
NCO	121286N	1C 1O 1	G	0300.00 5000.00 1000.00	1
0.05012045E+02	0.02626773E-01	-0.11082433E-05	0.02093860E-08	-0.14603470E-13	2
0.01737185E+06	-0.01830075E+02	0.02830320E+02	0.08871490E-01	-0.08945636E-04	3
0.05876918E-07	-0.01907734E-10	0.01800543E+06	0.09498831E+02		4
NF	121286N	1F 1	G	0300.00 5000.00 1000.00	1
0.03862176E+02	0.07551806E-02	-0.03044942E-05	0.05874447E-09	-0.04187479E-13	2

	0.02867242E+06	0.03457232E+02	0.02871947E+02	0.03312192E-01	-0.02691158E-04	3
	0.11219514E-08	-0.02475130E-11	0.02896257E+06	0.08640247E+02		4
NF0	121286N	1F	10	1	G 0300.00 5000.00 1000.00	1
	0.05174520E+02	0.01938472E-01	-0.08222701E-05	0.15642909E-09	-0.11044974E-13	2
	-0.09670935E+05	-0.05352460E+01	0.03352307E+02	0.07229966E-01	-0.06951136E-04	3
	0.03828526E-07	-0.10235582E-11	-0.09167035E+05	0.08854189E+02		4
NF02	121286N	1F	10	2	G 0300.00 5000.00 1000.00	1
	0.06816857E+02	0.03462639E-01	-0.14922156E-05	0.02869665E-08	-0.02041856E-12	2
	-0.15602619E+05	-0.09320129E+02	0.02447528E+02	0.15441095E-01	-0.13005952E-04	3
	0.04856383E-07	-0.06852266E-11	-0.14393999E+05	0.13283604E+02		4
NH	31387H	1N	1		G 0300.00 5000.00 1000.00	1
	0.02760249E+02	0.13753463E-02	-0.04451914E-05	0.07692791E-09	-0.05017592E-13	2
	0.04207828E+06	0.05857199E+02	0.03339758E+02	0.12530086E-02	-0.03491645E-04	3
	0.04218812E-07	-0.15576179E-11	0.04185047E+06	0.02507180E+02		4
NH2	121686N	1H	2		G 0300.00 5000.00 1000.00	1
	0.02961311E+02	0.02932699E-01	-0.09063600E-05	0.16172575E-09	-0.12042003E-13	2
	0.02191976E+06	0.05777878E+02	0.03432493E+02	0.03299540E-01	-0.06613600E-04	3
	0.08590947E-07	-0.03572046E-10	0.02177227E+06	0.03090110E+02		4
NH3	121386N	1H	3		G 0300.00 5000.00 1000.00	1
	0.02461904E+02	0.06059166E-01	-0.02004976E-04	0.03136003E-08	-0.01938317E-12	2
	-0.06493269E+05	0.07472097E+02	0.02204351E+02	0.10114765E-01	-0.14652648E-04	3
	0.14472350E-07	-0.05328509E-10	-0.06525488E+05	0.08127138E+02		4
NNH	120186N	2H	1		G 0250.00 4000.00 1000.00	1
	0.04415342E+02	0.16143879E-02	-0.16328943E-06	-0.08559846E-09	0.16147909E-13	2
	0.02788029E+06	0.09042888E+01	0.03501344E+02	0.02053586E-01	0.07170409E-05	3
	0.04921348E-08	-0.09671170E-11	0.02833347E+06	0.06391837E+02		4
NO	121286N	10	1		G 0300.00 5000.00 1000.00	1
	0.03245435E+02	0.12691383E-02	-0.05015890E-05	0.09169283E-09	-0.06275419E-13	2
	0.09800840E+05	0.06417293E+02	0.03376541E+02	0.12530634E-02	-0.03302750E-04	3
	0.05217810E-07	-0.02446262E-10	0.09817961E+05	0.05829590E+02		4
NO+	121286N	10	1E	-1	G 0300.00 5000.00 1000.00	1
	0.02914888E+02	0.14993349E-02	-0.05727972E-05	0.10177767E-09	-0.06825390E-13	2
	0.11818688E+06	0.06844346E+02	0.03297349E+02	0.14228899E-02	-0.04007441E-04	3
	0.05670551E-07	-0.02446971E-10	0.11808338E+06	0.04749948E+02		4
N02	121286N	10	2		G 0300.00 5000.00 1000.00	1
	0.04682859E+02	0.02462429E-01	-0.10422585E-05	0.01976902E-08	-0.13917168E-13	2
	0.02261292E+05	0.09885985E+01	0.02670600E+02	0.07838500E-01	-0.08063864E-04	3
	0.06161714E-07	-0.02320150E-10	0.02896290E+05	0.11612071E+02		4
N02-	121286N	10	2E	1	G 0300.00 5000.00 1000.00	1
	0.05043114E+02	0.02166427E-01	-0.09455454E-05	0.01816313E-08	-0.12383945E-13	2
	-0.02621553E+06	-0.14459051E+01	0.02448586E+02	0.08982507E-01	-0.07853431E-04	3
	0.03927276E-07	-0.10716939E-11	-0.02545097E+06	0.12130600E+02		4
N03	121286N	10	3		G 0300.00 5000.00 1000.00	1
	0.07120307E+02	0.03246228E-01	-0.14316134E-05	0.02797053E-08	-0.02013007E-12	2

	0.05864479E+05-0.12137301E+02	0.12210763E+01	0.01878797E+00-0.13443212E-04	3	
	0.12746013E-08	0.13540601E-11	0.07473144E+05	0.01840202E+03	4
Onr	1201860	1	G 0300.00 5000.00 1000.00	1	
	0.02542059E+02-0.02755061E-03-0.03102803E-07	0.04551067E-10-0.04368051E-14		2	
	0.02923080E+06	0.04920308E+02	0.02946428E+02-0.16381665E-02	0.02421031E-04	3
	-0.16028431E-08	0.03890696E-11	0.02914764E+06	0.02963995E+02	4
0	1201860	1	G 0300.00 5000.00 1000.00	1	
	0.02542059E+02-0.02755061E-03-0.03102803E-07	0.04551067E-10-0.04368051E-14		2	
	0.02923080E+06	0.04920308E+02	0.02946428E+02-0.16381665E-02	0.02421031E-04	3
	-0.16028431E-08	0.03890696E-11	0.02914764E+06	0.02963995E+02	4
0+	1212860	1E -1	G 0300.00 5000.00 1000.00	1	
	0.02501869E+02-0.06107262E-04	0.07324307E-07-0.03438353E-10	0.05506407E-14		2
	0.01879552E+07	0.04372826E+02	0.02499272E+02	0.05820598E-04-0.11209219E-07	3
	0.08232108E-10-0.01916378E-13	0.01879556E+07	0.04384825E+02		4
0-	905890	1E 1	G 0300.00 5000.00 1000.00	1	
	0.02559580E+02-0.07147887E-03	0.03301804E-06-0.06660944E-10	0.04900726E-14		2
