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POLYNOMIAL COEFFICIENTS OF

THERMOCHEMICAL DATA FOR THE C-H-O-N SYSTEM

By

N. T. Wakelyn and Allen G. McLain

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16. Abstract

Thermodynamic data are required input for the finite kinetics and equilibrium computer programs needed for modeling the combustion of hydrocarbons in the fields of energy and pollution research. Least squares determined coefficients of the curve-fitted thermodynamic data for 193 species in the C-H-O-N system are presented in card image form of suitable format for use by the commonly used computer programs.

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SUMMARY

The thermochemical data for the 179 chemical species presented by Bahn (NASA CR2178) for the C-H-O-N System have been curve-fitted to provide coefficients used as input data for equilibrium and finite chemistry computer programs such as Gordon and McBride (NASA SP-273), Bittker and Scullin (NASA TN D6586), and Pratt (Washington State University Bulletin 336). Polynomial coefficients are listed in the proper card image form for use in these computer programs. The thermochemical curve-fit coefficient data include many chemical species which are not included in the present data tapes used with the referenced computer programs. Hydrocarbon reaction mechanisms that were previously neglected because of lack of thermochemical data can now be included in combustion and pollutant formation analytical studies.

INTRODUCTION

In efforts to utilize the dwindling supply of hydrocarbon fuels in a more efficient way and in a manner less destructive to the environment, the use of computer combustor models as engineering tools to guide the development of combustion systems will be increasing. Realistic chemical reaction mechanisms describing the pyrolysis and subsequent oxidation of various hydrocarbon fuels and fuel mixtures are very important in combustor modeling. As more detailed reaction mechanisms are developed, a need arises for thermochemical data for the various hydrocarbon fuels and combustion intermediates. These data are used to assemble the complex reaction mechanisms that are required to describe the combustion of hydrocarbon fuels and the formation of pollutants. The need for thermochemical data becomes increasingly important as attempts are made to use fuels synthesized from coal or shale oil, where fuel

chemical structure may be an important factor in its combustion and pollutant formation characteristics.

The JANNAF tables (ref. 1) have provided thermochemical data for many of the lower molecular weight hydrocarbons and pyrolysis intermediates for combustion calculations in the past. However, thermochemical properties of the larger molecular weight hydrocarbons, which are the predominant constituents of present-day fuels, have been omitted from consideration. One reason for the omission has been the orientation of the efforts of the JANNAF organization toward tabulating thermochemical data primarily for the combustion products of rocket engines. Nevertheless, some numerical representation of the chemical thermodynamics of the higher molecular weight hydrocarbons is required if they are to be considered quantitatively in combustion kinetics.

A recent report by Bahn (ref. 2) provides approximate thermochemical properties for a number of the higher molecular weight fuels and intermediate species which may result from their pyrolysis. It is believed that, during the interim period until a recognized body such as the JANNAF organization compiles thermochemical data for these species, the data provided by Bahn can be used to upgrade computational procedures involving more complex reaction mechanisms in combustion models.

The compilation of Bahn presents thermochemical data for entropy, heat capacity, and enthalpy to temperatures of 6000°K in tabular form much like that of the JANNAF tables. The tables as issued by Bahn were prepared using the computer program of McBride and Gordon (ref. 3). This program creates least squares polynomial fit coefficients to express the pertinent thermochemical data as functions of temperature. Bahn used the program to smooth interpolated and extrapolated data. Being interested in applying the output of smoothed

tabular data, consistent with the data format of computer program FINEK*, he did not report the polynomial coefficients which had been created. The present work comprises a restoration of the coefficients from the smoothed tables presented by Bahn.

While the form of Bahn's data is convenient for observing the trends of the data or for comparing it with existing data, it is in a form not easily compatible with most existing computational models other than program FINEK. A number of computer programs now available for performing combustion calculations with either equilibrium or kinetically controlled chemistry rely on "packed" thermochemical data. The "packed" data are in the form of the least squares polynomial fit coefficients from which thermochemical properties can be calculated at required temperatures. To be more specific, the computer programs of Gordon and McBride (ref. 4), Bittker and Scullin (ref. 5), and Pratt (ref. 6), all of which deal with combustion of fuels, require the thermochemical data in the "packed" form. Therefore, in the present work, the thermochemical data of Bahn have been curve-fitted by the method of McBride and Gordon (ref. 3) and the coefficients are presented in the card form suitable for use with the specified computer programs or any other programs using the method of Gordon and McBride to calculate thermochemical properties.

A comparison is shown for the combustion of methane and air with the perfectly stirred reactor program of Pratt (ref. 6) using the original "packed" thermochemical data supplied by Gordon and McBride derived from the JANNAF tables and the "packed" thermochemical data derived from Bahn's tables. This comparison was performed to check the consistency between the two versions of thermochemical data during an actual combustion calculation. To illustrate the use of the new thermochemical data, a perfectly stirred reactor calculation

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*Program FINEK was created at the Marquardt Company by A. Widowsky and C. W. Brandenburg and used by Bahn both there and at LTV Aerospace Corporation for general finite-kinetics calculations.

of propane-air stoichiometric combustion was performed. The reaction mechanism for this calculation was a combination of the complex Chinitz-Baurer mechanism (ref. 7) and an accepted methane combustion mechanism (ref. 8), and involves many of the species previously neglected because of lack of thermochemical data.

SYMBOL LIST

C_p	heat capacity, constant pressure
h	enthalpy
$\dot{m}$	mass flow rate, $\frac{\text{gram}}{\text{sec}}$
R	universal gas constant
S	entropy
T	absolute temperature
v	volume, cc

CALCULATION OF COEFFICIENTS

The polynomial coefficients were calculated using the computer program of McBride and Gordon (ref. 3). The tabular thermochemical data issued by Bahn (ref. 2) were used to effect a simultaneous least squares polynomial fit of C_p/R, h/RT, and S/R in the form

$$\frac{C_p}{R} = A_1 + A_2T + A_3T^2 + A_4T^3 + A_5T^4$$

$$\frac{h}{RT} = A_1 + \frac{A_2}{2}T + \frac{A_3}{3}T^2 + \frac{A_4}{4}T^3 + \frac{A_5}{5}T^4 + \frac{A_6}{T}$$

$$\frac{S}{R} = A_1 \ln T + A_2T + \frac{A_3}{2}T^2 + \frac{A_4}{3}T^3 + \frac{A_5}{4}T^4 + A_7$$

where C_p is defined as heat capacity at constant pressure, h is enthalpy-based at the reference temperature of 298.15°K, S is entropy, R is universal gas constant, and T is temperature. The seven coefficients ($A_1 \cdots A_7$) calculated by the program for the upper (1000-5000°K) and lower (300-1000°K)

temperature ranges of the thermochemical data are presented in the card format suitable for use by the computer programs of references 4, 5, and 6. The format is as follows:

(a) Card 1 (Contains species name, reference, pertinent elemental symbols and stoichiometric coefficients, the temperature range, and the card number).

Columns 1 - 8	Species name
Columns 19 - 24	Reference
Columns 25 - 44	Elemental symbols and stoichiometric coefficients
Columns 45	State of species
Columns 49 - 55	Lowest temperature
Columns 58 - 65	Highest temperature
Column 80	Number of card

(b) Cards 2 through 4 (Contain coefficients ($A_1 \cdots A_7$) for the upper temperature range followed by coefficients ($A_1 \cdots A_7$) for the lower temperature range).

Card 2,	Columns 1 - 15	A_1	Upper Temperature Range
	Columns 16 - 30	A_2	
	Columns 31 - 45	A_3	
	Columns 46 - 60	A_4	
	Columns 61 - 75	A_5	
Card 3,	Columns 1 - 15	A_6	
	Columns 16 - 30	A_7	
Card 3,	Columns 31 - 45	A_1	
	Columns 46 - 60	A_2	
	Columns 61 - 75	A_3	

Card 4,	Columns 31 - 45	A_4	Lower Temperature Range
	Columns 16 - 30	A_5	
	Columns 31 - 45	A_6	
	Columns 46 - 60	A_7	

Each species is represented by a four-card set.

The cards were stored on a tape in the same manner as the original tape supplied by Gordon and McBride (ref. 4). The data of this form stored on a tape have been referred to as "packed" thermochemical data. The cards are listed in Appendix A, pages A1 - A14, for the Bahn data. The cards on page A15 (also last set on page A14) of the Appendix were added from the original data as reported in (ref. 4) to make a more complete C-H-O-N thermochemical package. In the case of species common to both data sets, the Bahn data were chosen for the present listing in order to provide a more unified data set, with the exception of water for which the listing of the two phases of the JANNAF data set was considered more appropriate.

RESULTS OF CALCULATIONS

Application of the species provided by Bahn and the curve fits reported here to the computer programs of ref. 4, 5, and 6 requires only slight modification of the different programs. Methane-air combustion calculations were performed using the stirred reactor computer program of ref. 6 and the methane mechanism from Jachimowski (ref. 8) with the original thermochemical data tape from Gordon and McBride as well as with the thermochemical data tape of this paper.

Figure 1 shows the variation of mole fractions of CO and NO with residence time within the reactor volume. The circular symbols represent a calculation using the original [old] tape and the square symbols represent a calculation performed using the [new] tape generated in this paper. The variation of

temperature with mass flow rate for methane-air combustion is shown in Figure 2 for the old and new thermochemical data tapes. These figures illustrate that although the curve-fitted polynomial coefficients listed in reference 4 appear different from those listed in Appendix A for the same species considered in the methane-air calculation, the results such as mole fractions of the chemical species and the temperature variation with mass flow rate per unit volume are comparable.

To illustrate the need for thermochemical data provided by Bahn and curve-fitted in this paper, a computer calculation of propane-air combustion was performed using a complex reaction mechanism. The reaction mechanism, which is a combination of the Chinitz-Baurer Mechanism (ref. 7) and an accepted methane reaction mechanism (ref. 8), is shown in Table I. This composite reaction mechanism contains many of the intermediate species for which thermochemical data in the form of polynomial coefficients were not previously available. The equilibrium combustion solution for the polynomial fits generated in this paper is shown in Table II. In Table III, the mole fractions of the combustion products at different stirred reactor stationary states are shown. As was stated earlier, this stirred reactor combustion solution was provided as an example of the type of reaction mechanism that may now be considered. Perhaps a more vivid example of the need for this interim thermochemical data is the fact that not even the simplest propane combustion calculations could be tested previously because as yet the JANNAF tables do not include propane.

CONCLUDING REMARKS

Least square polynomial coefficients for 179 species in C-H-O-N system have been calculated from the thermochemical data presented by Bahn in NASA CR-2178. These thermochemical data coefficients, along with some taken from NASA SP-273 which were not in the Bahn list of species, are presented in a

form suitable for use with equilibrium and finite rate chemistry computer programs such as those described in NASA SP-273, NASA TN D-6586, and Washington State University Bulletin 336. The thermochemical data provided by Bahn and for which polynomial curve-fit coefficients are listed in this report allow use of complex hydrocarbon species - important for combustion analyses - but missing from present compilations such as the JANNAF Tables. Results of calculations with species included in the thermochemical data coefficients listed in NASA SP-273 and those listed in this compilation agree very well. Results of the propane-air combustion could not be compared with the data of NASA SP-273 because no data for propane or its pyrolysis intermediates were included therein.

REFERENCES

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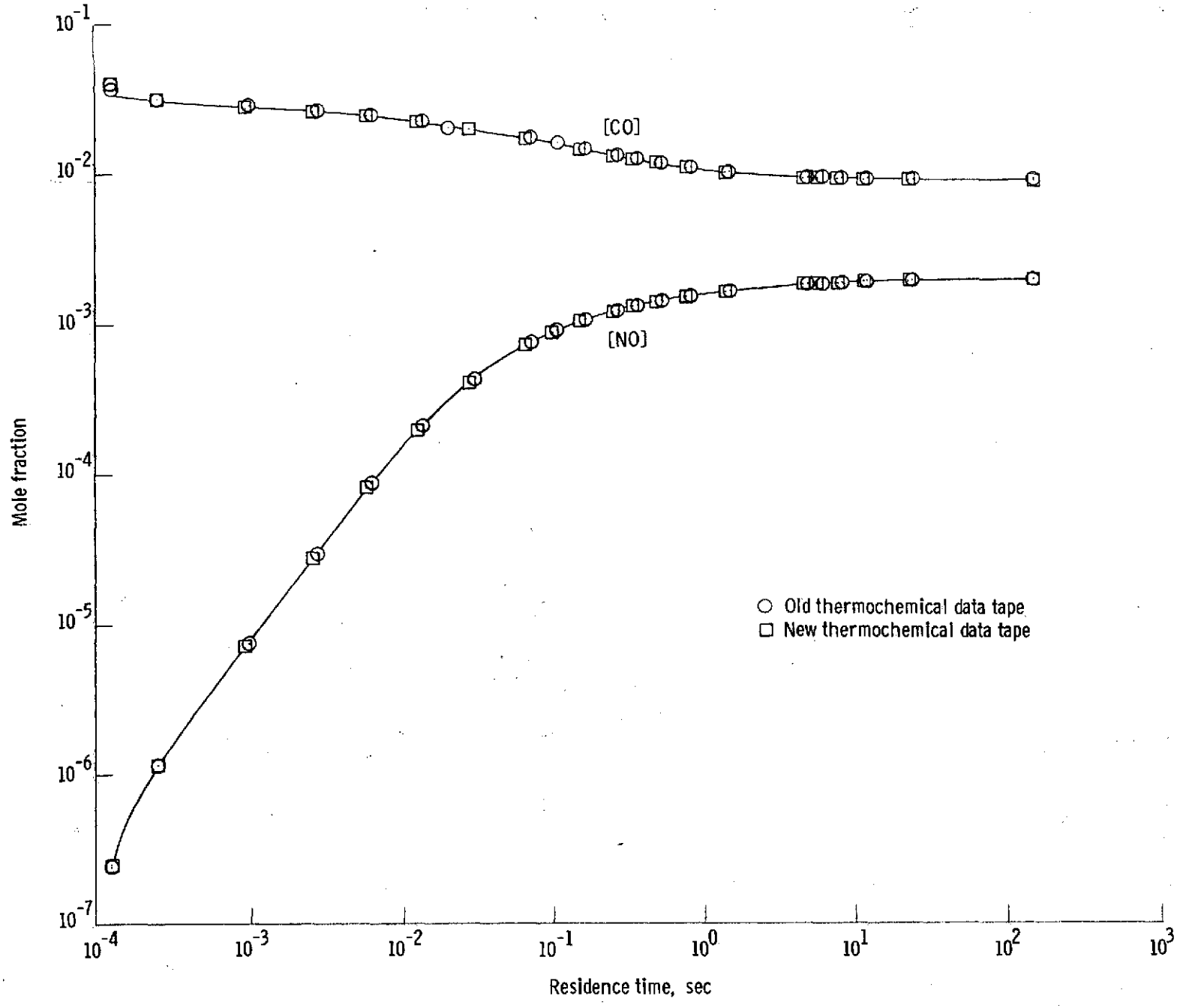

Figure 1. - Mole fraction CO and NO versus residence time.