	0.11489346E+05	0.04426186E+02	0.02747263E+02-0.05724860E-02	0.02712548E-05	3
	0.02691511E-08-0.02002357E-11	0.11443947E+05	0.03469852E+02		4
02	1213860	2	G 0300.00 5000.00 1000.00	1	
	0.03697578E+02	0.06135197E-02-0.12588420E-06	0.01775281E-09-0.11364354E-14		2
	-0.12339301E+04	0.03189165E+02	0.03212936E+02	0.11274864E-02-0.05756150E-05	3
	0.13138773E-08-0.08768554E-11-0.10052490E+04	0.06034737E+02			4
02-	1212860	2E 1	G 0300.00 5000.00 1000.00	1	
	0.03883013E+02	0.07407872E-02-0.02961776E-05	0.05724304E-09-0.04086547E-13		2
	-0.07121644E+05	0.02658211E+02	0.02872291E+02	0.03359716E-01-0.02664886E-04	3
	0.09807524E-08-0.16709571E-12-0.06829094E+05	0.07938372E+02			4
03	1212860	3	G 0300.00 5000.00 1000.00	1	
	0.05429371E+02	0.01820380E-01-0.07705607E-05	0.14992929E-09-0.10755629E-13		2
	0.15235267E+05-0.03266386E+02	0.02462608E+02	0.09582781E-01-0.07087359E-04		3
	0.13633683E-08	0.02969647E-11	0.16061522E+05	0.12141870E+02	4
0C(OH)2	103190C	1H 20 3	G 0300.00 4000.00 1500.00	1	
	0.11431961E+02	0.02555103E-01-0.04326538E-05-0.05781341E-09	0.15454611E-13		2
	-0.07904865E+06-0.03657200E+03	0.03540332E+01	0.03042527E+00-0.02939615E-03		3
	0.14529342E-07-0.02906245E-10-0.07522629E+06	0.02250923E+03			4
0CHCHO	103190C	2H 20 2	G 0300.00 4000.00 1500.00	1	
	0.10568433E+02	0.02907353E-01-0.03452401E-05-0.10375932E-09	0.02042134E-12		2
	-0.02952623E+06-0.03104084E+03	0.01863564E+02	0.02298297E+00-0.01917997E-03		3
	0.08558604E-07-0.16123463E-11-0.02634846E+06	0.16016745E+02			4
0CHNNHO	103190C	1H 2N 20 2G	0300.00 4000.00 1500.00	1	
	0.12413972E+02	0.04091550E-01-0.04547841E-05-0.01752323E-08	0.03271471E-12		2
	-0.06754774E+05-0.04078722E+03	0.14052751E+01	0.02776280E+00-0.02088465E-03		3
	0.08550259E-07-0.15434856E-11-0.02537630E+05	0.01937722E+03			4
0Hnr	1212860	1H 1	G 0300.00 5000.00 1000.00	1	
	0.02882730E+02	0.10139743E-02-0.02276877E-05	0.02174683E-09-0.05126305E-14		2

	0.03886888E+05	0.05595712E+02	0.03637266E+02	0.01850910E-02	-0.16761646E-05	3
	0.02387202E-07	-0.08431442E-11	0.03606781E+05	0.13588605E+01		4
OH	1212860	1H	1	G	0300.00 5000.00 1000.00	1
	0.02882730E+02	0.10139743E-02	-0.02276877E-05	0.02174683E-09	-0.05126305E-14	2
	0.03886888E+05	0.05595712E+02	0.03637266E+02	0.01850910E-02	-0.16761646E-05	3
	0.02387202E-07	-0.08431442E-11	0.03606781E+05	0.13588605E+01		4
OH+	1212860	1H	1E	-1	G 0300.00 5000.00 1000.00	1
	0.02719058E+02	0.15085714E-02	-0.05029369E-05	0.08261951E-09	-0.04947452E-13	2
	0.15763414E+06	0.06234536E+02	0.03326978E+02	0.13457859E-02	-0.03777167E-04	3
	0.04687749E-07	-0.01780982E-10	0.15740294E+06	0.02744042E+02		4
OH-	1212860	1H	1E	1	G 0300.00 5000.00 1000.00	1
	0.02846204E+02	0.10418347E-02	-0.02416850E-05	0.02483215E-09	-0.07775605E-14	2
	-0.01807280E+06	0.04422712E+02	0.03390037E+02	0.07922381E-02	-0.01943429E-04	3
	0.02001769E-07	-0.05702087E-11	-0.01830493E+06	0.12498923E+01		4
ONHNHO	103190H	2N	20	2	G 0300.00 4000.00 1500.00	1
	0.10055101E+02	0.03525461E-01	-0.03868361E-05	-0.12986541E-09	0.02398500E-12	2
	0.07381692E+05	-0.02950581E+03	0.07815142E+01	0.02605711E+00	-0.02264713E-03	3
	0.10499245E-07	-0.02012847E-10	0.10627777E+05	0.02017945E+03		4
ONHNOH	103190H	2N	20	2	G 0300.00 4000.00 1500.00	1
	0.11208735E+02	0.02650302E-01	-0.03760644E-05	-0.06355768E-09	0.14662515E-13	2
	-0.05721250E+05	-0.03476474E+03	0.10532706E+01	0.02809676E+00	-0.02637379E-03	3
	0.12707572E-07	-0.02478550E-10	-0.02244768E+05	0.01937010E+03		4
S	121286S	1		G	0300.00 5000.00 1000.00	1
	0.02902148E+02	-0.05484546E-02	0.02764576E-05	-0.05017114E-09	0.03150684E-13	2
	0.03249423E+06	0.03838471E+02	0.03187329E+02	-0.15957763E-02	0.02005531E-04	3
	-0.15070814E-08	0.04931282E-11	0.03242259E+06	0.02414441E+02		4
S(L)	120186S	1		L	0388.36 2000.00 1000.00	1
	0.03603667E+02	0.09903341E-02	-0.10114410E-05	0.04053632E-08	-0.05667913E-12	2
	-0.08453839E+04	-0.16344708E+02	-0.12706310E+02	0.09072521E+00	-0.01695178E-02	3
	0.13070636E-06	-0.03527615E-09	0.12346069E+04	0.05621016E+03		4
S(S)	120186S	1		S	0300.00 0388.36 1000.00	1
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	2
	0.00000000E+00	0.00000000E+00	-0.05063702E+02	0.02881935E-01	-0.02133020E-03	3
	0.08478786E-05	-0.01734496E-07	0.07148263E+04	0.02871407E+03		4
S+	121286S	1E	-1	G	0300.00 5000.00 1000.00	1
	0.02404600E+02	0.02410908E-02	-0.02041779E-05	0.06592945E-09	-0.05756939E-13	2
	0.15352225E+06	0.05924256E+02	0.02366100E+02	0.09130767E-02	-0.02140283E-04	3
	0.02076177E-07	-0.07133859E-11	0.15350910E+06	0.05993094E+02		4
S-TRIAZINE	41687C	3N	3H	3	G 0300.00 4000.00 1000.00	1
	0.13036170E+02	0.07711820E-01	-0.07724374E-05	-0.04385191E-08	0.08298992E-12	2
	0.02251663E+06	-0.04777676E+03	0.04493492E+01	0.02728306E+00	0.02309304E-04	3
	-0.14968443E-07	0.04546753E-10	0.02703032E+06	0.02178518E+03		4
S2	121386S	1		G	0300.00 5000.00 1000.00	1
	0.03904443E+02	0.06925733E-02	-0.12330970E-06	0.08783809E-11	0.13746621E-14	2

	0.14256933E+05	0.04956834E+02	0.03157672E+02	0.03099480E-01	-0.15607465E-05	3
	-0.13578905E-08	0.11374435E-11	0.14391873E+05	0.08596062E+02		4
SH	121286S	1H	1	G	0300.00 5000.00 1000.00	1
	0.03053810E+02	0.12588843E-02	-0.04249169E-05	0.06929591E-09	-0.04281691E-13	2
	0.15882250E+05	0.05973551E+02	0.04133326E+02	-0.03787893E-02	-0.02777854E-04	3
	0.05370112E-07	-0.02394006E-10	0.15558623E+05	0.16115348E+00		4
SI	32989SI	1		G	0300.00 4000.00 1000.00	1
	0.02775845E+02	-0.06213257E-02	0.04843696E-05	-0.12756146E-09	0.11344818E-13	2
	0.05339790E+06	0.04543298E+02	0.03113515E+02	-0.02330991E-01	0.03518530E-04	3
	-0.02417573E-07	0.06391902E-11	0.05335061E+06	0.03009718E+02		4
SI(L)	90589SI	1		L	0300.00 4500.00 1000.00	1
	0.03271263E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	2
	0.04855057E+05	-0.13290542E+02	0.03271263E+02	0.00000000E+00	0.00000000E+00	3
	0.00000000E+00	0.00000000E+00	0.04855058E+05	-0.13290542E+02		4
SI(NH2)3	42489SI	1N	3H	6	G	0300.00 3000.00 1000.00
	0.14065501E+02	0.07581744E-01	-0.05168510E-05	-0.06743626E-08	0.13979258E-12	2
	-0.14144028E+05	-0.04063873E+03	0.07598413E+02	0.02435266E+00	-0.04296202E-04	3
	-0.01756006E-06	0.10501017E-10	-0.12653434E+05	-0.07808647E+02		4
SI(NH2)4	22790SI	1N	4H	8	G	0300.00 4000.00 1000.00
	0.02032107E+03	0.08289798E-01	-0.07077612E-05	-0.04340724E-08	0.07747068E-12	2
	-0.05389855E+06	-0.07730464E+03	0.08454529E+02	0.03465772E+00	-0.04266782E-04	3
	-0.02495363E-06	0.13654663E-10	-0.05061518E+06	-0.15143013E+02		4
SI(S)	90589SI	1		S	0300.00 2500.00 1000.00	1
	0.02530275E+02	0.08522433E-02	-0.03223468E-05	0.12808208E-09	-0.01850849E-12	2
	-0.08395197E+04	-0.12514782E+02	0.05746418E+01	0.10264855E-01	-0.01775345E-03	3
	0.14575000E-07	-0.04491292E-10	-0.04969951E+04	-0.03400242E+02		4
SI2	90589SI	2		G	0300.00 2000.00 1000.00	1
	0.04232196E+02	0.04315355E-02	-0.02964833E-05	0.09823294E-09	-0.12962688E-13	2
	0.06964651E+06	0.03308527E+02	0.02993750E+02	0.06053689E-01	-0.10158575E-04	3
	0.07909737E-07	-0.02346083E-10	0.06987498E+06	0.09151741E+02		4
SI2C	112989C	1SI	2		G	0300.00 5000.00 1000.00
	0.06334110E+02	0.12102520E-02	-0.06798289E-05	0.02244432E-08	-0.02280177E-12	2
	0.06227189E+06	-0.07770097E+02	0.04157246E+02	0.07031825E-01	-0.07263033E-04	3
	0.04633583E-07	-0.14934475E-11	0.06292421E+06	0.03635125E+02		4
SI2F6	42489SI	2F	6		G	0300.00 3000.00 1000.00
	0.01830047E+03	0.02868752E-01	-0.04545576E-05	-0.02497900E-08	0.06630658E-12	2
	-0.02928185E+07	-0.05760425E+03	0.09998134E+02	0.02170313E+00	-0.03875091E-04	3
	-0.16702523E-07	0.09407529E-10	-0.02905482E+07	-0.14228863E+02		4
SI2H2	90589SI	2H	2		G	0300.00 2000.00 1000.00
	0.05778180E+02	0.04070596E-01	-0.04259125E-05	-0.07920228E-08	0.02379752E-11	2
	0.03980520E+06	-0.05392375E+02	0.16247229E+01	0.14871029E-01	-0.08707160E-04	3
	-0.01699554E-09	0.10972211E-11	0.04095325E+06	0.16165730E+02		4
SI2H3	90589SI	2H	3		G	0300.00 2000.00 1000.00
	0.07257627E+02	0.05123859E-01	-0.07633465E-05	-0.06662471E-08	0.02053052E-11	2

	0.05062055E+06-0.10314127E+02	0.03335404E+02	0.02155614E+00-0.02933937E-03	3	
	0.02287784E-06-0.07272827E-10	0.05146157E+06	0.08656853E+02	4	
SI2H5	90589SI	2H 5	G 0300.00 2000.00 1000.00	1	
	0.08451010E+02	0.09286371E-01-0.10911831E-05-0.14423673E-08	0.04250824E-11	2	
	0.02472718E+06-0.01710331E+03	0.15788481E+01	0.03549382E+00-0.04267511E-03	3	
	0.03059177E-06-0.09360425E-10	0.02630549E+06	0.16720734E+02	4	
SI2H6	90589SI	2H 6	G 0300.00 2000.00 1000.00	1	
	0.08882090E+02	0.11513955E-01-0.12162159E-05-0.01905085E-07	0.05542379E-11	2	
	0.05967241E+05-0.02265611E+03	0.05301921E+01	0.04184055E+00-0.04685249E-03	3	
	0.03179525E-06-0.09484526E-10	0.07950597E+05	0.01880453E+03	4	
SI3	32989SI	3	G 0300.00 4000.00 1000.00	1	
	0.07021584E+02	0.06981538E-02-0.04818729E-05	0.01720754E-08-0.01927024E-12	2	
	0.07429956E+06-0.08179232E+02	0.05312161E+02	0.05920180E-01-0.05075224E-04	3	
	0.05303866E-08	0.07031630E-11	0.07469501E+06	0.04036452E+01	4
SI3H8	90589SI	3H 8	G 0300.00 2000.00 1000.00	1	
	0.13422770E+02	0.15636323E-01-0.01936565E-04-0.02388329E-07	0.07120030E-11	2	
	0.09165887E+05-0.04163000E+03	0.06319791E+01	0.06412995E+00-0.07772444E-03	3	