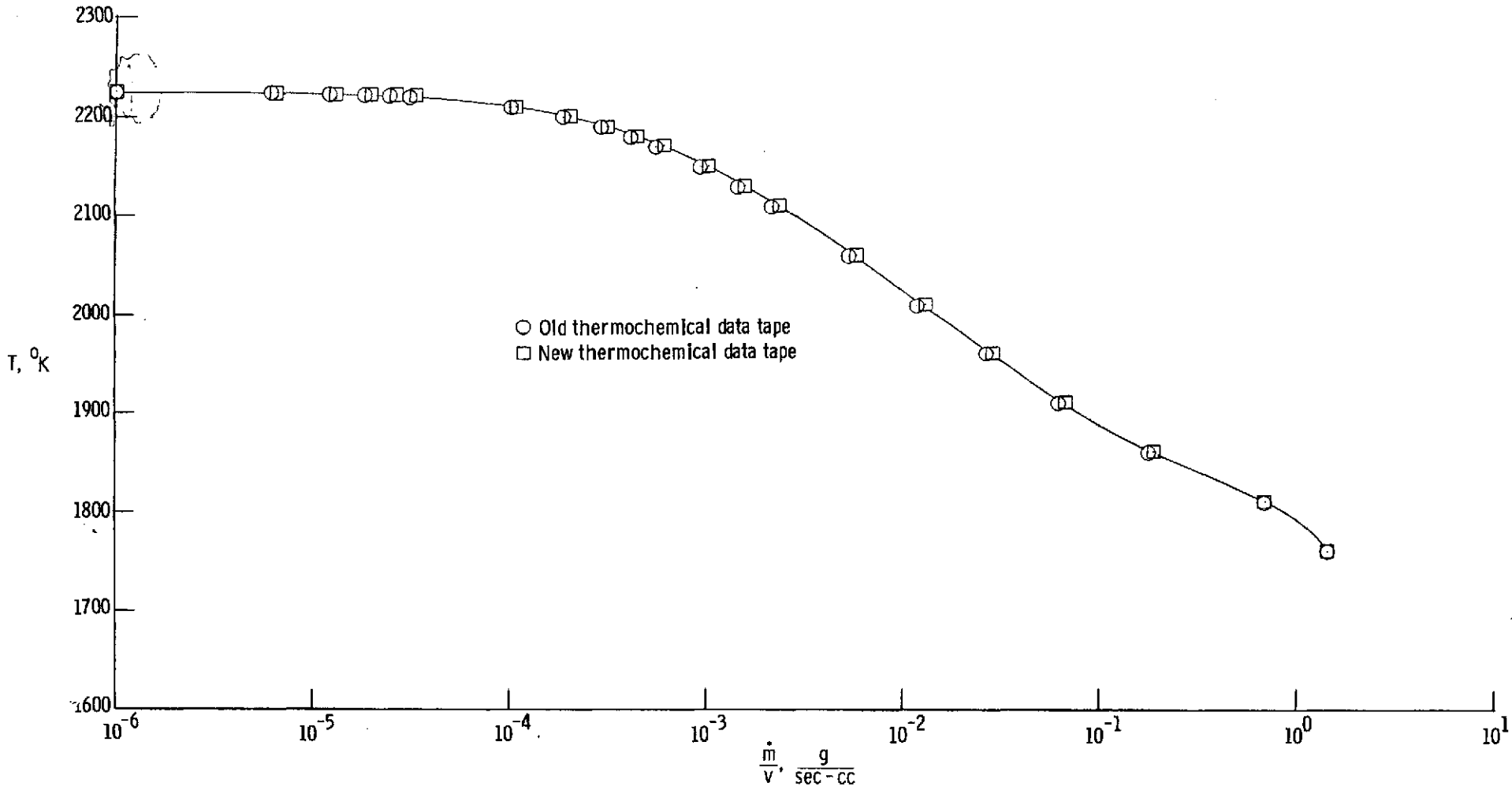

Figure 2. - Temperature versus mass flow rate per unit volume.

APPENDIX A

CARD IMAGES FOR THERMODYNAMIC DATA TAPE

```
0         1         2         3         4         5         6         7         8
12345678901234567890123456789012345678901234567890123456789012345678901234567890


   300.000  1000.000  5000.000

AR                  CR2178AR  10   00   00   0G   300.000  5000.000                1
 2.51062479E+00-1.38937567E-05 6.56665581E-09-1.34972376E-12 1.02693875E-16       2
-7.47627433E+02 4.30454989E+00 2.37763928E+00 9.51768376E-04-2.45748152E-06       3
 2.63504161E-09-1.00491710E-12-7.34217481E+02 4.86200098E+00                      4

H                   CR2178H   10   00   00   0G   300.000  5000.000                1
 2.51483889E+00-2.16303554E-05 1.10486229E-08-2.39405857E-12 1.87553969E-16       2
 2.54689942E+04-5.44696138E-01 2.37808007E+00 9.44383311E-04-2.43716893E-06       3
 2.61768927E-09-1.00093306E-12 2.54840220E+04 3.50145175E-02                      4

HNO                 CR2178H   1N   10   10   0G   300.000  5000.000                1
 3.26917547E+00 3.61417900E-03-1.39428801E-06 2.39192466E-10-1.51090771E-14       2
 1.08543496E+04 6.85488924E+00 3.39810073E+00 2.99061231E-03-4.37253320E-07       3
-2.49621217E-10 1.13113547E-14 1.08351155E+04 6.26568728E+00                      4

OH                  CR2178O   1H   10   00   0G   300.000  5000.000                1
 3.43261260E+00 1.83340682E-04 1.89076697E-07-6.29681174E-11 5.47860574E-15       2
 3.70046978E+03 2.44655445E+00 3.47034494E+00-6.92182499E-05 9.92224840E-07       3
-1.45504385E-09 8.09232796E-13 3.70856896E+03 2.29998029E+00                      4

HO2                 CR2178H   10   20   00   0G   300.000  5000.000                1
 3.46258881E+00 3.23382372E-03-1.21393310E-06 2.05886117E-10-1.29578066E-14       2
 1.35464935E+03 6.69569968E+00 3.44031955E+00 3.53735488E-03-2.45516407E-06       3
 2.12110065E-09-9.68203271E-13 1.35114215E+03 6.76702112E+00                      4

H2                  CR2178H   20   00   00   0G   300.000  5000.000                1
 3.32686011E+00 2.38917795E-04 1.52769123E-07-4.74507588E-11 3.97934156E-15       2
-1.00106600E+03-3.30446231E+00 2.84460248E+00 3.42801294E-03-7.40092798E-06       3
 7.63285252E-09-2.82946434E-12-9.48843987E+02-1.23713138E+00                      4

H2O                 CR2178H   20   10   00   0G   300.000  5000.000                1
 3.32449972E+00 2.02694711E-03-3.39108414E-07 7.45713395E-12 1.91874758E-15       2
-3.01784964E+04 3.15077706E+00 3.41291470E+00 1.42834687E-03 1.35410198E-06       3
-2.41252664E-09 1.23887739E-12-3.01744105E+04 2.78944463E+00                      4

H2O2                CR2178H   20   20   00   0G   300.000  5000.000                1
 3.78822153E+00 5.99894691E-03-2.69732390E-06 5.62126177E-10-3.91343711E-14       2
-1.77449352E+04 4.83336124E+00 3.56621321E+00 7.54415174E-03-6.12015182E-06       3
 3.49213181E-09-8.69508599E-13-1.77210132E+04 5.76407448E+00                      4

N                   CR2178N   10   00   00   0G   300.000  5000.000                1
 2.48030982E+00 7.90306735E-05-7.06336763E-08 2.01786188E-11-1.29926580E-15       2
 5.61041313E+04 4.26762042E+00 2.35851956E+00 9.46816790E-04-2.25072254E-06       3
 2.30570085E-09-8.52728501E-13 5.61176301E+04 4.78219255E+00                      4

NO                  CR2178N   10   10   00   0G   300.000  5000.000                1
 3.20190007E+00 1.26773610E-03-4.65949701E-07 7.71671459E-11-4.70512320E-15       2
 9.84597543E+03 6.70393834E+00 3.39864387E+00 1.57097556E-04 1.91755989E-06       3
-2.37681305E-09 9.79660217E-13 9.82666968E+03 5.83566612E+00                      4

NO2                 CR2178N   10   20   00   0G   300.000  5000.000                1
 3.68493822E+00 3.87290924E-03-1.69517738E-06 3.18379349E-10-2.15361430E-14       2
 2.74234758E+03 6.74942849E+00 3.53583593E+00 5.19702970E-03-5.90524264E-06       3
 6.09785069E-09-2.76596040E-12 2.73676173E+03 7.31991839E+00                      4
```

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-9.77928186E+02 5.05783761E+00 3.15539314E+00 9.06017877E-04 1.56189555E-07        3
-6.86385052E-10 4.11577494E-13-9.81267815E+02 4.77456433E+00                       4

N2O                 CR2178N   20   10   00   0G   300.000  5000.000                1
 3.82025413E+00 4.14595688E-03-1.78113181E-06 3.30769791E-10-2.21921812E-14        2
 8.58720047E+03 3.52296257E+00 3.25082261E+00 8.18288843E-03-1.23645697E-05        3
 1.27480024E-08-5.32348696E-12 8.62192965E+03 5.89748973E+00                       4

O                   CR2178O   10   00   00   0G   300.000  5000.000                1
 2.68095645E+00-2.46685190E-04 1.11184175E-07-1.95839215E-11 1.34055109E-15        2
 2.91793188E+04 4.13395046E+00 2.65344834E+00-4.22648660E-07-5.31001897E-07        3
 5.55303343E-10-1.50115070E-13 2.91843269E+04 4.24503508E+00                       4

O2                  CR2178O   20   00   00   0G   300.000  5000.000                1
 3.26494072E+00 1.23593056E-03-4.26006473E-07 7.82654492E-11-5.52335861E-15        2
-1.02084632E+03 5.68230627E+00 3.23218536E+00 1.68340068E-03-2.04681420E-06        3
 2.31269101E-09-1.03385594E-12-1.02449665E+03 5.78378066E+00                       4

O3                  CR2178O   30   00   00   0G   300.000  5000.000                1
 4.48462136E+00 3.21494804E-03-1.44261930E-06 2.79112833E-10-1.92576344E-14        2
 1.57129121E+04 2.14703555E+00 4.17207609E+00 5.25104785E-03-7.49923318E-06        3
 8.79972883E-09-4.20681429E-12 1.57336361E+04 3.50491274E+00                       4

NH                  CR2178N   1H   10   00   0G   300.000  5000.000                1
 3.20923723E+00 6.57041432E-04-4.72280340E-08-1.58449721E-11 2.20606241E-15        2
 3.88619172E+04 3.30411806E+00 3.16545065E+00 9.93827531E-04-7.29092517E-07        3
 2.48404805E-10 1.26821244E-13 3.88736134E+04 3.49149410E+00                       4

NH2                 CR2178N   1H   20   00   0G   300.000  5000.000                1
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 1.92042800E+04 3.66089880E+00 3.38414151E+00 1.30603093E-03 2.23845177E-06        3
-3.52224209E-09 1.67773246E-12 1.91994583E+04 2.95973532E+00                       4

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-6.58324973E+03 6.52738734E+00 3.02337157E+00 2.82820572E-03 4.59233142E-06        3
-6.72751162E-09 2.87991827E-12-6.61139991E+03 4.89744032E+00                       4

N2H2                CR2178N   2H   20   00   0G   300.000  5000.000                1
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 2.45213732E+04 8.71190369E+00 3.04569098E+00 5.01546979E-03 9.66227368E-07        3
-2.36706498E-09 7.13479788E-13 2.44791257E+04 7.34864237E+00                       4

N2H3                CR2178N   2H   30   00   0G   300.000  5000.000                1
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 1.72050778E+04 6.50133444E+00 3.03851382E+00 1.05091498E-02-7.85211180E-06        3
 6.78063685E-09-3.07236318E-12 1.72031902E+04 7.27962239E+00                       4

N2H4                CR2178N   2H   40   00   0G   300.000  5000.000                1
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 9.65648660E+03-2.16312736E+00 3.75888927E+00 1.62030627E-02-2.26184582E-05        3
 2.45788792E-08-1.07894553E-11 9.76390755E+03 2.93210952E+00                       4

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-1.50337745E+04-1.09190625E+02 6.08769135E+00 7.70726892E-02-2.08570758E-04        3
 2.38530076E-07-1.00039289E-10-1.29104309E+04-3.71940811E+01                       4

C*                  CR2178C   10   00   00   0S   300.000  5000.000                1
 4.71671368E-01 3.21934214E-03-1.46570497E-06 2.84789091E-10-1.96212204E-14        2
-2.46859407E+02-2.89887105E+00 1.60397456E-01 5.43110417E-03-7.51534731E-06        3
 7.92631839E-09-3.51199630E-12-2.36826374E+02-1.60969057E+00                       4
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C                   CR2178C    10    00    00    0G    300.000  5000.000                1
 2.54938901E+00-1.10991572E-04 6.41947669E-08-7.79422112E-12 2.07477096E-16     2
 8.52429614E+04 4.50171277E+00 2.42570857E+00 8.26693742E-04-2.38936810E-06     3
 2.68709302E-09-1.05512176E-12 8.52529975E+04 5.01069968E+00                    4

CH                  CR2178C    1H    10    00    0G    300.000  5000.000                1
 2.99894814E+00 1.13921473E-03-1.08970024E-07-3.00768113E-11 4.56759521E-15     2
 7.04983069E+04 4.57529939E+00 3.03628689E+00 8.12550256E-04 1.13108987E-06     3
-2.22491529E-09 1.24867191E-12 7.05108359E+04 4.44459372E+00                    4

HCN                 CR2178H    1C    1N    10    0G    300.000  5000.000                1
 3.40733200E+00 3.86371845E-03-1.39459604E-06 2.34276889E-10-1.46247732E-14     2
 1.45381781E+04 3.76606724E+00 3.02692358E+00 6.51581942E-03-8.12949023E-06     3
 7.80119918E-09-3.11834543E-12 1.45665143E+04 5.36280435E+00                    4

HNCO                CR2178H    1C    1N    10    1G    300.000  5000.000                1
 4.21527465E+00 5.68050857E-03-2.25406090E-06 3.98571421E-10-2.58812903E-14     2
-1.54990361E+04 3.03936069E+00 3.53392346E+00 1.04032295E-02-1.44244668E-05     3
 1.45280187E-08-6.02629243E-12-1.54545230E+04 5.89873699E+00                    4

HCO                 CR2178H    1C    10    10    0G    300.000  5000.000                1
 3.24055175E+00 3.44818293E-03-1.27300604E-06 2.10700204E-10-1.29181764E-14     2
-2.56983116E+03 7.54836666E+00 3.40254146E+00 2.58617114E-03 4.18740813E-07     3
-1.31452946E-09 5.20586721E-13-2.59012415E+03 6.82055346E+00                    4

CH2                 CR2178C    1H    20    00    0G    300.000  5000.000                1
 2.62660433E+00 4.38474164E-03-1.55238195E-06 2.48931881E-10-1.48751685E-14     2
 4.53656196E+04 5.54134933E+00 2.76358289E+00 3.59677330E-03 1.18947602E-07     3
-1.35442834E-09 5.68145275E-13 4.53497513E+04 4.93613685E+00                    4

CH2O                CR2178C    1H    20    10    0G    300.000  5000.000                1
 2.33936516E+00 7.41087604E-03-2.85116622E-06 4.87878128E-10-3.07631510E-14     2
-1.49456605E+04 1.08129291E+01 2.95815982E+00 3.66686713E-03 5.33335501E-06     3
-7.32112828E-09 2.71893628E-12-1.50183128E+04 8.10577264E+00                    4