	0.05486969E-06-0.16460971E-10	0.12092580E+05	0.02133318E+03	4	
SI3N4(A)	42589N	4SI 3	S 0300.00 3000.00 1000.00	1	
	0.09667453E+02	0.11927212E-01-0.01709281E-04-0.10846074E-08	0.02713018E-11	2	
	-0.09324734E+06-0.04556492E+03	0.06631384E+02	0.02293928E+00-0.02152875E-03	3	
	0.01766237E-06-0.06632214E-10-0.09241684E+06-0.03021795E+03			4	
SIC	112989C	1SI 1	G 0300.00 5000.00 1000.00	1	
	0.05024270E+02-0.04920894E-02	0.03109315E-05-0.06901344E-09	0.05215735E-13	2	
	0.08531026E+06-0.02478798E+02	0.02427812E+02	0.09551934E-01-0.02796633E-04	3	
	-0.13600122E-07	0.09196322E-10	0.08546512E+06	0.09179253E+02	4
SIC(B)	112989C	1SI 1	S 0300.00 4000.00 1000.00	1	
	0.03548056E+02	0.03636817E-01-0.01734872E-04	0.03912869E-08-0.03337952E-12	2	
	-0.10188585E+05-0.01967253E+03-0.03551395E+01	0.15998806E-01-0.13933268E-04		3	
	0.03314914E-07	0.07825957E-11-0.09294352E+05-0.15153885E+00		4	
SIC2	112989C	2SI 1	G 0300.00 5000.00 1000.00	1	
	0.05753725E+02	0.02067546E-01-0.11325346E-05	0.03106456E-08-0.02799936E-12	2	
	0.07200461E+06-0.05294926E+02	0.03647724E+02	0.08765100E-01-0.10798686E-04	3	
	0.07974287E-07-0.02617042E-10	0.07258578E+06	0.05481049E+02	4	
SICL	121986SI	1CL 1	G 0300.00 2000.00 1000.00	1	
	0.04258459E+02	0.04020317E-02-0.02888145E-05	0.10097771E-09-0.14110117E-13	2	
	0.01775613E+06	0.04134521E+02	0.03096406E+02	0.05738623E-01-0.09740903E-04	3
	0.07643597E-07-0.02279178E-10	0.01796794E+06	0.09603212E+02	4	
SICL2	121986SI	1CL 2	G 0300.00 2000.00 1000.00	1	
	0.06491204E+02	0.08242384E-02-0.05767737E-05	0.01972405E-08-0.02713757E-12	2	
	-0.02232408E+06-0.03570531E+02	0.03826666E+02	0.13082964E-01-0.02234087E-03	3	
	0.01760741E-06-0.05267404E-10-0.02183869E+06	0.08965448E+02		4	
SICL2H2	121986SI	1H 2CL 2	G 0300.00 2000.00 1000.00	1	
	0.07727079E+02	0.05034188E-01-0.10957459E-05-0.04419587E-08	0.16311241E-12	2	

-0.04028605E+06-0.11708156E+02 0.11002086E+01 0.03262361E+00-0.04691994E-03	3
0.03494565E-06-0.10362847E-10-0.03892086E+06 0.02022693E+03	4
SICL3 121986SI 1CL 3 G 0300.00 2000.00 1000.00	1
0.09098097E+02 0.14053526E-02-0.09317005E-05 0.02982296E-08-0.03822010E-12	2
-0.04140193E+06-0.14550117E+02 0.04485690E+02 0.02241754E+00-0.03794196E-03	3
0.02973183E-06-0.08861335E-10-0.04055264E+06 0.07198771E+02	4
SICL3H 121986SI 1H 1CL 3 G 0300.00 2000.00 1000.00	1
0.09663121E+02 0.03563367E-01-0.12149114E-05-0.16090094E-10 0.05641710E-12	2
-0.06295557E+06-0.01894777E+03 0.02883769E+02 0.03308240E+00-0.05169241E-03	3
0.03949918E-06-0.11721043E-10-0.06163323E+06 0.13374664E+02	4
SICL4 121986SI 1CL 4 G 0300.00 2000.00 1000.00	1
0.11709377E+02 0.01972091E-01-0.12690771E-05 0.03900188E-08-0.04756468E-12	2
-0.08347808E+06-0.02791153E+03 0.05252110E+02 0.03122067E+00-0.05254593E-03	3
0.04102707E-06-0.12199071E-10-0.08228177E+06 0.02575727E+02	4
SICLH3 121986SI 1H 3CL 1 G 0300.00 2000.00 1000.00	1
0.05964237E+02 0.06278087E-01-0.08205634E-05-0.09280558E-08 0.02796642E-11	2
-0.01854309E+06-0.06395305E+02 0.05057173E+01 0.02703377E+00-0.03301474E-03	3
0.02302732E-06-0.06778703E-10-0.01730819E+06 0.02043167E+03	4
SIF 42489SI 1F 1 G 0300.00 3000.00 1000.00	1
0.04120066E+02 0.03548820E-02-0.07200222E-06-0.02190434E-09 0.06764591E-13	2
-0.07561378E+05 0.02784246E+02 0.03144947E+02 0.02588557E-01-0.05795912E-05	3
-0.01807278E-07 0.10411718E-11-0.07294439E+05 0.07876774E+02	4
SIF(NH2)2 22790SI 1F 1N 2H 4G 0300.00 4000.00 1000.00	1
0.12879436E+02 0.04598535E-01-0.04004440E-05-0.02374189E-08 0.04255211E-12	2
-0.05238278E+06-0.03653418E+03 0.07210094E+02 0.01764697E+00-0.02542059E-04	3
-0.12422138E-07 0.06989787E-10-0.05086706E+06-0.07024622E+02	4
SIF(NH2)3 42489SI 1N 3H 6F 1G 0300.00 3000.00 1000.00	1
0.16111795E+02 0.08329222E-01-0.06023787E-05-0.07470125E-08 0.15707311E-12	2
-0.09137007E+06-0.05098123E+03 0.08388268E+02 0.02746622E+00-0.04455674E-04	3
-0.01955732E-06 0.11407210E-10-0.08947806E+06-0.11381777E+02	4
SIF2 42489SI 1F 2 G 0300.00 3000.00 1000.00	1
0.06142470E+02 0.07807974E-02-0.13393119E-06-0.06264839E-09 0.01725138E-12	2
-0.07744042E+06-0.04712327E+02 0.03845345E+02 0.06038465E-01-0.11677323E-05	3
-0.04579553E-07 0.02607414E-10-0.07681633E+06 0.07272983E+02	4
SIF2(NH2)2 42489SI 1N 2H 4F 2G 0300.00 3000.00 1000.00	1
0.14414775E+02 0.06110646E-01-0.04871145E-05-0.05455935E-08 0.11727140E-12	2
-0.12927572E+06-0.04308682E+03 0.07634268E+02 0.02315843E+00-0.04193827E-04	3
-0.01715350E-06 0.10164619E-10-0.12764102E+06-0.08419031E+02	4
SIF2N 42489SI 1N 1F 2 G 0300.00 3000.00 1000.00	1
0.08687337E+02 0.11934885E-02-0.01992660E-05-0.09951333E-09 0.02704383E-12	2
-0.03463832E+06-0.14940526E+02 0.05102583E+02 0.09456606E-01-0.01819383E-04	3
-0.07309616E-07 0.04178902E-10-0.03367293E+06 0.03734423E+02	4
SIF2NH2 42489SI 1N 1F 2H 2G 0300.00 3000.00 1000.00	1
0.09872415E+02 0.03722112E-01-0.03271338E-05-0.03321674E-08 0.07293692E-12	2



-0.08751628E+06-0.01899095E+03 0.05890444E+02 0.12851282E-01-0.01863556E-04	3
-0.08718963E-07 0.04848951E-10-0.08644527E+06 0.01756162E+02	4
SIF3                    42489SI 1F 3                    G 0300.00 3000.00 1000.00	1
0.08524790E+02 0.13237924E-02-0.02104278E-05-0.11495040E-09 0.03055301E-12	2
-0.12235223E+06-0.15502343E+02 0.04662868E+02 0.10087878E-01-0.01805544E-04	3
-0.07769299E-07 0.04377851E-10-0.12129652E+06 0.04672966E+02	4
SIF3NH                    42489SI 1N 1F 3H 1G 0300.00 3000.00 1000.00	1
0.11637665E+02 0.02880768E-01-0.03357310E-05-0.02584594E-08 0.06162371E-12	2
-0.12958909E+06-0.02590717E+03 0.06013822E+02 0.15977294E-01-0.02791466E-04	3
-0.12141200E-07 0.06927415E-10-0.12809741E+06 0.03316770E+02	4
SIF3NH2                    42489SI 1N 1F 3H 2G 0300.00 3000.00 1000.00	1
0.12109636E+02 0.04383282E-01-0.04142245E-05-0.03989090E-08 0.08958954E-12	2
-0.16417679E+06-0.03046928E+03 0.06229403E+02 0.01778015E+00-0.02612304E-04	3
-0.12672434E-07 0.07044556E-10-0.16258489E+06 0.02045440E+01	4
SIF3NHSIH3                    42489SI 2N 1H 4F 3G 0300.00 3000.00 1000.00	1
0.16699406E+02 0.07789784E-01-0.08110570E-05-0.07650199E-08 0.01773956E-11	2
-0.16734123E+06-0.05080007E+03 0.06216046E+02 0.02939330E+00-0.02717745E-04	3
-0.01982877E-06 0.10027676E-10-0.16422818E+06 0.04858261E+02	4
SIF3NSIH3                    42489SI 2N 1H 3F 3G 0300.00 3000.00 1000.00	1
0.15991462E+02 0.06371085E-01-0.07256823E-05-0.06292690E-08 0.14951566E-12	2
-0.13311576E+06-0.04495265E+03 0.06404371E+02 0.02601982E+00-0.02491543E-04	3
-0.01769542E-06 0.08919883E-10-0.13025197E+06 0.06002945E+02	4
SIF4                    41389F 4SI 1                    G 0300.00 2000.00 1000.00	1
0.09985301E+02 0.03532637E-01-0.11973776E-05-0.10365486E-09 0.08661585E-12	2
-0.01977199E+07-0.02472643E+03 0.02147416E+02 0.03402219E+00-0.04756873E-03	3
0.03252196E-06-0.08819304E-10-0.01960449E+07 0.13463150E+02	4
SIFH3                    42489SI 1F 1H 3                    G 0300.00 3000.00 1000.00	1
0.06799678E+02 0.04747086E-01-0.04767066E-05-0.04814665E-08 0.11077613E-12	2
-0.04577024E+06-0.12614326E+02 0.02032189E+02 0.13413632E-01-0.02806381E-05	3
-0.07803291E-07 0.03337474E-10-0.04421627E+06 0.13187677E+02	4
SIFNH                    42489SI 1N 1F 1H 1G 0300.00 3000.00 1000.00	1
0.07163298E+02 0.15213245E-02-0.15363371E-06-0.11959331E-09 0.02684099E-12	2
-0.09065496E+05-0.06764144E+02 0.05390691E+02 0.06071319E-01-0.13594903E-05	3
-0.04267435E-07 0.02603153E-10-0.08644237E+05 0.02272064E+02	4
SIFNH2                    22790F 1SI 1N 1H 2G 0300.00 4000.00 1000.00	1
0.08017582E+02 0.03209103E-01-0.03361364E-05-0.01796536E-08 0.03385552E-12	2
-0.04313426E+06-0.14870236E+02 0.04214050E+02 0.11054231E-01-0.10147254E-05	3
-0.07143728E-07 0.03634922E-10-0.04200629E+06 0.05318889E+02	4
SIH                    121986SI 1H 1                    G 0300.00 2000.00 1000.00	1
0.03110430E+02 0.10949460E-02 0.02898628E-06-0.02745104E-08 0.07051799E-12	2
0.04516897E+06 0.04193487E+02 0.03836009E+02-0.02702656E-01 0.06849070E-04	3
-0.05424184E-07 0.14721313E-11 0.04507593E+06 0.09350778E+01	4
SIH2                    42489SI 1H 2                    G 0300.00 3000.00 1000.00	1
0.04142390E+02 0.02150191E-01-0.02190730E-05-0.02073725E-08 0.04741018E-12	2

0.03110483E+06	0.02930745E+01	0.03475092E+02	0.02139338E-01	0.07672305E-05	3
0.05217668E-08	-0.09898824E-11	0.03147397E+06	0.04436585E+02		4
SIH2CL	121986SI	1H 2CL 1	G	0300.00 2000.00 1000.00	1
0.05555901E+02	0.04046479E-01	-0.06581751E-05	-0.05027548E-08	0.15991101E-12	2
0.01912428E+05	-0.01906889E+02	0.01699256E+02	0.01961407E+00	-0.02622973E-03	3
0.01936416E-06	-0.05846399E-10	0.02743661E+05	0.01683132E+03		4
SIH2F	42489SI	1F 1H 2	G	0300.00 3000.00 1000.00	1
0.06020398E+02	0.03074039E-01	-0.03248886E-05	-0.03052243E-08	0.07098090E-12	2
-0.02347670E+06	-0.05919595E+02	0.02782566E+02	0.09148257E-01	-0.04186787E-05	3
-0.05388971E-07	0.02412133E-10	-0.02244201E+06	0.11528536E+02		4
SIH2F2	42489SI	1H 2F 2	G	0300.00 3000.00 1000.00	1
0.07997762E+02	0.03911538E-01	-0.04222679E-05	-0.03913812E-08	0.09171569E-12	2
-0.09682880E+06	-0.16223999E+02	0.02701455E+02	0.14565451E-01	-0.11633003E-05	3