CH3                 CR2178C    1H    30    00    0G    300.000  5000.000                1
 3.09341682E+00 5.59964963E-03-1.86446048E-06 2.82403921E-10-1.59953741E-14     2
 1.63617506E+04 4.10833246E+00 3.18127093E+00 5.10354492E-03-7.38827505E-07     3
-1.02028941E-09 5.69315586E-13 1.63553490E+04 3.72264937E+00                    4

CH2OH               CR2178C    1H    30    10    0G    300.000  5000.000                1
 3.65756222E+00 8.61103635E-03-4.17975483E-06 8.44566424E-10-5.94839367E-14     2
-8.43960375E+03 4.10409518E+00 3.59145095E+00 9.89325055E-03-9.25616061E-06     3
 8.73947858E-09-4.09409324E-12-8.48927050E+03 4.19377930E+00                    4

CH4                 CR2178C    1H    40    00    0G    300.000  5000.000                1
 1.47128753E+00 1.02071503E-02-3.66612409E-06 5.93978401E-10-3.58125627E-14     2
-9.88510477E+03 1.10329845E+01 2.49979471E+00 3.65425574E-03 1.16204547E-05     3
-1.52431531E-08 6.03912763E-12-9.98839606E+03 6.59822256E+00                    4

CH3OH               CR2178C    1H    40    10    0G    300.000  5000.000                1
 3.59160306E+00 1.07118619E-02-5.47218110E-06 1.13437990E-09-8.22617005E-14     2
-2.55462745E+04 5.36931055E+00 4.19130491E+00 8.84143852E-03-5.86253906E-06     3
 7.43806752E-09-4.72486987E-12-2.57280456E+04 2.35174207E+00                    4

CO                  CR2178C    10    10    00    0G    300.000  5000.000                1
 3.08842913E+00 1.27942328E-03-4.43765694E-07 6.95081740E-11-4.00164665E-15     2
-1.42732120E+04 5.78104805E+00 3.16642056E+00 9.22686436E-04 2.34641794E-07     3
-7.17367948E-10 3.83212395E-13-1.42796946E+04 5.42532394E+00                    4

CO2                 CR2178C    10    20    00    0G    300.000  5000.000                1
 3.68670706E+00 4.00800104E-03-1.57810292E-06 2.73434503E-10-1.71576389E-14     2
-4.85701573E+04 3.62968598E+00 3.03788318E+00 8.44740343E-03-1.15395893E-05     3
 9.72999552E-09-3.30281078E-12-4.85275488E+04 6.32216965E+00                    4
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CN                  CR2178C   1N   10   00   0G   300.000  5000.000                1
 3.32057915E+00 6.56001520E-04 1.45845747E-09-9.81578114E-12 2.34310104E-16        2
 5.38362168E+04 5.22307847E+00 3.33010967E+00 9.01536511E-04-1.16016772E-06        3
 1.66129187E-09-7.64312683E-13 5.38262600E+04 5.12662292E+00                        4

C2*                 CR2178C   20   00   00   0S   300.000  5000.000                1
 9.84804505E-01 6.36003447E-03-2.88885480E-06 5.60516803E-10-3.85675365E-14        2
-5.04862247E+02-6.01386133E+00 2.83222651E-01 1.12077478E-02-1.59810002E-05        3
 1.69417450E-08-7.47378178E-12-4.71352775E+02-3.07075201E+00                        4

C2                  CR2178C   20   00   00   0G   300.000  5000.000                1
 4.82079323E+00-9.92861645E-04 7.33948362E-07-1.71113119E-10 1.29832258E-14        2
 9.87354021E+04-3.17176252E+00 4.22957183E+00 3.18082722E-03-8.96091445E-06        3
 8.74337694E-09-2.78911148E-12 9.88031964E+04-6.84980205E-01                        4

C2H                 CR2178C   2H   10   00   0G   300.000  5000.000                1
 3.80698272E+00 3.07871683E-03-9.87229393E-07 1.64334330E-10-1.09820407E-14        2
 5.61257711E+04 2.38256144E+00 3.28411373E+00 6.76845529E-03-1.05034560E-05        3
 1.10616219E-08-4.55891255E-12 5.61611106E+04 4.56734072E+00                        4

C2HO                CR2178C   2H   10   10   0G   300.000  5000.000                1
 5.69321526E+00 4.40687363E-03-1.10849657E-06 7.94020863E-11 2.21021113E-15        2
 2.53531116E+04-5.42913812E+00 4.07144948E+00 1.53047806E-02-2.89925150E-05        3
 3.24872036E-08-1.37977140E-11 2.54786312E+04 1.46510585E+00                        4

C2HO2               CR2178C   2H   10   20   0G   300.000  5000.000                1
 6.53125340E+00 6.50646217E-03-2.25174117E-06 3.32957827E-10-1.72147113E-14        2
 1.39565711E+04-7.44672280E+00 4.96866101E+00 1.72785935E-02-2.99431719E-05        3
 3.24616136E-08-1.36639786E-11 1.40607636E+04-8.76993806E-01                        4

C2H2                CR2178C   2H   20   00   0G   300.000  5000.000                1
 3.98766152E+00 5.98459934E-03-2.16237963E-06 3.64783506E-10-2.28709722E-14        2
 2.58648149E+04-2.11528178E-01 3.03904911E+00 1.23084836E-02-1.77821709E-05        3
 1.77033539E-08-7.11692190E-12 2.59422499E+04 3.82125488E+00                        4

C2H2O               CR2178C   2H   20   10   0G   300.000  5000.000                1
 5.41210425E+00 7.06080094E-03-2.13786641E-06 2.73703627E-10-1.17627890E-14        2
 1.79239962E+02-4.51226732E+00 4.00668319E+00 1.69352685E-02-2.79809210E-05        3
 3.08516290E-08-1.32156800E-11 2.58080895E+02 1.35143470E+00                        4

C2H2O2              CR2178C   2H   20   20   0G   300.000  5000.000                1
 6.19828993E+00 9.70517256E-03-3.70225912E-06 6.26663407E-10-3.88250851E-14        2
-6.20933959E+03-5.80339553E+00 4.72807322E+00 1.96724949E-02-2.93039899E-05        3
 3.05359643E-08-1.28435008E-11-6.10526385E+03 4.17446817E-01                        4

C2H3                CR2178C   2H   30   00   0G   300.000  5000.000                1
 3.91828714E+00 7.10447061E-03-1.98355545E-06 2.02007740E-10-3.95303041E-15        2
 3.22388006E+04 3.03714467E+00 3.65517039E+00 9.50926265E-03-9.48490849E-06        3
 1.03811014E-08-4.82336893E-12 3.22190821E+04 4.01239803E+00                        4

C2H3O               CR2178C   2H   30   10   0G   300.000  5000.000                1
 4.72368767E+00 1.06097943E-02-3.75368497E-06 5.90702236E-10-3.41445431E-14        2
-6.82917000E+03-8.37213414E-01 3.66756991E+00 1.77593928E-02-2.23106408E-05        3
 2.26574027E-08-9.63736986E-12-6.75822957E+03 3.63230863E+00                        4

CH3CO               CR2178C   2H   30   10   0G   300.000  5000.000                1
 4.08969012E-01 1.85625284E-02-8.36753943E-06 1.59287441E-09-1.08787589E-13        2
-3.94094469E+03 2.36220518E+01 2.28725654E+00 6.86246638E-03 1.96960490E-05        3
-2.93487184E-08 1.25909913E-11-4.12828825E+03 1.54544886E+01                        4

C2H3O2              CR2178C   2H   30   20   0G   300.000  5000.000                1
 5.89753730E+00 1.28447671E-02-5.13420238E-06 9.19869042E-10-6.06632518E-14        2
-1.53102248E+04-4.30132049E+00 4.55523711E+00 2.19461986E-02-2.84883542E-05        3
 2.81808991E-08-1.17266729E-11-1.52159787E+04 1.37609747E+00                        4
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C2O2H3              CR2178C    20    2H    30    0G    300.000  5000.000                1
 7.11508476E+00 8.98053640E-03-3.51985467E-06 6.19814636E-10-4.01892860E-14      2
-2.41500676E+03-1.28741449E+01 5.00707131E+00 2.30445808E-02-3.87151529E-05      3
 4.04612350E-08-1.66423423E-11-2.24717390E+03-3.90883434E+00                     4

C2H4                CR2178C    2H    40    00    0G    300.000  5000.000                1
 2.23312189E+00 1.32141704E-02-5.11224078E-06 8.83920914E-10-5.63643039E-14      2
 5.10533922E+03 9.88961110E+00 2.41824020E+00 1.22921229E-02-4.24080278E-06      3
 2.13889678E-09-1.44584897E-12 5.05491829E+03 9.02623346E+00                     4

H4C2O               CR2178C    2H    40    10    0G    300.000  5000.000                1
 4.08386664E+00 1.40763627E-02-5.33737007E-06 9.03788690E-10-5.64536850E-14      2
-2.79379479E+04 2.59898573E+00 3.34350564E+00 1.88685143E-02-1.75177180E-05      3
 1.52338591E-08-6.25796670E-12-2.78757617E+04 5.78492888E+00                     4

CH3CHO              CR2178C    2H    40    10    0G    300.000  5000.000                1
 2.34943696E+00 1.75870386E-02-8.05272231E-06 1.53897860E-09-1.04797289E-13      2
-2.13467214E+04 1.34220214E+01 2.80579309E+00 1.54153926E-02-4.78260662E-06      3
 4.76039212E-10-5.96683759E-13-2.14431810E+04 1.12834979E+01                     4

C2H4O2              CR2178C    2H    40    20    0G    300.000  5000.000                1
 4.63265231E+00 1.85201055E-02-8.03208639E-06 1.53904130E-09-1.07027257E-13      2
-4.13413243E+04 1.97054410E+00 3.66168038E+00 2.50382471E-02-2.48334678E-05      3
 2.14479053E-08-8.76167958E-12-4.12752482E+04 6.08770475E+00                     4

C2O2H4              CR2178C    20    2H    40    0G    300.000  5000.000                1
 5.89753730E+00 1.28447671E-02-5.13420238E-06 9.19869042E-10-6.06632518E-14      2
-4.23920422E+03-4.30132049E+00 4.55523711E+00 2.19461986E-02-2.84883542E-05      3
 2.81808991E-08-1.17266729E-11-4.14495812E+03 1.37609747E+00                     4

C2H5                CR2178C    2H    50    00    0G    300.000  5000.000                1
 2.32839159E+00 1.54249686E-02-5.81801008E-06 9.82013719E-10-6.13927665E-14      2
 1.19386390E+04 9.74205262E+00 2.97925920E+00 1.11580715E-02 3.70471303E-06      3
-7.71404829E-09 2.72797559E-12 1.18631207E+04 6.95289922E+00                     4

C2H4OH              CR2178C    2H    50    10    0G    300.000  5000.000                1
 4.04771018E+00 1.66974043E-02-7.70925619E-06 1.47364213E-09-1.00063933E-13      2
-1.38461882E+04 4.91571288E+00 3.86473732E+00 1.98561552E-02-2.04007597E-05      3
 2.17695825E-08-1.06802789E-11-1.39700317E+04 5.24638576E+00                     4

C2H6                CR2178C    2H    60    00    0G    300.000  5000.000                1
 1.67107058E+00 1.88078150E-02-6.98943156E-06 1.16385735E-09-7.17707692E-14      2
-1.14683543E+04 1.26317347E+01 1.92453270E+00 1.68224303E-02-2.24906498E-06      3
-3.40875417E-09 1.49239675E-12-1.14789269E+04 1.16292438E+01                     4

C2H5OH              CR2178C    2H    60    10    0G    300.000  5000.000                1
 4.07928885E+00 1.99448500E-02-1.03391268E-05 2.18924488E-09-1.62465786E-13      2
-3.01364507E+04 5.15237578E+00 4.05660285E+00 2.27314459E-02-2.39257902E-05      3
 2.57251945E-08-1.28756619E-11-3.03195231E+04 4.64880338E+00 0.                  4

C2N2                CR2178C    2N    20    00    0G    300.000  5000.000                1
 5.67975220E+00 5.19447889E-03-2.17021877E-06 3.95325286E-10-2.61329962E-14      2
 3.53056634E+04-4.72842915E+00 4.59656802E+00 1.26965425E-02-2.10870659E-05      3
 2.15419464E-08-8.67478630E-12 3.53865069E+04-1.76408289E-01 0.                  4

C2O                 CR2178C    20    10    00    0G    300.000  5000.000                1
 4.36968556E+00 3.63689770E-03-1.41453611E-06 2.39665088E-10-1.49829137E-14      2
 3.30396533E+04 2.12103265E+00 3.70503786E+00 8.21925889E-03-1.30057185E-05      3
 1.32342356E-08-5.33608448E-12 3.30924256E+04 4.92423824E+00 0.                  4

C2O2                CR2178C    20    20    00    0G    300.000  5000.000                1
 5.03257176E+00 6.26246660E-03-2.72195339E-06 5.09908358E-10-3.44468985E-14      2
 2.95007060E+04-1.06546898E+00 3.71718074E+00 1.56054238E-02-2.63876709E-05      3
 2.69563030E-08-1.08426902E-11 2.95832409E+04 4.39742778E+00 0.                  4
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C3*                 CR2178C    30    00    00    0S    300.000  5000.000                1
 1.41748909E+00 9.65888581E-03-4.39984059E-06 8.55369856E-10-5.89652625E-14      2
-7.40837440E+02-8.71401834E+00 4.41908110E-01 1.65790640E-02-2.32569673E-05      3
 2.45436475E-08-1.08347135E-11-7.06556446E+02-4.66871405E+00 0.                  4

C3                  CR2178C    30    00    00    0G    300.000  5000.000                1
 3.84688132E+00 2.07933866E-03-6.29245249E-07 9.21967001E-11-5.13282996E-15      2
 9.73802920E+04 5.94563882E+00 4.39695616E+00-1.30482003E-03 7.16223848E-06      3
-8.19797148E-09 3.32763548E-12 9.73311237E+04 3.56447059E+00 0.                  4

C3H                 CR2178C    3H    10    00    0G    300.000  5000.000                1
 3.87768217E+00 6.72429692E-03-2.60557340E-06 4.41633303E-10-2.70827040E-14      2
 6.25643380E+04 3.82652971E+00 3.34466073E+00 1.06876056E-02-1.33121389E-05      3
 1.33896016E-08-5.69877273E-12 6.25819062E+04 6.00041845E+00 0.                  4

C3H2                CR2178C    3H    20    00    0G    300.000  5000.000                1
 5.35285383E+00 7.20414402E-03-2.22961757E-06 2.93790631E-10-1.31202676E-14      2
 5.18692712E+04-4.20881663E+00 3.90939393E+00 1.72387449E-02-2.83086137E-05      3
 3.09546819E-08-1.31861564E-11 5.19578137E+04 1.84011020E+00 0.                  4

C3H3                CR2178C    3H    30    00    0G    300.000  5000.000                1
 4.42121734E+00 1.16586316E-02-4.85432110E-06 9.08320547E-10-6.24101500E-14      2
 3.71413875E+04 1.69502468E+00 3.66436750E+00 1.68596717E-02-1.82928161E-05      3
 1.66849198E-08-6.84470460E-12 3.71895247E+04 4.87807284E+00 0.                  4