-0.09685830E-07	0.04769590E-10	-0.09522440E+06	0.12006887E+02		4
SIH3	42489SI	1H 3	G	0300.00 3000.00 1000.00	1
0.05015906E+02	0.03732750E-01	-0.03609053E-05	-0.03729193E-08	0.08468491E-12	2
0.02190233E+06	-0.04291368E+02	0.02946733E+02	0.06466763E-01	0.05991653E-05	3
-0.02218413E-07	0.03052669E-11	0.02270173E+06	0.07347948E+02		4
SIH3NH2	42489SI	1N 1H 5	G	0300.00 3000.00 1000.00	1
0.08109945E+02	0.07215752E-01	-0.06052251E-05	-0.07086088E-08	0.15578638E-12	2
-0.08999782E+05	-0.16516504E+02	0.02936348E+02	0.16747041E-01	-0.03232858E-05	3
-0.09171970E-07	0.03979516E-10	-0.07334716E+05	0.11414373E+02		4
SIH3NHSIH3	42489SI	2N 1H 7	G	0300.00 3000.00 1000.00	1
0.12652963E+02	0.10667481E-01	-0.10073358E-05	-0.10812221E-08	0.02452363E-11	2
-0.12497210E+05	-0.03441428E+03	0.02468749E+02	0.02940254E+00	-0.06248179E-05	3
-0.01731461E-06	0.07545261E-10	-0.09209690E+05	0.02059559E+03		4
SIH3NSIH3	42489SI	2N 1H 6	G	0300.00 3000.00 1000.00	1
0.12014620E+02	0.09187517E-01	-0.09159516E-05	-0.09380967E-08	0.02156435E-11	2
0.01965065E+06	-0.02978185E+03	0.02827574E+02	0.02580646E+00	-0.04200477E-05	3
-0.15038588E-07	0.06388324E-10	0.02265351E+06	0.01997012E+03		4
SIH4	121386SI	1H 4	G	0300.00 4000.00 1000.00	1
0.06893873E+02	0.04030500E-01	-0.04183314E-05	-0.02291394E-08	0.04384766E-12	2
0.11070374E+04	-0.01749116E+03	0.02475166E+02	0.09003721E-01	0.02185394E-04	3
-0.02681423E-07	0.06621080E-11	0.02925488E+05	0.07751014E+02		4
SIHCL2	121986SI	1H 1CL 2	G	0300.00 2000.00 1000.00	1
0.07229734E+02	0.02869205E-01	-0.08849876E-05	-0.07495865E-09	0.05752338E-12	2
-0.01971399E+06	-0.07052663E+02	0.02368353E+02	0.02401088E+00	-0.03717219E-03	3
0.02851997E-06	-0.08530494E-10	0.01875884E+06	0.16145866E+02		4
SIHF	42489SI	1F 1H 1	G	0300.00 3000.00 1000.00	1
0.05073508E+02	0.15332789E-02	-0.01840658E-05	-0.14400376E-09	0.03452517E-12	2
-0.01973879E+06	-0.10795069E+01	0.03223727E+02	0.04981220E-01	-0.03173051E-05	3
-0.02822231E-07	0.12478316E-11	-0.01914167E+06	0.08906423E+02		4
SIHF2	42489SI	1H 1F 2	G	0300.00 3000.00 1000.00	1
0.07216536E+02	0.02253240E-01	-0.02737472E-05	-0.02173460E-08	0.05255331E-12	2

-0.07280241E+06-0.09783487E+02 0.03377237E+02 0.10366072E-01-0.12390823E-05	3
-0.07267981E-07 0.03794989E-10-0.07168358E+06 0.10521894E+02	4
SIHF3 42489SI 1H 1F 3 G 0300.00 3000.00 1000.00	1
0.09363567E+02 0.02947555E-01-0.03577633E-05-0.02858224E-08 0.06915728E-12	2
-0.14860736E+06-0.02169452E+03 0.03918053E+02 0.14639172E-01-0.01856069E-04	3
-0.10582003E-07 0.05617543E-10-0.14704386E+06 0.07024261E+02	4
SIN 42489SI 1N 1 G 0300.00 3000.00 1000.00	1
0.04122909E+02 0.03521457E-02-0.07161080E-06-0.02154956E-09 0.06667570E-13	2
0.05683927E+06 0.02389837E+02 0.03149181E+02 0.02584376E-01-0.05804624E-05	3
-0.01805626E-07 0.10410949E-11 0.05710563E+06 0.07474389E+02	4
SINH 42489SI 1N 1H 1 G 0300.00 3000.00 1000.00	1
0.04928800E+02 0.16286244E-02-0.13671971E-06-0.13904604E-09 0.02998968E-12	2
0.01767789E+06-0.02823472E+02 0.03166974E+02 0.05805822E-01-0.09524443E-05	3
-0.03991892E-07 0.02283188E-10 0.01813560E+06 0.06298439E+02	4
SINH2 42489SI 1N 1H 2 G 0300.00 3000.00 1000.00	1
0.05186435E+02 0.03016656E-01-0.02165476E-05-0.02722658E-08 0.05706182E-12	2
0.02270507E+06-0.12421399E+01 0.03362769E+02 0.07261175E-01-0.08721233E-05	3
-0.04400014E-07 0.02419532E-10 0.02318445E+06 0.08223867E+02	4
SN 121286S 1N 1 G 0300.00 5000.00 1000.00	1
0.03888286E+02 0.06778427E-02-0.02725308E-05 0.05135927E-09-0.03593836E-13	2
0.03044496E+06 0.04194291E+02 0.03407345E+02 0.01797887E-01-0.02018969E-04	3
0.02107857E-07-0.09527593E-11 0.03062373E+06 0.06821481E+02	4
SO 121286S 10 1 G 0300.00 5000.00 1000.00	1
0.04021077E+02 0.02584856E-02 0.08948142E-06-0.03580144E-09 0.03228430E-13	2
-0.07119620E+04 0.03452522E+02 0.03080401E+02 0.01803105E-01 0.06705022E-05	3
-0.02069005E-07 0.08514657E-11-0.03986163E+04 0.08581028E+02	4
SO2 121286S 10 2 G 0300.00 5000.00 1000.00	1
0.05254498E+02 0.01978545E-01-0.08204226E-05 0.15763830E-09-0.11204512E-13	2
-0.03756885E+06-0.11460563E+01 0.02911438E+02 0.08103022E-01-0.06906710E-04	3
0.03329015E-07-0.08777121E-11-0.03687881E+06 0.11117403E+02	4
SO3 121286S 10 3 G 0300.00 5000.00 1000.00	1
0.07050668E+02 0.03246560E-01-0.14088974E-05 0.02721535E-08-0.01942364E-12	2
-0.05020667E+06-0.11064426E+02 0.02575282E+02 0.15150916E-01-0.12298717E-04	3
0.04240257E-07-0.05266812E-11-0.04894410E+06 0.12195116E+02	4
NA20 tpis82NA 2.0 1. 0. 0.G 200.000 6000.000 1000.	1
7.22445198E+00 2.89517146E-04-1.15117270E-07 1.98465646E-11-1.24263508E-15	2
-4.22757052E+03-8.78254668E+00 4.47778382E+00 1.41517070E-02-2.77158315E-05	3
2.49680245E-08-8.46422797E-12-3.75620660E+03 3.92861915E+00	4
NA02 D=37.2NA 10 2 0 G 300.000 2000.000 1000.00	1
.24373729D+01 .11708054D-01 -.12465450D-04 .60394798D-08 -.10877028D-11	2
-.68349080D+04 .15175355D+02 .24373729D+01 .11708054D-01 -.12465450D-04	3
.60394798D-08 -.10877028D-11 -.68349080D+04 .15175355D+02	4
HCL 42189CL 1H 1 G 300.000 2000.000 1000.00	1
.37039792D+01 -.12852596D-02 .24168090D-05 -.12493998D-08 .21730232D-12	2

-	12167451D+05	.16516317D+01	.37039792D+01	-	12852596D-02	.24168090D-05	3		
-	12493998D-08	.21730232D-12	-	12167451D+05	.16516317D+01		4		
CL	42189CL	1		G	300.000	2000.000	1000.00	1	
	.21819488D+01	.23933914D-02	-	34824719D-05	.19618096D-08	-	38542551D-12	2	
	.13858705D+05	.68500574D+01	.21819488D+01		.23933914D-02	-	34824719D-05	3	
	.19618096D-08	-	38542551D-12	.13858705D+05	.68500574D+01			4	
CL2	42189CL	2		G	300.000	2000.000	1000.00	1	
	.33474856D+01	.35465402D-02	-	41020340D-05	.21051260D-08	-	39180420D-12	2	
-	11234604D+04	.68564007D+01	.33474856D+01		.35465402D-02	-	41020340D-05	3	
	.21051260D-08	-	39180420D-12	-	11234604D+04	.68564007D+01		4	
NAS02	EST-VZNA	1S	10	2	OG	300.000	2000.000	1000.00	1
	.10564578D+02	.12021251D-02	.23902747D-05	-	21589178D-08	.52044716D-12		2	
-	49517463D+05	-	45542840D+02	.10564578D+02	.12021251D-02	.23902747D-05		3	
-	21589178D-08	.52044716D-12	-	49517463D+05	-	45542840D+02		4	
NA2S04	80792NA	20	4S	1	G	300.000	2000.000	1000.00	1
	.45889397D+01	.38040129D-01	-	41096543D-04	.20017107D-07	-	36046429D-11	2	
-	12705639D+06	.58915156D+01	.45889397D+01		.38040129D-01	-	41096543D-04	3	
	.20017107D-07	-	36046429D-11	-	12705639D+06	.58915156D+01		4	
NA2S03	BAR 77NA	2S	10	3	OL	300.000	2000.000	1000.00	1
	.21890427D+02	.00000000D+00	.00000000D+00		.00000000D+00	.00000000D+00		2	
-	13847832D+06	-	11136788D+03	.21890427D+02	.00000000D+00	.00000000D+00		3	
	.00000000D+00	.00000000D+00	-	13847832D+06	-	11136788D+03		4	
NACL	81092CL	1NA	1		G	300.000	2000.000	1000.00	1
	.38609970D+01	.21586897D-02	-	25630874D-05	.13632700D-08	-	26045355D-12	2	
-	23047048D+05	.50924911D+01	.38609970D+01		.21586897D-02	-	25630874D-05	3	
	.13632700D-08	-	26045355D-12	-	23047048D+05	.50924911D+01		4	
NAOH	J12/70NA	10	1H	100	OG	300.000	2000.000	1000.00	1
	.45711116D+01	.61346093D-02	-	76237353D-05	.43706135D-08	-	89064713D-12	2	
-	25359026D+05	-	95321963D-01	.45711116D+01	.61346093D-02	-	76237353D-05	3	
	.43706135D-08	-	89064713D-12	-	25359026D+05	-	95321963D-01	4	
NA	L 4/93NA	100	000	000	OG	300.000	2000.000	1000.00	1
	.25010442D+01	.00000000D+00	.00000000D+00		.00000000D+00	.00000000D+00		2	
	.12157060D+05	.42385793D+01	.25010442D+01		.00000000D+00	.00000000D+00		3	
	.00000000D+00	.00000000D+00	.12157060D+05		.42385793D+01			4	
NAO	J12/67NA	10	100	000	OG	300.000	2000.000	1000.00	1
	.36192660D+01	.29441938D-02	-	35206654D-05	.18827273D-08	-	36198896D-12	2	
	.88821327D+04	.62033018D+01	.36192660D+01		.29441938D-02	-	35206654D-05	3	
	.18827273D-08	-	36198896D-12	.88821327D+04	.62033018D+01			4	
NA2C03(S)	J 3/66NA	2C	10	3	OS	300.000	2000.000	1000.00	1
	.12014036D+02	-	50536347D-02	.25519440D-04	-	13688606D-07	.27714728D-11	2	
-	13815566D+06	-	48715125D+02	.12014036D+02	-	50536347D-02	.25519440D-04	3	
-	13688606D-07	.27714728D-11	-	13815566D+06	-	48715125D+02		4	
NA2C03(L)	J 3/66NA	2C	10	3	OL	300.000	2000.000	1000.00	1
	.22796238D+02	.00000000D+00	.00000000D+00		.00000000D+00	.00000000D+00		2	

- .14229112D+06	- .11622189D+03	.22796238D+02	.00000000D+00	.00000000D+00	3				
.00000000D+00	.00000000D+00	- .14229112D+06	- .11622189D+03		4				
NA2C03	BENSONNA	2C	10	3	OG	300.000	2000.000	1000.00	1
.56157861D+01	.25916438D-01	.25963740D-05	- .15866667D-07	.51192999D-11					2
- .13627651D+06	- .21019356D+02	.56157861D+01	.25916438D-01	.25963740D-05					3
- .15866667D-07	.51192999D-11	- .13627651D+06	- .21019356D+02						4
HS03	T 3/96H	1S	10	3	OG	300.000	2000.00	1000.00	1
.29221355D+01	.24537632D-01	- .28258748D-04	.14728290D-07	- .28007910D-11					2
- .48042084D+05	.12532987D+02	.29221355D+01	.24537632D-01	- .28258748D-04					3
.14728290D-07	- .28007910D-11	- .48042084D+05	.12532987D+02						4
S02	121286S	10	2		G	0300.00	5000.00	1000.00	1
0.05254498E+02	0.01978545E-01	-0.08204226E-05	0.15763830E-09	-0.11204512E-13					2
-0.03756885E+06	-0.11460563E+01	0.02911438E+02	0.08103022E-01	-0.06906710E-04					3
0.03329015E-07	-0.08777121E-11	-0.03687881E+06	0.11117403E+02						4