C3H4                CR2178C    3H    40    00    0G    300.000  5000.000                1
 4.11563623E+00 1.39956296E-02-5.29010702E-06 8.94318329E-10-5.58506042E-14      2
 2.13822256E+04 2.43963682E+00 3.38119240E+00 1.87778042E-02-1.75134727E-05      3
 1.53583176E-08-6.34421504E-12 2.14417104E+04 5.59326125E+00 0.                  4

C3H5                CR2178C    3H    50    00    0G    300.000  5000.000                1
 3.98400596E+00 1.69312231E-02-6.28120531E-06 1.03004414E-09-6.19805342E-14      2
 1.57334259E+04 8.83528102E+00 3.62796589E+00 1.99300881E-02-1.60428741E-05      3
 1.52297312E-08-7.14282368E-12 1.57101700E+04 1.02136699E+01 0.                  4

C2H5CO              CR2178C    3H    50    10    0G    300.000  5000.000                1
-8.46878054E-01 3.15739885E-02-1.45528906E-05 2.77483660E-09-1.87702346E-13      2
-5.58405584E+03 3.19574435E+01 1.20279388E+00 1.87918737E-02 1.60835231E-05      3
-3.04859639E-08 1.31691273E-11-5.81097408E+03 2.30104455E+01 0.                  4

C3H6                CR2178C    3H    60    00    0G    300.000  5000.000                1
 2.55583323E+00 2.14012996E-02-8.26898180E-06 1.43903008E-09-9.29062010E-14      2
 8.22366737E+02 1.14621524E+01 2.43798592E+00 2.19510872E-02-1.00483298E-05      3
 4.54037599E-09-1.84684440E-12 8.33887415E+02 1.20208018E+01 0.                  4

C2H6CO              CR2178C    3H    60    10    0G    300.000  5000.000                1
 2.55520097E+00 2.67728564E-02-1.19321200E-05 2.18220493E-09-1.40952691E-13      2
-2.59106875E+04 1.45241547E+01 2.97307949E+00 2.57414927E-02-1.35099913E-05      3
 9.32153522E-09-5.08892650E-12-2.60821649E+04 1.23150682E+01 0.                  4

C3H7                CR2178C    3H    70    00    0G    300.000  5000.000                1
 2.63075453E+00 2.42979573E-02-9.62786424E-06 1.71216523E-09-1.12767794E-13      2
 9.17147226E+03 1.08721288E+01 3.43473677E+00 1.89905564E-02 2.26298908E-06      3
-9.34591044E-09 3.55787331E-12 9.08796344E+03 7.44875556E+00 0.                  4

C3H6OH              CR2178C    3H    70    10    0G    300.000  5000.000                1
 4.01258970E+00 2.69189876E-02-1.29040868E-05 2.54156183E-09-1.76735542E-13      2
-1.82323145E+04 7.19497814E+00 3.79423960E+00 3.05698564E-02-2.78984027E-05      3
 2.73591962E-08-1.34325728E-11-1.83945346E+04 7.59099088E+00 0.                  4

C3H8                CR2178C    3H    80    00    0G    300.000  5000.000                1
 2.61363612E+00 2.60693233E-02-9.56070819E-06 1.56557291E-09-9.47193731E-14      2
-1.43392842E+04 1.00666551E+01 2.19458112E+00 2.82910276E-02-1.58606143E-05      3
 1.05635674E-08-4.59545710E-12-1.42804637E+04 1.20154862E+01 0.                  4
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C3H7OH              CR2178C   3H   8O   1O   0G   300.000  5000.000          1
 5.72357110E+00 2.57263785E-02-1.27850324E-05 2.60280499E-09-1.86486039E-13   2
-3.36153160E+04-8.39331908E-01 5.32730810E+00 3.19623241E-02-3.81054084E-05   3
 4.39070115E-08-2.20099992E-11-3.38582495E+04 1.00077400E-02 0.               4

C3O2                CR2178C   3O   2O   0O   0G   300.000  5000.000          1
 6.25090440E+00 8.18909055E-03-3.52887809E-06 6.56958175E-10-4.41490502E-14   2
-6.30855441E+03-7.02634617E+00 4.70638642E+00 1.88917640E-02-3.08216920E-05   3
 3.18454393E-08-1.30979717E-11-6.20412427E+03-5.46165127E-01 0.               4

C4*                 CR2178C   4O   0O   0O   0S   300.000  5000.000          1
 1.88913226E+00 1.28759411E-02-5.86305643E-06 1.13941522E-09-7.85200945E-14   2
-9.88719380E+02-1.16119242E+01 6.42490342E-01 2.17334991E-02-3.00975877E-05   3
 3.17460068E-08-1.40614964E-11-9.47731973E+02-6.44717240E+00 0.               4

C4                  CR2178C   4O   0O   0O   0G   300.000  5000.000          1
 4.80290718E+00 6.68890075E-03-2.95140576E-06 5.58156050E-10-3.79343083E-14   2
 1.15103502E+05-1.73882047E+00 3.52514698E+00 1.55384532E-02-2.56787417E-05   3
 2.68539646E-08-1.11781992E-11 1.15186365E+05 3.62154648E+00 0.               4

C4H                 CR2178C   4H   1O   0O   0G   300.000  5000.000          1
 6.53125340E+00 6.50646217E-03-2.25174117E-06 3.32957827E-10-1.72147113E-14   2
 7.53504126E+04-7.44672280E+00 4.96866101E+00 1.72785935E-02-2.99431719E-05   3
 3.24616136E-08-1.36639786E-11 7.54546051E+04-8.76993806E-01 0.               4

C4H2                CR2178C   4H   2O   0O   0G   300.000  5000.000          1
 7.11508476E+00 8.98053640E-03-3.51985467E-06 6.19814636E-10-4.01892860E-14   2
 5.35942929E+04-1.28741449E+01 5.00707131E+00 2.30445808E-02-3.87151529E-05   3
 4.04612350E-08-1.66423423E-11 5.37621258E+04-3.90883434E+00 0.               4

C4H3                CR2178C   4H   3O   0O   0G   300.000  5000.000          1
 5.89753730E+00 1.28447671E-02-5.13420238E-06 9.19869042E-10-6.06632518E-14   2
 5.26004220E+04-4.30132049E+00 4.55523711E+00 2.19461986E-02-2.84883542E-05   3
 2.81808991E-08-1.17266729E-11 5.26946681E+04 1.37609747E+00 0.               4

C4H4                CR2178C   4H   4O   0O   0G   300.000  5000.000          1
 4.63265231E+00 1.85201055E-02-8.03208639E-06 1.53904130E-09-1.07027257E-13   2
 2.95383690E+04 1.97054410E+00 3.66168038E+00 2.50382471E-02-2.48334678E-05   3
 2.14479053E-08-8.76167958E-12 2.96044450E+04 6.08770475E+00 0.               4

C4H5                CR2178C   4H   5O   0O   0G   300.000  5000.000          1
 4.44020972E+00 2.06997069E-02-8.17384169E-06 1.44524452E-09-9.43158963E-14   2
 3.87383060E+04 3.28299330E+00 4.09539209E+00 2.32840045E-02-1.50725994E-05   3
 9.67687539E-09-3.66666900E-12 3.87471236E+04 4.67920168E+00 0.               4

C4H6                CR2178C   4H   6O   0O   0G   300.000  5000.000          1
 4.43098352E+00 2.24282232E-02-8.59171047E-06 1.47461640E-09-9.35672369E-14   2
 1.54683211E+04 3.42850266E+00 3.40277307E+00 2.87651345E-02-2.45720259E-05   3
 2.03612642E-08-8.30860042E-12 1.55761924E+04 7.94258428E+00 0.               4

C4H7                CR2178C   4H   7O   0O   0G   300.000  5000.000          1
 3.52666591E+00 2.72743607E-02-1.13977731E-05 2.12009066E-09-1.44700172E-13   2
 1.74958381E+04 7.78106058E+00 3.87907764E+00 2.47950888E-02-6.52610968E-06   3
-8.52955289E-10 8.35425746E-14 1.74567874E+04 6.32408143E+00 0.               4

C4H7O4              CR2178C   4H   7O   4O   0G   300.000  5000.000          1
 7.43472191E+00 5.74671537E-02-2.52342204E-05 4.67052780E-09-3.09740604E-13   2
-5.59725718E+04-1.07439529E+01 1.15142106E+01 3.03127360E-02 3.65072269E-05   3
-5.51101394E-08 2.08044084E-11-5.63329970E+04-2.79920162E+01                 4

C4H8                CR2178C   4H   8O   0O   0G   300.000  5000.000          1
 3.58352143E+00 2.94161684E-02-1.17841176E-05 2.08265924E-09-1.35140195E-13   2
-4.30675911E+03 6.69676777E+00 4.74222795E+00 2.23143438E-02 3.28090615E-06   3
-1.12045573E-08 4.03017064E-12-4.44748596E+03 1.64976386E+00 0.
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C4H9                CR2178C    4H    90    00    0G    300.000  5000.000                1
 3.94203795E+00 3.13699971E-02-1.25699881E-05 2.19576133E-09-1.40231806E-13    2
 4.78191368E+03 4.92919702E+00 6.42117608E+00 1.61266657E-02 2.13829420E-05    3
-3.10370756E-08 1.19038683E-11 4.50618711E+03-5.86262882E+00                    4

C4H10               CR2178C    4H   100    00    0G    300.000  5000.000                1
 4.27672407E+00 3.28008540E-02-1.26283431E-05 2.10021571E-09-1.26950379E-13    2
-1.88268203E+04 2.84236871E+00 6.96165373E+00 1.64578986E-02 2.33155288E-05    3
-3.25197791E-08 1.22071983E-11-1.91333939E+04-8.87698772E+00                    4

C5                  CR2178C    50    00    00    0G    300.000  5000.000                1
 5.67967482E+00 9.24365225E-03-4.09941097E-06 7.78212058E-10-5.30407626E-14    2
 1.15773338E+05-5.76697644E+00 3.72681940E+00 2.26491373E-02-3.82603957E-05    3
 4.00684104E-08-1.66348839E-11 1.15904265E+05 2.44660629E+00                    4

C5H                 CR2178C    5H    10    00    0G    300.000  5000.000                1
 7.89957802E+00 8.65499890E-03-3.29389928E-06 5.43403306E-10-3.22345528E-14    2
 9.06747482E+04-1.29484180E+01 5.76437471E+00 2.30569269E-02-3.99910175E-05    3
 4.30109463E-08-1.80693840E-11 9.08319044E+04-3.89888526E+00                    4

C5H2                CR2178C    5H    20    00    0G    300.000  5000.000                1
 7.37309582E+00 1.25292951E-02-5.07002453E-06 9.14773750E-10-6.05104550E-14    2
 8.04067078E+04-1.21423162E+01 5.23219119E+00 2.67872287E-02-4.10917187E-05    3
 4.24213136E-08-1.76623850E-11 8.05696170E+04-3.03560200E+00                    4

C5H3                CR2178C    5H    30    00    0G    300.000  5000.000                1
 6.72458417E+00 1.63076641E-02-6.63012025E-06 1.20358719E-09-8.02895819E-14    2
 6.96760026E+04-9.26818386E+00 4.80149759E+00 2.91500466E-02-3.94022762E-05    3
 3.95479007E-08-1.65717430E-11 6.98141623E+04-1.09885131E+00                    4

C5H4                CR2178C    5H    40    00    0G    300.000  5000.000                1
 6.29409217E+00 1.89832534E-02-7.50788446E-06 1.32047274E-09-8.55205219E-14    2
 4.64854807E+04-6.90413286E+00 4.80908267E+00 2.90269322E-02-3.37695164E-05    3
 3.29467307E-08-1.40088159E-11 4.65806227E+04-6.20175608E-01                    4

C5H5                CR2178C    5H    50    00    0G    300.000  5000.000                1
 4.63182693E+00 2.54220063E-02-1.09521039E-05 2.09577765E-09-1.46464484E-13    2
 5.01639816E+04 1.87502179E+00 3.59387109E+00 3.21289782E-02-2.83896360E-05    3
 2.33055313E-08-9.58770207E-12 5.02467713E+04 6.34715240E+00                    4

C5H6                CR2178C    5H    60    00    0G    300.000  5000.000                1
 4.29266987E+00 2.84301488E-02-1.21707440E-05 2.30441758E-09-1.59390333E-13    2
 2.69309767E+04 3.60155851E+00 4.14521151E+00 2.95271905E-02-1.63216425E-05    3
 9.42159764E-09-4.07525520E-12 2.69174250E+04 4.20514523E+00                    4

C5H7                CR2178C    5H    70    00    0G    300.000  5000.000                1
 4.04069506E+00 3.14262778E-02-1.34707144E-05 2.54751482E-09-1.75953709E-13    2
 3.61313642E+04 4.82432546E+00 4.60432806E+00 2.80249314E-02-6.94029066E-06    3
-1.82824298E-09 5.07093767E-13 3.60489264E+04 2.35484525E+00                    4

C5H8                CR2178C    5H    80    00    0G    300.000  5000.000                1
 4.12896891E+00 3.35832983E-02-1.42026413E-05 2.63670017E-09-1.78744092E-13    2
 1.28017450E+04 4.43958284E+00 5.51026293E+00 2.49363184E-02 4.48192598E-06    3
-1.41426355E-08 5.18171021E-12 1.26384949E+04-1.54436364E+00                    4

C5H9                CR2178C    5H    90    00    0G    300.000  5000.000                1
 5.03610093E+00 3.36132436E-02-1.34046516E-05 2.31886028E-09-1.46170737E-13    2
 1.60139828E+04-6.94029811E-02 7.43866915E+00 1.93807864E-02 1.67855939E-05    3
-2.48255308E-08 8.63786386E-12 1.56935189E+04-1.06763001E+01                    4

C5H10               CR2178C    5H   100    00    0G    300.000  5000.000                1
 5.47754916E+00 3.51266606E-02-1.37969042E-05 2.32699006E-09-1.42311989E-13    2
-7.38876020E+03-2.24269020E+00 9.10290447E+00 1.35146527E-02 3.31811937E-05    3
-4.19601645E-08 1.51533972E-11-7.85483075E+03-1.82243410E+01                    4
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C5H11               CR2178C   5H  110   00   0G   300.000  5000.000          1
 5.31923524E+00 3.85588510E-02-1.57070977E-05 2.74658136E-09-1.74352078E-13   2
 9.75263998E+02-1.45174886E+00 1.03193996E+01 7.76851220E-03 5.36807810E-05   3
-6.60061724E-08 2.49806974E-11 3.98154685E+02-2.32664388E+01                 4

C5H12               CR2178C   5H  120   00   0G   300.000  5000.000          1
 6.10174775E+00 3.94595075E-02-1.57755320E-05 2.67456217E-09-1.63602187E-13   2
-2.27527707E+04-5.33357910E+00 1.26604527E+01-6.13641200E-04 7.45625118E-05   3
-8.73257444E-08 3.30131044E-11-2.35228472E+04-3.40294556E+01                 4

C6                  CR2178C   60   00   00   0G   300.000  5000.000          1
 2.23918997E+00 1.32016152E-02-5.10462744E-06 8.82151541E-10-5.62243371E-14   2
 9.94606336E+04 9.85750088E+00 2.41729946E+00 1.23043351E-02-4.28636449E-06   3
 2.20171316E-09-1.47487834E-12 9.94122502E+04 9.03012232E+00                 4

C6H                 CR2178C   6H   10   00   0G   300.000  5000.000          1
 9.33072908E+00 1.06499048E-02-4.24704120E-06 7.34612471E-10-4.58557360E-14   2
 1.03219061E+05-1.87341950E+01 6.58711823E+00 2.91118115E-02-5.09629667E-05   3
 5.42594367E-08-2.25730504E-11 1.03427927E+05-7.09575611E+00                 4

C6H2                CR2178C   6H   20   00   0G   300.000  5000.000          1
 7.76750537E+00 1.61428701E-02-6.82435437E-06 1.29114123E-09-8.93460175E-14   2
 8.19597405E+04-1.35356056E+01 5.34045460E+00 3.20519579E-02-4.65553375E-05   3
 4.67031488E-08-1.92524074E-11 8.21555188E+04-3.16029948E+00                 4

C6OH2               CR2178C   60   1H   20   0G   300.000  5000.000          1
 2.55583323E+00 2.14012996E-02-8.26898180E-06 1.43903008E-09-9.29062010E-14   2
 2.75538492E+04 1.14621524E+01 2.43798592E+00 2.19510872E-02-1.00483298E-05   3
 4.54037599E-09-1.84684440E-12 2.75653699E+04 1.20208018E+01                 4

C6H3                CR2178C   6H   30   00   0G   300.000  5000.000          1
 7.45328661E+00 1.86390006E-02-7.59030388E-06 1.37494267E-09-9.15024655E-14   2
 8.04596707E+04-1.21982228E+01 5.50055685E+00 3.17431991E-02-4.12863060E-05   3
 4.11330694E-08-1.73050958E-11 8.05954889E+04-3.91475144E+00                 4

C6H4                CR2178C   6H   40   00   0G   300.000  5000.000          1
 7.14745406E+00 2.11186604E-02-8.34579079E-06 1.45614764E-09-9.34406393E-14   2
 5.72478848E+04-1.09067196E+01 5.68709109E+00 3.12733519E-02-3.56354873E-05   3
 3.51678012E-08-1.52097262E-11 5.73228113E+04-4.78687929E+00                 4

C6O2H4              CR2178C   60   2H   40   0G   300.000  5000.000          1
 3.58733571E+00 2.87356101E-02-1.09276767E-05 1.86509101E-09-1.17901333E-13   2
-3.64721968E+04 6.74942091E+00 2.69334897E+00 3.35803816E-02-2.27096916E-05   3
 1.59336379E-08-6.35521797E-12-3.63429309E+04 1.08409121E+01                 4

H5C6                CR2178H   5C   60   00   0G   300.000  5000.000          1
 6.83580894E+00 2.36101654E-02-9.10914573E-06 1.53936015E-09-9.55509769E-14   2
 6.64959637E+04-9.58309877E+00 5.84523053E+00 3.09822733E-02-3.04091897E-05   3
 2.96385849E-08-1.32762612E-11 6.65118387E+04-5.53374206E+00                 4

C6H5                CR2178C   6H   50   00   0G   300.000  5000.000          1
 6.83576837E+00 2.32272601E-02-8.89219788E-06 1.49330001E-09-9.23324636E-14   2
 3.23347600E+04-9.51072968E+00 5.77996503E+00 3.13863489E-02-3.25371792E-05   3
 3.24224931E-08-1.44798298E-11 3.23378805E+04-5.26695349E+00                 4

H6C6                CR2178H   6C   60   00   0G   300.000  5000.000          1
 6.52891445E+00 2.60916541E-02-9.86554521E-06 1.62071705E-09-9.74954389E-14   2
 4.32846433E+04-8.28568161E+00 6.01265860E+00 3.06462241E-02-2.51038844E-05   3
 2.40562617E-08-1.13330150E-11 4.32412783E+04-6.32454791E+00                 4

C6H6                CR2178C   6H   60   00   0G   300.000  5000.000          1
 4.36367372E+00 2.93791648E-02-1.12705781E-05 1.88724983E-09-1.14981578E-13   2
 7.58222595E+03-4.84978232E-01 2.69773694E+00 4.09514438E-02-4.31447697E-05   3
 4.26444782E-08-1.89043606E-11 7.65532248E+03 6.49932413E+00                 4
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C603H6              CR2178C    60    3H    60    0G    300.000  5000.000                1
 5.48708602E+00 3.50988122E-02-1.37780313E-05 2.32257179E-09-1.41977763E-13     2
-6.44612528E+04-2.28927065E+00 9.11272047E+00 1.34967281E-02 3.31517589E-05     3
-4.18874945E-08 1.51147480E-11-6.49279372E+04-1.82745698E+01                     4

C6H7                CR2178C    6H    70    00    0G    300.000  5000.000                1
 6.32883516E+00 2.88992529E-02-1.08958109E-05 1.77814337E-09-1.06102832E-13     2
 4.67038100E+04-7.65466155E+00 6.61063416E+00 2.88321685E-02-1.59530082E-05     3
 1.41771554E-08-7.66263224E-12 4.65528385E+04-9.24944879E+00                     4

C6H8                CR2178C    6H    80    00    0G    300.000  5000.000                1
 6.47429853E+00 3.09447605E-02-1.14085783E-05 1.79536834E-09-1.02129723E-13     2
 2.33808900E+04-8.46759439E+00 7.51651654E+00 2.63881296E-02-6.56879652E-06     3
 4.52947505E-09-4.16160532E-12 2.31320953E+04-1.34267413E+01                     4

C604H8              CR2178C    60    4H    80    0G    300.000  5000.000                1
 5.88556039E+00 4.51369701E-02-1.87790596E-05 3.34373856E-09-2.15801926E-13     2
-9.27093838E+04-4.46780917E+00 1.05763394E+01 1.59744221E-02 4.66320005E-05     3
-6.05958265E-08 2.27844721E-11-9.32377390E+04-2.48504249E+01                     4

C6H9                CR2178C    6H    90    00    0G    300.000  5000.000                1
 5.40444124E+00 3.67178130E-02-1.47976523E-05 2.58971281E-09-1.65979087E-13     2
 3.26701929E+04-3.10788303E+00 7.36515874E+00 2.53404410E-02 8.03139631E-06     3
-1.57936556E-08 4.80499506E-12 3.23901258E+04-1.18041462E+01                     4

C6H10               CR2178C    6H   100    00    0G    300.000  5000.000                1
 6.19881581E+00 3.74681540E-02-1.45072819E-05 2.40208649E-09-1.44230839E-13     2
 9.20993622E+03-6.85309512E+00 8.89937429E+00 2.19272623E-02 1.69075206E-05     3
-2.35628823E-08 7.24626871E-12 8.82136505E+03-1.88670370E+01                     4

C6H+05              CR2178C    6H   100    50    0G    300.000  5000.000                1
 5.47912554E+00 3.51233241E-02-1.37945531E-05 2.32633858E-09-1.42251521E-13     2
-7.20088356E+04-2.25121649E+00 9.10290447E+00 1.35146527E-02 3.31811937E-05     3
-4.19601645E-08 1.51533972E-11-7.24743651E+04-1.82243410E+01                     4

C605H+              CR2178C    60    5H   100    0G    300.000  5000.000                1
 7.26995565E+00 5.21455831E-02-2.14214069E-05 3.76775468E-09-2.40023768E-13     2
-1.20086912E+05-9.69241136E+00 1.16070916E+01 2.47991217E-02 3.91503582E-05     3
-5.37225141E-08 1.96878053E-11-1.20554404E+05-2.84102408E+01                     4

H+05C6              CR2178H   100    5C    60    0G    300.000  5000.000                1
 7.97241368E+00 5.79583779E-02-2.48487606E-05 4.46746475E-09-2.87137784E-13     2
-1.14518427E+05-1.35885448E+01 1.24120044E+01 2.83752238E-02 4.13484816E-05     3
-5.74192321E-08 2.05458805E-11-1.14927117E+05-3.23509732E+01                     4

C6H11               CR2178C    6H   110    00    0G    300.000  5000.000                1
 4.70945518E+00 4.50172349E-02-1.94023085E-05 3.61353960E-09-2.44779703E-13     2
 1.27450309E+04 8.28228604E-01 8.66651578E+00 2.01105903E-02 3.71497513E-05     3
-5.24841929E-08 2.02504771E-11 1.23159878E+04-1.63001329E+01                     4

C6H12               CR2178C    6H   120    00    0G    300.000  5000.000                1
 5.88488423E+00 4.51365903E-02-1.87783200E-05 3.34353677E-09-2.15787004E-13     2
-1.08083036E+04-4.46306485E+00 1.05667982E+01 1.60550448E-02 4.64070879E-05     3
-6.03405199E-08 2.26824932E-11-1.13365560E+04-2.48122908E+01                     4

C6H13               CR2178C    6H   130    00    0G    300.000  5000.000                1
 6.09038245E+00 4.83649468E-02-2.05966354E-05 3.73975738E-09-2.45330911E-13     2
-2.73222948E+03-4.84917568E+00 1.18044712E+01 1.22988467E-02 6.17209049E-05     3
-7.86674041E-08 3.01963015E-11-3.33898441E+03-2.95547266E+01                     4

C6H14               CR2178C    6H   140    00    0G    300.000  5000.000                1
 6.93509523E+00 4.99837642E-02-2.12653951E-05 3.82923887E-09-2.48012709E-13     2
-2.65184374E+04-8.24828574E+00 1.36589425E+01 7.56989398E-03 7.59075336E-05     3
-9.41922345E-08 3.62905549E-11-2.72286710E+04-3.73283891E+01                     4
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C7H                 CR2178C   7H   10   00   0G   300.000  5000.000                1
 9.95961268E+00 1.38815773E-02-5.92169501E-06 1.10050501E-09-7.39611621E-14        2
 1.17373214E+05-2.23941662E+01 6.71100284E+00 3.58433013E-02-6.16573211E-05        3
 6.52114623E-08-2.71624065E-11 1.17609454E+05-8.64568323E+00                        4

C7H2                CR2178C   7H   20   00   0G   300.000  5000.000                1
 8.40401146E+00 1.86100610E-02-7.88269607E-06 1.49502480E-09-1.03748325E-13        2
 1.07528503E+05-1.55451548E+01 5.70072495E+00 3.62099847E-02-5.13656013E-05        3
 5.03723393E-08-2.03947947E-11 1.07765010E+05-3.94966076E+00                        4

C7H14               CR2178C   7H  140   00   0G   300.000  5000.000                1
 7.26883972E+00 5.21472992E-02-2.14221290E-05 3.76788638E-09-2.40033484E-13        2
-1.30196455E+04-9.68609928E+00 1.16026162E+01 2.48269960E-02 3.90842636E-05        3
-5.36537165E-08 1.96617034E-11-1.34870147E+04-2.83905601E+01                        4

C7H15               CR2178C   7H  150   00   0G   300.000  5000.000                1
 7.44151150E+00 5.74626986E-02-2.52344178E-05 4.67095893E-09-3.09792667E-13        2
-5.21873986E+03-1.07859274E+01 1.15223944E+01 3.02562318E-02 3.66499313E-05        3
-5.52163740E-08 2.08187751E-11-5.57838605E+03-2.80310733E+01                        4

C7H16               CR2178C   7H  160   00   0G   300.000  5000.000                1
 7.97404170E+00 5.79562438E-02-2.48474252E-05 4.46710521E-09-2.87104229E-13        2
-2.85874506E+04-1.35982128E+01 1.23924786E+01 2.85096113E-02 4.10203599E-05        3
-5.70695773E-08 2.04099888E-11-2.89937476E+04-3.22689995E+01                        4

C8H                 CR2178C   8H   10   00   0G   300.000  5000.000                1
 1.12137780E+01 1.50488466E-02-6.01689908E-06 1.04022405E-09-6.48160608E-14        2
 1.30565263E+05-2.84954890E+01 7.43356164E+00 4.07220219E-02-7.16169041E-05        3
 7.70967508E-08-3.24142967E-11 1.30831326E+05-1.25206573E+01                        4

C8H2                CR2178C   8H   20   00   0G   300.000  5000.000                1
 1.17338513E+01 1.76350130E-02-7.45335759E-06 1.39194449E-09-9.45403749E-14        2
 1.09168109E+05-3.33713193E+01 7.45648506E+00 4.61406382E-02-7.90485520E-05        3
 8.30200725E-08-3.43557329E-11 1.09502934E+05-1.51764256E+01                        4

C8H16               CR2178C   8H  160   00   0G   300.000  5000.000                1
 8.72631842E+00 6.01905027E-02-2.52169779E-05 4.49843351E-09-2.89944768E-13        2
-1.69309000E+04-1.68095263E+01 1.40465955E+01 2.63865047E-02 4.97834592E-05        3
-6.66792297E-08 2.43710023E-11-1.74870973E+04-3.06962680E+01                        4

C8H17               CR2178C   8H  170   00   0G   300.000  5000.000                1
 1.02042144E+01 6.35429051E-02-2.75949900E-05 4.97199413E-09-3.18203666E-13        2
-9.17131464E+03-2.45217938E+01 1.37698320E+01 3.88591826E-02 2.74041606E-05        3
-4.51419759E-08 1.59147207E-11-9.44621356E+03-3.93216349E+01                        4

C8H18               CR2178C   8H  180   00   0G   300.000  5000.000                1
 9.54307684E+00 6.64615226E-02-2.86115458E-05 5.11117032E-09-3.24491047E-13        2
-3.25581143E+04-2.18448517E+01 1.38773424E+01 3.67381109E-02 3.83142718E-05        3
-5.73704055E-08 2.06204134E-11-3.29078668E+04-3.99334289E+01                        4

C9H                 CR2178C   9H   10   00   0G   300.000  5000.000                1
 1.21519596E+01 1.87476296E-02-8.35513101E-06 1.61937302E-09-1.13045465E-13        2
 1.42217900E+05-3.27929826E+01 7.65113658E+00 4.86037270E-02-8.32385062E-05        3
 8.69742429E-08-3.59398145E-11 1.42578436E+05-1.36117395E+01                        4

C9H2                CR2178C   9H   20   00   0G   300.000  5000.000                1
 1.35477500E+01 1.83833809E-02-7.46552045E-06 1.33402157E-09-8.66834796E-14        2
 1.31774466E+05-4.11853269E+01 8.91266665E+00 4.93189974E-02-8.58366007E-05        3
 9.19537121E-08-3.86358269E-11 1.32120341E+05-2.14866595E+01                        4

C9H18               CR2178C   9H  180   00   0G   300.000  5000.000                1
 1.03245382E+01 6.83721069E-02-2.92405938E-05 5.29939835E-09-3.46415657E-13        2
-2.02427104E+04-2.49645955E+01 1.65643628E+01 2.82080220E-02 6.02262272E-05        3
-7.97393901E-08 2.91498121E-11-2.08623146E+04-5.16648961E+01                        4
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C9H19               CR2178C   9H  190   00   0G   300.000  5000.000          1
 1.16908553E+01 7.40732964E-02-3.33404488E-05 6.16610847E-09-4.03043281E-13  2
-1.25696513E+04-3.22311720E+01 1.49406990E+01 4.93001248E-02 2.38501888E-05  3
-4.70813175E-08 1.71770729E-11-1.27006219E+04-4.51483311E+01                 4

C9H20               CR2178C   9H  200   00   0G   300.000  5000.000          1
 1.00188713E+01 7.85810011E-02-3.49786228E-05 6.42191973E-09-4.17671790E-13  2
-3.57480027E+04-2.51260724E+01 1.40256839E+01 4.85642511E-02 3.56312062E-05  3
-6.24104003E-08 2.38147567E-11-3.59214556E+04-4.12063180E+01                 4