S03	121286S	10	3		G	0300.00	5000.00	1000.00	1
0.07050668E+02	0.03246560E-01	-0.14088974E-05	0.02721535E-08	-0.01942364E-12					2
-0.05020667E+06	-0.11064426E+02	0.02575282E+02	0.15150916E-01	-0.12298717E-04					3
0.04240257E-07	-0.05266812E-11	-0.04894410E+06	0.12195116E+02						4
CH302	L184	C 1H	30	2	G	300.000	5000.00	1000.00	1
0.66812963E 01	0.80057271E-02	-0.27188507E-05	0.40631365E-09	-0.21927725E-13					2
0.52621851E 03	-0.99423847E 01	0.20986490E 01	0.15786357E-01	0.75683261E-07					3
-0.11274587E-07	0.56665133E-11	0.20695879E 04	0.15007068E 02						4
CH302H	BENSON/Vit C	1H	40	2	G	300.000	2000.000	1000.00	1
.70880631D+02	- .34336913D+00	.54005126D-03	- .32136525D-06	.65219886D-10					2
- .24541521D+05	- .29072672D+03	.70880631D+02	- .34336913D+00	.54005126D-03					3
- .32136525D-06	.65219886D-10	- .24541521D+05	- .29072672D+03						4
CH2*	L S/93C	1H	2	00	00G	200.000	3500.000	1000.000	1
2.29203842E+00	4.65588637E-03	-2.01191947E-06	4.17906000E-10	-3.39716365E-14					2
5.09259997E+04	8.62650169E+00	4.19860411E+00	-2.36661419E-03	8.23296220E-06					3
-6.68815981E-09	1.94314737E-12	5.04968163E+04	-7.69118967E-01	9.93967200E+03					4
HN02	120186H	1N	10	2	G	0200.00	6000.00	1000.00	1
0.57900059E+01	0.36505061E-02	-0.12902803E-05	0.20751067E-09	-0.12300051E-13					2
-0.11563080E+05	-0.40550308E+01	0.32100428E+01	0.81300665E-02	0.16621031E-05					3
-0.95328431E-08	0.48700696E-11	-0.10700764E+05	0.98200995E+01						4
HN03	121286H	1N	10	3	G	0300.00	5000.00	1000.00	1
0.07003844E+02	0.05811493E-01	-0.02333788E-04	0.04288814E-08	-0.02959385E-12					2
-0.01889952E+06	-0.10478628E+02	0.13531850E+01	0.02220024E+00	-0.01978811E-03					3
0.08773908E-07	-0.16583844E-11	-0.01738562E+06	0.01851868E+03						4
H202+	120186H	20	2		G	0300.00	5000.00	1000.00	1
0.04573167E+02	0.04336136E-01	-0.14746888E-05	0.02348903E-08	-0.14316536E-13					2
-0.01800696E+06	0.05011369E+01	0.03388753E+02	0.06569226E-01	-0.14850125E-06					3
-0.04625805E-07	0.02471514E-10	-0.01766314E+06	0.06785363E+02						4
NH20H	JWB/SAND88	N 1H	30	1	OG	300.000	5000.000	1412.000	11
5.12276969E+00	5.73428233E-03	-1.86277359E-06	2.78938290E-10	-1.57685159E-14					2

-7. 42648110E+03-3. 34064363E+00 1. 59842441E+00 1. 54722273E-02-1. 24132635E-05 3  
5. 50996715E-09-1. 00114333E-12-6. 34935610E+03 1. 50585859E+01 4  
H2NN M93/JBPM3 96 N 2H 2 0 OG 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  
NH2NO M/JB189 N 2H 20 1 OG 300.000 5000.000 1376.000 11  
8. 29632310E+00 4. 68893443E-03-1. 88894635E-06 3. 25848090E-10-2. 03763038E-14 2  
5. 26778509E+03-2. 04554254E+01 1. 30310075E+00 1. 94969032E-02-1. 34642223E-05 3  
4. 29560204E-09-5. 24866242E-13 7. 86417421E+03 1. 76712406E+01 4  
HON HF MELIUS93H 1N 10 1 OG 300.000 5000.000 1671.000 01  
3. 78577430E+00 2. 86062728E-03-1. 02423922E-06 1. 64463139E-10-9. 77943616E-15 2  
2. 93319701E+04 3. 12193293E+00 3. 33656431E+00 2. 67682939E-03 5. 61801303E-07 3  
-1. 11362279E-09 2. 84076438E-13 2. 95979751E+04 5. 96343188E+00 4  
C2H5CHO T 9/92C 3H 60 1 OG 273.150 5000.000 1000. 1  
0. 33137982E+01 0. 26619606E-01-0. 10475596E-04 0. 18815334E-08-0. 12761310E-12 2  
-0. 25459603E+05 0. 96608447E+01 0. 76044596E+01-0. 86403564E-02 0. 73930097E-04 3  
-0. 79687398E-07 0. 28004927E-10-0. 25489789E+05-0. 67643691E+01 4  
CH3CN Methyl-Cya T01/03C 2.H 3.N 1. 0.G 200.000 6000.000 1000. 1  
5. 09921882E+00 9. 69585649E-03-3. 48051966E-06 5. 61420173E-10-3. 35835856E-14 2  
6. 60967324E+03-3. 36087178E+00 3. 82392803E+00 4. 08201943E-03 2. 16209537E-05 3  
-2. 89807789E-08 1. 12962700E-11 7. 44430382E+03 5. 52656156E+00 4  
CH2CN Radical T01/03C 2.H 2.N 1. 0.G 200.000 6000.000 1000. 1  
6. 14873620E+00 6. 06600240E-03-2. 17174620E-06 3. 49750387E-10-2. 09004207E-14 2  
2. 86491222E+04-6. 59235995E+00 2. 63064017E+00 1. 73644377E-02-1. 70284117E-05 3  
9. 86551140E-09-2. 46033517E-12 2. 95791691E+04 1. 12776223E+01 4  
C2H5CO T 9/92C 3H 50 1 OG 298.150 5000.000 1500.00 1  
0. 30445698E+01 0. 23236429E-01-0. 86317936E-05 0. 14799550E-08-0. 96860829E-13 2  
-0. 61787211E+04 0. 13122302E+02 0. 67368294E+01-0. 26945299E-02 0. 49927017E-04 3  
-0. 50025808E-07 0. 15011503E-10-0. 65703366E+04-0. 23398732E+01 4  
C2H2OH C 2H 30 1 OG 300.000 5000.000 1432.000 1  
6. 22800189E 00 7. 49055727E-03-2. 50690816E-06 3. 83916588E-10-2. 20740476E-14 2  
1. 46499099E 04-6. 13007793E 00 4. 65202956E 00 4. 18808988E-03 9. 02055130E-06 3  
-8. 66939586E-09 2. 17803441E-12 1. 58770986E 04 4. 78089988E 00 4  
END