C10H                CR2178C  10H   10   00   0G   300.000  5000.000          1
 1.37279214E+01 1.99097333E-02-8.60835904E-06 1.61762986E-09-1.09689141E-13  2
 1.58318882E+05-3.85575885E+01 9.07615867E+00 5.10126770E-02-8.70499610E-05  3
 9.14059997E-08-3.79076380E-11 1.58678871E+05-1.87864619E+01                 4

C10H2               CR2178C  10H   20   00   0G   300.000  5000.000          1
 1.54959909E+01 1.88297655E-02-7.31103086E-06 1.24141992E-09-7.63722096E-14  2
 1.36736225E+05-4.96292961E+01 1.00704220E+01 5.54051513E-02-1.00095074E-04  3
 1.07996365E-07-4.51970904E-11 1.37137523E+05-2.66389601E+01                 4

C+H+O+              CR2178C  12H  200  100   0G   300.000  5000.000          1
 2.46438698E+01 8.48715937E-02-3.97368102E-05 9.32823166E-09-8.51879012E-13  2
-2.41899031E+05-6.25797739E+01 2.58520779E+01 8.61504174E-02-6.05707552E-05  3
 5.14360726E-08-2.46128069E-11-2.42576777E+05-6.98833466E+01                 4

C2H4O               CR2178C   2H   40   10   0G   300.000  5000.000          1
 2.13948577E+00 1.70856105E-02-6.88202446E-06 1.22653337E-09-8.00697707E-14  2
-7.42022823E+03 1.21482939E+01 2.16422597E+00 1.74017280E-02-9.97336799E-06  3
 8.36036869E-09-4.46341933E-12-7.47936829E+03 1.19248412E+01                 4

HNO2-C              CR2178H   1N   10   20   0G   300.000  5000.000          1
 4.30604728E+00 5.91182934E-03-2.43942101E-06 4.43498473E-10-2.93988482E-14  2
-1.07189986E+04 3.79795719E+00 3.59576057E+00 1.08733125E-02-1.54580086E-05  3
 1.59003603E-08-6.71886954E-12-1.06762456E+04 6.77233505E+00                 4

HNO2-T              CR2178H   1N   10   20   0G   300.000  5000.000          1
 4.43870342E+00 5.70860007E-03-2.34523219E-06 4.25740051E-10-2.82109227E-14  2
-1.10001222E+04 3.08613279E+00 3.63354168E+00 1.12930921E-02-1.68361763E-05  3
 1.74076706E-08-7.29852767E-12-1.09483111E+04 6.46590876E+00                 4

HNO3                CR2178H   1N   10   30   0G   300.000  5000.000          1
 4.79323295E+00 9.03583689E-03-3.87230132E-06 7.22178336E-10-4.87541785E-14  2
-1.78850328E+04 2.21642863E+00 3.60437427E+00 1.73117667E-02-2.56339565E-05  3
 2.67946927E-08-1.14466844E-11-1.78187965E+04 7.19231572E+00                 4

NO3                 CR2178N   10   30   00   0G   300.000  5000.000          1
 4.77225841E+00 6.73895322E-03-3.14060934E-06 6.15718184E-10-4.29487552E-14  2
 6.92766593E+03 1.31305815E+00 3.57596133E+00 1.50262846E-02-2.50214655E-05  3
 2.70557232E-08-1.16931318E-11 6.99395144E+03 6.32909317E+00                 4

N2O3                CR2178N   20   30   00   0G   300.000  5000.000          1
 6.54535847E+00 7.09780993E-03-3.15533138E-06 5.99393828E-10-4.08684304E-14  2
 7.78092403E+03-2.05597467E+00 5.34742727E+00 1.55649231E-02-2.52749971E-05  3
 2.64887086E-08-1.10796995E-11 7.85395807E+03 2.94169677E+00                 4

N2O4                CR2178N   20   40   00   0G   300.000  5000.000          1
 7.45489228E+00 1.03944998E-02-4.68048202E-06 8.96984652E-10-6.15569250E-14  2
-1.46226768E+03-8.73815330E+00 5.66999956E+00 2.29012754E-02-3.73602726E-05  3
 3.94435054E-08-1.66501699E-11-1.35640679E+03-1.27711848E+00                 4

N2O5                CR2178N   20   50   00   0G   300.000  5000.000          1
 1.06649774E+01 9.85194976E-03-4.70528496E-06 9.35573686E-10-6.57040205E-14  2
-2.06659206E+03-2.19681157E+01 6.12134308E+00 3.99827623E-02-8.07086823E-05  3
 8.79303802E-08-3.66442913E-11-1.68688234E+03-2.56453741E+00                 4
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C5*                 CR2178C   50   00   00   0S   300.000  5000.000          1
 2.32216176E+00 1.61254319E-02-7.32039303E-06 1.41745664E-09-9.73074827E-14   2
-1.23218228E+03-1.42947782E+01 8.71728386E-01 2.62112427E-02-3.50842047E-05   3
 3.71110925E-08-1.66625092E-11-1.18041907E+03-8.23602263E+00                 4

C6*                 CR2178C   60   00   00   0S   300.000  5000.000          1
 2.78990133E+00 1.93405316E-02-8.77694855E-06 1.69891949E-09-1.16590639E-13   2
-1.47952574E+03-1.71693201E+01 1.03976837E+00 3.15009516E-02-4.22337296E-05   3
 4.46826430E-08-2.00538200E-11-1.41582739E+03-9.85545979E+00                 4

HCOOH               CR2178H   2C   1O   2O   0G   300.000  5000.000          1
 5.39320914E+00 7.09819421E-03-2.15400045E-06 2.75928893E-10-1.18231146E-14   2
-4.91351708E+04-2.56394343E+00 3.94463499E+00 1.70961328E-02-2.82246368E-05   3
 3.11909973E-08-1.34056196E-11-4.90453616E+04 3.52325822E+00                 4

CH4COO              CR2178C   2H   4O   2O   0G   300.000  5000.000          1
 4.62254108E+00 1.85020263E-02-7.99623944E-06 1.52604400E-09-1.05712297E-13   2
-5.78934530E+04 3.68557661E+00 3.70459613E+00 2.45976606E-02-2.38051164E-05   3
 2.05699879E-08-8.51846852E-12-5.78321343E+04 7.59052765E+00                 4

HE                  CR2178HE  1O   00   00   0G   300.000  5000.000          1
 2.50798024E+00-2.85843494E-06-9.81288200E-10 4.68497405E-13-4.22177436E-17   2
-7.45672974E+02 8.61331375E-01 2.30618881E+00 1.47176892E-03-3.75122677E-06   3
 4.00985852E-09-1.53202268E-12-7.27064805E+02 1.70228436E+00                 4

E                   CR2178E   1O   00   00   0G   300.000  5000.000          1
 2.37626905E+00 2.07741476E-04-1.13104855E-07 2.43930105E-11-1.80291089E-15   2
-7.01451155E+02-1.10375409E+01 1.66876530E+00 5.09538278E-03-1.20629758E-05   3
 1.26590984E-08-4.86677487E-12-6.40159685E+02-8.05830942E+00                 4

H+                  CR2178H   1E  -1O   00   0G   300.000  5000.000          1
 2.51219345E+00-1.87486335E-05 1.02778322E-08-2.36835211E-12 1.93130549E-16   2
 1.84031157E+05-1.22388651E+00 2.38182132E+00 9.44649108E-04-2.46590480E-06   3
 2.66489474E-09-1.02391294E-12 1.84043230E+05-6.81675321E-01                 4

H-                  CR2178H   1E   1O   00   0G   300.000  5000.000          1
 2.51419332E+00-2.28909272E-05 1.30827419E-08-3.09332412E-12 2.55620167E-16   2
 1.59593097E+04-1.23322554E+00 2.38484372E+00 9.26528104E-04-2.43085170E-06   3
 2.63943134E-09-1.01840403E-12 1.59716953E+04-6.93338666E-01                 4

O-                  CR2178O   1E   1O   00   0G   300.000  5000.000          1
 2.60116573E+00-1.35802068E-04 6.48410678E-08-1.29758820E-11 9.25105350E-16   2
 1.14574644E+04 4.18971288E+00 2.47078527E+00 8.07591100E-04-2.31433265E-06   3
 2.46878479E-09-9.14674559E-13 1.14718860E+04 4.73818925E+00                 4

OH+                 CR2178O   1H   1E  -1O   0G   300.000  5000.000          1
 3.16242504E+00 8.11313055E-04-1.36069212E-07 4.03829741E-12 9.43424569E-16   2
 1.57429408E+05 3.70909077E+00 3.14413183E+00 9.74911382E-04-3.94564618E-07   3
-1.91457623E-10 3.09629637E-13 1.57439204E+05 3.78909893E+00                 4

OH-                 CR2178O   1H   1E   1O   0G   300.000  5000.000          1
 3.31275361E+00 3.46121399E-04 1.04635693E-07-4.53217659E-11 4.19012546E-15   2
-1.83220961E+04 1.74337768E+00 3.19134270E+00 1.13327900E-03-1.61064012E-06   3
 1.32977579E-09-3.21378308E-13-1.83011661E+04 2.27556109E+00                 4

H3O+                CR2178H   3O   1E  -1O   0G   300.000  5000.000          1
 2.82208892E+00 4.87691336E-03-1.37875395E-06 1.81084151E-10-9.18536687E-15   2
 6.88286235E+04 5.74675582E+00 3.97117949E+00-1.25072927E-03 1.28908296E-05   3
-1.66263750E-08 7.50724222E-12 6.86854057E+04 5.25349683E-01                 4

NO+                 CR2178N   1O   1E  -1O   0G   300.000  5000.000          1
 3.09453628E+00 1.16390462E-03-3.68121074E-07 5.21412009E-11-2.68737891E-15   2
 1.18116546E+05 5.84919244E+00 3.14570870E+00 9.55519742E-04 4.94798549E-08   3
-5.82257176E-10 3.71322532E-13 1.18114163E+05 5.61325399E+00                 4
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NO2-                CR2178N   1O   2E   1O   0G   300.000  5000.000          1
 4.06241241E+00 3.59270888E-03-1.62012918E-06 3.10339051E-10-2.12622600E-14   2
-4.45340517E+04 4.19850644E+00 3.55126544E+00 7.10743338E-03-1.12990554E-05   3
 1.25125017E-08-5.54807621E-12-4.44991361E+04 6.36843918E+00                 4

O2-                 CR2178O   2E   1O   0O   0G   300.000  5000.000          1
 3.39445694E+00 1.40226776E-03-6.15282283E-07 1.17574100E-10-7.98957275E-15   2
-6.78960204E+03 5.36570261E+00 3.11413119E+00 3.39699169E-03-5.94269297E-06   3
 6.45268380E-09-2.73008678E-12-6.77019268E+03 6.53992675E+00                 4

H2+                 CR2178H   2E  -1O   0O   0G   300.000  5000.000          1
 3.32871562E+00 2.50506781E-04 1.42245209E-07-4.45902420E-11 3.73375638E-15   2
 1.79974709E+05-3.32902789E+00 2.81737505E+00 3.65761027E-03-7.96554877E-06   3
 8.26140297E-09-3.09022840E-12 1.80027389E+05-1.14519278E+00                 4

H2O+                CR2178H   2O   1E  -1O   0G   300.000  5000.000          1
 3.32039240E+00 2.04286948E-03-3.49732956E-07 9.99066468E-12 1.71730071E-15   2
 1.15532710E+05 3.16321608E+00 3.29838370E+00 2.28639358E-03-7.86762475E-07   3
-1.63090920E-10 3.90313009E-13 1.15544184E+05 3.25078237E+00                 4

N+                  CR2178N   1E  -1O   0O   0G   300.000  5000.000          1
 2.47957220E+00 8.58290701E-05-7.51191467E-08 2.11968565E-11-1.37667111E-15   2
 2.24086690E+05 4.94417869E+00 2.29485807E+00 1.42410056E-03-3.44624981E-06   3
 3.57489851E-09-1.33750503E-12 2.24104779E+05 5.71689741E+00                 4

NO2+                CR2178N   1O   2E  -1O   0G   300.000  5000.000          1
 3.67553609E+00 3.88427165E-03-1.69480705E-06 3.16837396E-10-2.13183545E-14   2
 1.30354391E+05 6.79523637E+00 3.41846010E+00 5.93994993E-03-7.69435773E-06   3
 7.95625738E-09-3.45978995E-12 1.30361318E+05 7.82829601E+00                 4

N2+                 CR2178N   2E  -1O   0O   0G   300.000  5000.000          1
 3.09476368E+00 1.17122886E-03-3.70803092E-07 5.22559219E-11-2.63943973E-15   2
 1.78953470E+05 5.04447470E+00 3.04870303E+00 1.66691862E-03-1.69948507E-06   3
 1.22924435E-09-3.00574994E-13 1.78959920E+05 5.21345604E+00                 4

N2O+                CR2178N   2O   1E  -1O   0G   300.000  5000.000          1
 3.81881552E+00 4.14546701E-03-1.77463453E-06 3.27891977E-10-2.18702496E-14   2
 1.58239437E+05 3.52246527E+00 3.20425869E+00 8.43496006E-03-1.29484263E-05   3
 1.33967700E-08-5.59189267E-12 1.58280630E+05 6.10128921E+00                 4

O+                  CR2178O   1E  -1O   0O   0G   300.000  5000.000          1
 2.68420332E+00-2.47148101E-04 1.10854689E-07-1.95207915E-11 1.33909023E-15   2
 1.86372113E+05 3.80817902E+00 2.56134251E+00 7.07794011E-04-2.32396110E-06   3
 2.44900956E-09-8.64456773E-13 1.86385135E+05 4.31294272E+00                 4

O2+                 CR2178O   2E  -1O   0O   0G   300.000  5000.000          1
 3.25680775E+00 1.24798926E-03-4.28714608E-07 7.79714406E-11-5.44049135E-15   2
 1.43993928E+05 5.72232395E+00 3.12931650E+00 2.38851052E-03-3.76502512E-06   3
 4.08884445E-09-1.69303299E-12 1.43998062E+05 6.21557675E+00                 4

O3-                 CR2178O   3E   1O   0O   0G   300.000  5000.000          1
 4.42157839E+00 3.34012071E-03-1.51730860E-06 2.96605113E-10-2.06677042E-14   2
-1.90720301E+04 2.48267275E+00 4.05447843E+00 6.07948435E-03-9.58748864E-06   3
 1.09399959E-08-4.96614210E-12-1.90563047E+04 4.00280748E+00                 4

AR+                 CR2178AR  1E  -1O   0O   0G   300.000  5000.000          1
 2.50796905E+00-2.81899817E-06-1.02114189E-09 4.81392447E-13-4.35087371E-17   2
 1.81156733E+05 4.31252422E+00 2.30618882E+00 1.47176883E-03-3.75122654E-06   3
 4.00985828E-09-1.53202259E-12 1.81175339E+05 5.15342336E+00                 4

CNN                 J 6/66C   1N   2O0  0O0  0G   300.000  5000.000          1
 0.48209077E 01 0.24790014E-02-0.94644109E-06 0.16548764E-09-0.10899129E-13   2
 0.68685948E 05-0.48484039E 00 0.35077779E 01 0.72023958E-02-0.75574589E-05   3
 0.42979217E-08-0.94257935E-12 0.68994281E 05 0.60234964E 01                 4
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CN2                 J12/70C    1N    20    00    0G    300.000  5000.000                1
 0.55626268E+01 0.20860606E-02-0.88123724E-06 0.16505783E-09-0.11366697E-13      2
 0.54897907E+05-0.55989355E+01 0.32524003E+01 0.70010737E-02-0.22653599E-05      3
-0.28939808E-08 0.18270077E-11 0.55609085E+05 0.66966778E+01                      4

C2N                 J 3/67C    2N    100   000   0G    300.000  5000.000                1
 0.61931308E 01 0.14327539E-02-0.61255161E-06 0.11578707E-09-0.80401339E-14      2
 0.64818372E 05-0.84132298E 01 0.32670394E 01 0.98211307E-02-0.83284733E-05      3
 0.17650559E-08 0.59632768E-12 0.65589057E 05 0.65682304E 01                      4

H2O(S)              L11/65H    2O    100   000   0S    200.000   273.150                1
 0.              0.              0.              0.              0.                  2
 0.              0.             -0.39269330E-01 0.16920420E-01 0.                  3
 0.              0.             -0.35949581E 05 0.56933784E 00                      4

H2O(L)              L11/65H    2O    100   000   0L    273.150   1000.0                 1
 0.              0.              0.              0.              0.                  2
 0.              0.              0.12712782E 02-0.17662790E-01-0.22556661E-04      3
 0.20820908E-06-0.24078614E-09-0.37483200E 05-0.59115345E 02                      4

NCO                 J12/70N    1C    10    10    0G    300.000  5000.000                1
 0.49964357E+01 0.26250880E-02-0.10928387E-05 0.20309111E-09-0.13915195E-13      2
 0.17379356E+05-0.17325320E+01 0.31092021E+01 0.66201022E-02-0.26070086E-05      3
-0.14966380E-08 0.10922032E-11 0.17977514E+05 0.83561334E+01                      4

N3                  J12/70N    3O    00    00    0G    300.000  5000.000                1
 0.51996828E+01 0.24335678E-02-0.10192340E-05 0.19062350E-09-0.13212412E-13      2
 0.47963131E+05-0.35547759E+01 0.30624389E+01 0.73590658E-02-0.38229374E-05      3
-0.71824202E-09 0.91110236E-12 0.48614547E+05 0.77570129E+01                      4

C+                  L12/66C    1E   -100   000   0G    300.000  5000.000                1
 0.25118274E 01-0.17359784E-04 0.95042676E-08-0.22188518E-11 0.18621892E-15      2
 0.21667721E 06 0.42861298E 01 0.25953840E 01-0.40686645E-03 0.68923669E-06      3
-0.52664878E-09 0.15083377E-12 0.21666281E 06 0.38957298E 01                      4

C-                  J 9/65C    1E    100   000   0G    300.000  5000.000                1
 0.24470591E 01 0.11286428E-03-0.78591462E-07 0.19778614E-10-0.11105555E-14      2
 0.69972969E 05 0.42356992E 01 0.24925640E 01 0.53153068E-04-0.13307994E-06      3
 0.13951379E-09-0.52150992E-13 0.69955757E 05 0.39811657E 01                      4

CN+                 J12/70C    1N    1E   -10    0G    300.000  5000.000                1
 0.36522919E+01 0.81427579E-03-0.20853348E-06 0.29071604E-10-0.17865094E-14      2
 0.21560182E+06 0.43916910E+01 0.36175018E+01-0.20179550E-02 0.79359855E-05      3
-0.77300616E-08 0.24798477E-11 0.21578134E+06 0.53579527E+01                      4

CN-                 J12/70C    1N    1E    10    0G    300.000  5000.000                1
 0.29471725E+01 0.14988427E-02-0.57579547E-06 0.10177789E-09-0.67478503E-14      2
 0.63644338E+04 0.63743952E+01 0.37034310E+01-0.14896426E-02 0.31864701E-05      3
-0.14831305E-08 0.48121663E-13 0.62335826E+04 0.27722843E+01                      4

CO2-                J12/66C    1O    2E    100   0G    300.000  5000.000                1
 0.45454640E 01 0.26054316E-02-0.10928732E-05 0.20454421E-09-0.14184542E-13      2
-0.54761968E 05 0.18317369E 01 0.34743737E 01 0.16913805E-02 0.73533803E-05      3
-0.99554255E-08 0.36846719E-11-0.54249049E 05 0.83834329E 01                      4

C2-                 J12/69C    2E    10    00    0G    300.000  5000.000                1
 0.36926257E 01 0.41576040E-03 0.11654211E-07 0.23755880E-11-0.14585314E-14      2
 0.52118953E 05 0.22470173E 01 0.37342914E 01-0.23034649E-02 0.68417833E-05      3
-0.58120827E-08 0.16604296E-11 0.52281427E 05 0.27860423E 01                      4

HCO+                J12/70H    1C    10    1E   -1G    300.000  5000.000                1
 0.37411880E+01 0.33441517E-02-0.12397121E-05 0.21189388E-09-0.13704150E-13      2
 0.98884078E+05 0.20654768E+01 0.24739736E+01 0.86715590E-02-0.10031500E-04      3
 0.67170527E-08-0.17872674E-11 0.99146608E+05 0.81625751E+01                      4
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TABLE I - REACTION MECHANISM

UNITS: CM,CAL,KELVIN,MOLE,SEC. M IS ANY COLLISION PARTNER. RATE OF REVERSE REACTION CALCULATED FROM EQUILIBRIUM CONSTANT

	REACTIONS BEING CONSIDERED								K=A*(T**N)*EXP(-E/RT) A	N	E, CAL
1.	O2	+	M	=	O	+ O	+	M	2.550E+18	-1.00	118700.0
2.	H2	+ OH		=	H2O	+ H			2.190E+13	0.00	5150.0
3.	H	+ O2		=	OH	+ O			2.240E+14	0.00	16800.0
4.	O	+ H2		=	OH	+ H			1.800E+10	1.00	8900.0
5.	O	+ H2O		=	OH	+ OH			5.750E+13	0.00	18000.0
6.	H	+ H	+ M	=	H2	+		M	1.000E+18	-1.00	0.0
7.	H	+ OH	+ M	=	H2O	+		M	7.500E+23	-2.60	0.0
8.	CO	+ O2		=	O	+ CO2			1.600E+13	0.00	41000.0
9.	NO	+ O	+ M	=	NO2	+		M	1.050E+15	0.00	-1870.0
10.	NO2	+ O		=	NO	+ O2			1.000E+13	0.00	600.0
11.	NO2	+ H		=	NO	+ OH			7.200E+14	0.00	1930.0
12.	N	+ O	+ M	=	NO	+		M	6.400E+16	-.50	0.0
13.	N	+ O2		=	NO	+ O			6.400E+09	1.00	6250.0
14.	O	+ N2		=	NO	+ N			1.360E+14	0.00	75400.0
15.	CH4	+	M	=	CH3	+ H	+	M	4.000E+17	0.00	88421.0
16.	CO	+ OH		=	CO2	+ H			5.600E+11	0.00	1080.0
17.	CH4	+ O		=	OH	+ CH3			2.000E+13	0.00	9220.0
18.	CH4	+ H		=	CH3	+ H2			6.900E+13	0.00	11823.0
19.	CH4	+ OH		=	CH3	+ H2O			2.800E+13	0.00	4968.0
20.	CH3	+ O2		=	CH2O	+ OH			1.200E+12	0.00	15000.0
21.	CH3	+ O		=	CH2O	+ H			1.950E+13	0.00	2000.0
22.	CH2O	+	M	=	H2	+ CO	+	M	2.100E+16	0.00	35000.0
23.	HCO	+ OH		=	CO	+ H2O			2.000E+13	0.00	0.0
24.	HCO	+	M	=	H	+ CO	+	M	2.000E+12	.50	28613.0
25.	CH2O	+ OH		=	HCO	+ H2O			2.000E+13	0.00	0.0
26.	CO	+ O	+ M	=	CO2	+		M	4.000E+13	0.00	0.0
27.	C3H8	+ OH		=	C3H7	+ H2O			1.000E+11	.50	7200.0
28.	C3H8	+ O		=	C2H6	+ CH2O			1.000E+12	.50	0.0
29.	C3H8	+ H		=	C3H7	+ H2			3.600E+12	.50	7200.0
30.	C3H7	+ O		=	C2H6CO	+ H			8.800E+11	.50	0.0
31.	C3H7	+ O		=	C3H6	+ OH			8.800E+11	.50	0.0
32.	C3H7	+ OH		=	C3H6	+ H2O			8.800E+10	.50	0.0
33.	C3H7	+ O2		=	C2H6CO	+ OH			1.000E+11	.50	0.0
34.	C3H6	+ O2		=	CH3CHO	+ CH2O			9.800E+10	.50	0.0
35.	C3H6	+ OH		=	CH3CHO	+ CH3			8.100E+10	.50	1000.0
36.	C3H6	+ O		=	C3H4	+ H2O			8.100E+11	.50	0.0
37.	C3H6	+ O		=	CH2O	+ C2H4			8.100E+11	.50	0.0
38.	C3H4	+ O2		=	CH3CO	+ HCO			1.000E+11	.50	0.0
39.	C2H6	+ O		=	C2H5	+ OH			8.800E+11	.50	7000.0
40.	C2H6	+ OH		=	C2H5	+ H2O			8.900E+10	.50	5500.0
41.	C2H6	+ H		=	C2H5	+ H2			2.000E+12	0.00	6200.0
42.	C2H6CO	+ OH		=	C2H5CO	+ H2O			9.600E+10	.50	6700.0
43.	C2H6CO	+ H		=	C2H5CO	+ H2			3.500E+12	.50	10500.0
44.	C2H5CO	+ O		=	C2H5	+ CO2			9.000E+11	.50	0.0
45.	C2H5CO	+ OH		=	C2H5OH	+ CO			9.000E+10	.50	0.0
46.	C2H5CO	+ O2		=	C2H4OH	+ CO2			1.000E+11	.50	0.0
47.	C2H5CO	+ H		=	C2H5	+ HCO			3.300E+12	.50	5300.0
48.	C2H5OH	+ H		=	C2H5	+ H2O			3.000E+12	.50	4600.0
49.	C2H4OH	+ H		=	C2H5	+ OH			3.000E+12	.50	9800.0
50.	C2H5	+ O2		=	CH3CHO	+ OH			1.100E+11	.50	0.0
51.	C2H5	+ O		=	C2H4	+ OH			8.800E+11	.50	0.0
52.	C2H5	+ O		=	CH3CHO	+ H			8.800E+11	.50	0.0
53.	C2H5	+ OH		=	C2H4	+ H2O			8.900E+10	.50	0.0
54.	CH3CHO	+ OH		=	CH3CO	+ H2O			6.500E+10	.50	4000.0
55.	CH3CHO	+ H		=	CH3CO	+ H2			2.400E+12	.50	11000.0
56.	CH3CO	+ O		=	CH3	+ CO2			6.100E+11	.50	0.0
57.	CH3CO	+ O2		=	CH2OH	+ CO2			7.800E+10	.50	1500.0
58.	CH3CO	+ OH		=	CH3OH	+ CO			6.200E+10	.50	0.0
59.	CH3CO	+ H		=	CH3	+ HCO			2.200E+12	.50	5400.0
60.	CH3OH	+ H		=	CH3	+ H2O			2.300E+12	.50	5300.0
61.	CH2OH	+ H		=	CH3	+ OH			2.200E+12	.50	10700.0
62.	C2H4	+ O		=	CH3	+ HCO			3.000E+13	0.00	0.0
63.	C2H4	+ O		=	C2H2	+ H2O			3.000E+13	0.00	0.0
64.	C2H4	+ OH		=	CH3	+ CH2O			1.000E+11	.50	7100.0
65.	C2H2	+ O		=	C2H	+ OH			3.400E+15	-.64	18700.0
66.	C2H2	+ OH		=	C2H	+ H2O			2.200E+14	0.00	7000.0
67.	C2H	+ O2		=	CH	+ CO2			1.000E+14	0.00	23000.0
68.	CH	+ O2		=	CO	+ OH			8.100E+10	.50	0.0

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TABLE II - THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES

O/F= 15.6030 PERCENT FUEL= 6.0230 EQUIVALENCE RATIO= 1.0000

THERMODYNAMIC PROPERTIES	
P, ATM	1.0000
T, DEG K	2267
RHO, G/CC	1.5084-4
H, CAL/G	-33.4
S, CAL/(G)(K)	2.3180
M, MOL WT	28.064
(DLV/DLP)T	-1.00299
(DLV/DLT)P	1.0885
CP, CAL/(G)(K)	.5423
GAMMA (S)	1.1788
SON VEL,M/SEC	889.9

MOLE FRACTIONS

H	4.6931-4	N2O	1.1711-7	CH2O	2.478-11
HNO	5.9868-8	O	3.0935-4	CO	1.2288-2
OH	3.2027-3	O2	5.7614-3	CO2	1.0271-1
HO2	3.2382-7	O3	6.249-11	CN	5.714-16
H2	3.3605-3	NH	1.2687-8	HNO2-C	9.3494-9
H2O	1.4813-1	NH2	1.5114-9	HNO2-T	1.0745-8
H2O2	5.0460-8	NH3	1.8315-9	HNO3	5.382-13
N	2.3046-8	N2H2	3.280-14	NO3	1.504-13
NO	2.4479-3	HCN	3.207-11	HCOOH	4.1768-9
NO2	4.3392-7	HNCO	3.029-10	NCO	6.286-12
N2	7.2132-1	HCO	2.0927-8	N3	2.081-13

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 1.00000E-15

N2H3	N2H4	NH3*	C*	C	CH	CH2	CH3	CH2OH	CH4
CH3OH	C2*	C2	C2H	C2HO	C2HO2	C2H2	C2H2O	C2H2O2	C2H3
C2H3O	CH3CO	C2H3O2	C2O2H3	C2H4	H4C2O	CH3CHO	C2H4O2	C2O2H4	C2H5
C2H4OH	C2H6	C2H5OH	C2N2	C2O	C2O2	C3*	C3	C3H	C3H2
C3H3	C3H4	C3H5	C2H5CO	C3H6	C2H6CO	C3H7	C3H6OH	C3H8	C3H7OH
C3O2	C4*	C4	C4H	C4H2	C4H3	C4H4	C4H5	C4H6	C4H7
C4H7O4	C4H8	C4H9	C4H10	C5	C5H	C5H2	C5H3	C5H4	C5H5
C5H6	C5H7	C5H8	C5H9	C5H10	C5H11	C5H12	C6	C6H	C6H2
C6OH2	C6H3	C6H4	C6O2H4	H5C6	C6H5	H6C6	C6H6	C6O3H6	C6H7
C6H8	C6O4H8	C6H9	C6H10	C6H+O5	C6O5H+	H+O5C6	C6H11	C6H12	C6H13
C6H14	C7H	C7H2	C7H14	C7H15	C7H16	C8H	C8H2	C8H16	C8H17
C8H18	C9H	C9H2	C9H18	C9H19	C9H20	C10H	C10H2	C+H+O+	C2H4O
N2O3	N2O4	N2O5	C5*	C6*	CH4COO	CNN	CN2	C2N	H2O(S)
H2O(L)									

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TABLE III - STIRRED REACTOR STATIONARY STATES

T, DEG K	2.2674 3	2.2675 3	2.2673 3	2.2663 3	2.2653 3	2.2643 3	2.2633 3	2.2623 3	2.2523 3	2.2423 3	2.2323 3	2.2223 3	2.2123 3
EM/V, G/S-CC	1.000-15	1.000 -6	5.000 -6	4.014 -5	7.340 -5	1.058 -4	1.379 -4	1.699 -4	5.085 -4	9.146 -4	1.420 -3	2.056 -3	2.868 -3
RES TM, SEC	5.3746 9	1.5083 2	3.0168 1	3.7588 0	2.0565 0	1.4271 0	1.0954 0	8.8922-1	2.9825-1	1.6642-1	1.0763-1	7.4573-2	5.3667-2
SM, MOLX/GMX	1.0000 0	3.5633-2	3.5633-2	3.5636-2	3.5640-2	3.5643-2	3.5646-2	3.5649-2	3.5678-2	3.5705-2	3.5733-2	3.5760-2	3.5787-2
W, CAL/GMX	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0
O2 CONS EFF	1.0000 0	9.9999-1	9.9990-1	9.9922-1	9.9863-1	9.9809-1	9.9759-1	9.9711-1	9.9304-1	9.8949-1	9.8616-1	9.8295-1	9.7983-1
T-RISE RATIO	1.0000 0	1.0000 0	9.9993-1	9.9942-1	9.9891-1	9.9840-1	9.9789-1	9.9739-1	9.9230-1	9.8722-1	9.8214-1	9.7705-1	9.7197-1
O2 COMB RATE	1.8999-5	1.8998-5	1.8997-5	1.8984-5	1.8973-5	1.8962-5	1.8953-5	1.8944-5	1.8866-5	1.8799-5	1.8736-5	1.8675-5	1.8615-5

MOLE FRACTIONS X(I)

H	4.6931-4	4.6947-4	4.7107-4	4.8337-4	4.9492-4	5.0610-4	5.1705-4	5.2787-4	6.3486-4	7.4662-4	8.6592-4	9.9352-4	1.1296-3
OH	3.2027-3	3.2033-3	3.2096-3	3.2560-3	3.2975-3	3.3360-3	3.3725-3	3.4074-3	3.7148-3	3.9879-3	4.2442-3	4.4883-3	4.7219-3
H2	3.3605-3	3.3609-3	3.3650-3	3.3970-3	3.4280-3	3.4585-3	3.4886-3	3.5185-3	3.8105-3	4.0979-3	4.3836-3	4.6679-3	4.9506-3
H2O	1.4813-1	1.4813-1	1.4812-1	1.4806-1	1.4797-1	1.4789-1	1.4783-1	1.4776-1	1.4712-1	1.4650-1	1.4589-1	1.4529-1	1.4469-1
N	2.3046-8	2.0224-7	2.3417-6	2.4411-6	2.5443-6	2.6381-6	2.7251-6	2.8068-6	3.4719-6	4.0037-6	4.4651-6	4.8736-6	5.2351-6
NO	2.4479-3	2.4477-3	2.4269-3	2.2943-3	2.1902-3	2.1034-3	2.0286-3	1.9629-3	1.5419-3	1.2926-3	1.1064-3	9.5256-4	8.1863-4
NO2	4.3392-7	5.0254-7	4.2956-7	4.0152-7	3.7908-7	3.6006-7	3.4348-7	3.2874-7	2.3207-7	1.7546-7	1.3592-7	1.0625-7	8.3196-8
N2	7.2132-1	7.2132-1	7.2133-1	7.2132-1	7.2131-1	7.2129-1	7.2127-1	7.2124-1	7.2087-1	7.2043-1	7.1997-1	7.1949-1	7.1901-1
O	3.0935-4	3.0946-4	3.1078-4	3.2053-4	3.2945-4	3.3791-4	3.4608-4	3.5403-4	4.2571-4	5.0569-4	5.8493-4	6.6814-4	7.5549-4
O2	5.7614-3	5.7627-3	5.7802-3	5.9051-3	6.0142-3	6.1139-3	6.2071-3	6.2953-3	7.0466-3	7.6985-3	8.3100-3	8.8982-3	9.4702-3
CH	9.852-18	1.866 -7	4.385 -9	1.217 -8	2.188 -8	3.110 -8	4.000 -8	4.868 -8	1.325 -7	2.214 -7	3.225 -7	4.411 -7	5.833 -7
HCO	2.0927-8	2.0125-7	2.1740-6	2.5583-6	2.9449-6	3.3236-6	3.6992-6	4.0746-6	6.1128-6	1.3055-7	1.9278-7	2.7181-7	3.7271-7
CH2O	2.478-11	1.889 -7	3.499 -9	3.860-10	6.206-10	8.859-10	1.149 -9	1.413 -9	4.268 -9	7.820 -9	1.239 -8	1.834 -8	2.614 -8
CH3	9.843-17	1.946 -7	5.065 -8	3.953 -7	7.024 -7	9.866 -7	1.254 -6	1.509 -6	3.690 -6	5.592 -6	7.440 -6	9.356 -6	1.144 -5
CH2OH	5.792-17	1.933 -7	4.060 -8	3.134 -7	5.530 -7	7.715 -7	9.736 -7	1.163 -6	2.648 -6	3.747 -6	4.670 -6	5.518 -6	6.357 -6
CH4	2.848-17	1.904 -7	1.516 -8	1.125 -7	1.973 -7	2.738 -7	3.442 -7	4.097 -7	9.146 -7	1.285 -6	1.599 -6	1.895 -6	2.195 -6
CH3OH	3.206-18	1.890 -7	5.740 -9	2.721 -8	4.768 -8	6.607 -8	8.291 -8	9.849 -8	2.143 -7	2.928 -7	3.544 -7	4.085 -7	4.604 -7
CO	1.2288-2	1.2289-2	1.2302-2	1.2408-2	1.2508-2	1.2604-2	1.2700-2	1.2795-2	1.3709-2	1.4587-2	1.5439-2	1.6268-2	1.7076-2
CO2	1.0271-1	1.0270-1	1.0269-1	1.0257-1	1.0246-1	1.0235-1	1.0224-1	1.0213-1	1.0111-1	1.0013-1	9.9170-2	9.8235-2	9.7320-2
C2H	4.436-22	1.898 -7	1.077 -8	7.750 -8	1.397 -7	1.989 -7	2.564 -7	3.127 -7	8.685 -7	1.482 -6	2.204 -6	3.079 -6	4.159 -6
C2H2	2.305-21	1.945 -7	5.115 -8	3.472 -7	7.056 -7	9.923 -7	1.263 -6	1.523 -6	3.825 -6	5.995 -6	8.261 -6	1.076 -5	1.362 -5
CH3CO	2.031-24	1.890 -7	5.491 -9	2.505 -8	4.481 -8	6.336 -8	8.103 -8	9.805 -8	2.510 -7	3.946 -7	5.415 -7	6.996 -7	8.759 -7
C2H4	1.434-26	1.891 -7	5.845 -9	2.881 -8	5.134 -8	7.232 -8	9.219 -8	1.112 -7	2.786 -7	4.315 -7	5.855 -7	7.495 -7	9.313 -7
CH3CHO	8.790-26	1.906 -7	1.711 -8	1.316 -7	2.360 -7	3.343 -7	4.282 -7	5.188 -7	1.337 -6	2.107 -6	2.895 -6	3.742 -6	4.687 -6
C2H5	2.363-32	1.890 -7	5.111 -9	2.076 -6	3.717 -8	5.260 -8	6.734 -8	8.157 -8	2.114 -7	3.366 -7	4.677 -7	6.116 -7	7.746 -7
C2H4OH	7.098-32	1.900 -7	1.244 -8	9.535 -8	1.692 -7	2.373 -7	3.011 -7	3.615 -7	8.589 -7	1.260 -6	1.621 -6	1.970 -6	2.330 -6
C2H6	8.692-33	1.905 -7	1.654 -8	1.271 -7	2.284 -7	3.241 -7	4.159 -7	5.049 -7	1.328 -6	2.135 -6	2.990 -6	3.937 -6	5.019 -6
C2H5OH	3.429-33	1.887 -7	4.010 -9	7.379 -9	1.298 -8	1.804 -8	2.271 -8	2.706 -8	6.039 -8	8.410 -8	1.034 -7	1.206 -7	1.373 -7
C3H4	2.613-36	1.887 -7	3.661 -9	2.896 -9	5.212 -9	7.416 -9	9.548 -9	1.164 -8	3.221 -8	5.486 -8	8.144 -8	1.135 -7	1.526 -7
C2H5CO	0.0000 0	1.8876-7	4.0511-9	7.955e-9	1.4213-8	2.0068-8	2.5637-8	3.0990-8	7.8848-8	1.2352-7	1.6919-7	2.1834-7	2.7323-7
C3H6	0.0000 0	1.8874-7	3.9440-9	6.5879-9	1.1747-8	1.6564-8	2.1143-8	2.5544-8	6.5209-8	1.0312-7	1.4285-7	1.8655-7	2.3624-7
C2H6CO	0.0000 0	1.8949-7	8.6489-9	5.7304-8	1.0244-7	1.4468-7	1.8484-7	2.2341-7	5.6511-7	8.7790-7	1.1922-6	1.5260-6	1.8952-6
C3H7	0.0000 0	1.8887-7	4.6396-9	1.5170-8	2.7073-8	3.8205-8	4.8790-8	5.8969-8	1.5051-7	2.3731-7	3.2750-7	4.2593-7	5.3718-7
C3H8	0.0000 0	1.8947-7	8.5350-9	5.6054-8	9.9908-8	1.4073-7	1.7935-7	2.1627-7	5.3704-7	8.2234-7	1.1031-6	1.3965-6	1.7172-6

T, DEG K	2.1923 3	2.1723 3	2.1523 3	2.1023 3	2.0523 3	2.0023 3	1.9523 3	1.9316 3					
EM/V, G/S-CC	5.2541-3	9.3435-3	1.6722-2	8.4765-2	3.0065-1	5.1637-1	6.0229-1	6.0852-1					
RES TM, SEC	2.9519-2	1.6728-2	9.4202-3	1.8977-3	5.3758-4	3.2799-4	2.8929-4	2.8978-4					
SM, MOLX/GMX	3.5841-2	3.5894-2	3.5944-2	3.6037-2	3.6021-2	3.5937-2	3.5826-2	3.5779-2					
W, CAL/GMX	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0	0.0000 0					
O2 CONS EFF	1.0000 0	9.9392-1	9.8790-1	9.7097-1	9.4439-1	9.1168-1	8.7878-1	8.6567-1					
T-RISE RATIO	1.0000 0	9.8943-1	9.7886-1	9.5244-1	9.2602-1	8.9959-1	8.7317-1	8.6223-1					
O2 COMB RATE	3.9250-3	3.9012-3	3.8775-3	3.8111-3	3.7068-3	3.5784-3	3.4492-3	3.3978-3					

MOLE FRACTIONS X(I)

H	1.4204-3	1.7525-3	2.0968-3	2.7784-3	2.4401-3	1.6921-3	1.1067-3	9.3012-4
OH	5.1595-3	5.5562-3	5.9051-3	6.4084-3	5.9287-3	4.9312-3	3.9528-3	3.5993-3
H2	5.5085-3	6.0492-3	6.5569-3	7.3658-3	6.8233-3	5.9042-3	5.1470-3	4.8896-3
H2O	1.4348-1	1.4229-1	1.4111-1	1.3839-1	1.3609-1	1.3301-1	1.2891-1	1.2704-1
N	5.8140-8	6.1775-8	6.2870-8	5.1612-8	2.6267-8	1.0615-8	4.1313-9	2.6285-9
NO	5.9097-4	4.0542-4	2.5847-4	5.3230-5	9.7514-6	2.9890-6	1.2101-6	8.6496-7
NO2	5.035 -8	2.935 -8	1.613 -8	2.526 -9	4.399-10	1.418-10	6.109-11	4.490-11
N2	7.1805-1	7.1709-1	7.1616-1	7.1441-1	7.1476-1	7.1644-1	7.1865-1	7.1960-1
O	9.4176-4	1.1411-3	1.3474-3	1.7748-3	1.6936-3	1.3108-3	9.4935-4	8.2689-4
O2	1.0580-2	1.1657-2	1.2721-2	1.5717-2	2.0484-2	2.6403-2	3.2409-2	3.4815-2
CH	9.7019-7	1.5779-6	2.5891-6	9.9881-6	2.1839-5	2.0431-5	1.3428-5	1.0790-5
HCO	6.6975-7	1.1762-6	2.0835-6	1.0254-5	3.4874-5	5.2710-5	5.2644-5	4.9502-5
CH2O	5.0139-8	9.3509-8	1.7562-7	1.0174-6	4.2605-6	8.3174-6	1.1212-5	1.2033-5
CH3	1.6523-5	2.3825-5	3.5465-5	1.2994-4	4.6003-4	9.0927-4	1.2909-3	1.4070-3
CH2OH	8.2300-6	1.0700-5	1.4726-5	4.9278-5	2.2691-4	6.9887-4	1.5424-3	1.9831-3
CH4	2.6939-6	3.8819-6	5.4714-6	1.8795-5	6.7782-5	1.4209-4	2.1729-4	2.4453-4
CH3OH	5.7429-7	7.2763-7	9.6766-7	2.9918-6	1.1683-5	2.7750-5	4.5425-5	5.1573-5
CO	1.8623-2	2.0073-2	2.1408-2	2.3907-2	2.4729-2	2.4623-2	2.3697-2	2.2837-2
CO2	9.5550-2	9.3856-2	9.2235-2	8.8427-2	8.4474-2	8.0623-2	7.7530-2	7.6428-2
C2H	7.2232-6	1.2277-5	2.1074-5	5.1416-5	2.2642-4	2.4113-4	1.8138-4	1.5455-4
C2H2	2.1025-5	3.2226-5	5.0523-5	1.8752-4	4.6702-4	5.5195-4	4.7274-4	4.2485-4
CH3CO	1.3175-6	1.9632-6	3.0032-6	1.1634-5	4.2870-5	8.2830-5	1.0674-4	1.0997-4
C2H4	1.3842-6	2.0428-6	3.0962-6	1.1443-5	3.6718-5	6.0081-5	6.7667-5	6.6805-5
CH3CHO	7.0583-6	1.0543-5	1.6212-5	6.6044-5	2.9137-4	7.4359-4	1.3359-3	1.5925-3
C2H5	1.1905-6	1.8079-6	2.8091-6	1.0942-5	3.6795-5	6.2459-5	7.1993-5	7.1505-5
C2H4OH	3.1504-6	4.2859-6	6.0476-6	2.0965-5	8.9692-5	2.4245-4	4.7313-4	5.8257-4
C2H6	7.8111-6	1.2016-5	1.8944-5	7.8814-5	3.1600-4	7.0459-4	1.1382-3	1.3149-3
C2H5OH	1.7365-7	2.2199-7	2.9605-7	9.0845-7	3.3420-6	7.2976-6	1.0913-5	1.1932-5
C3H4	2.6207-7	4.3827-7	7.3646-7	2.9290-6	5.9248-6	4.4455-6	2.1199-6	1.4713-6
C2H5CO	4.1101-7	6.1290-7	9.3812-7	3.5969-6	1.2578-5	2.2650-5	2.7171-5	2.7198-5
C3H6	3.6351-7	5.5285-7	8.5864-7	3.2063-6	8.8768-6	1.1101-5	8.9690-6	7.6567-6
C2H6CO	2.8146-6	4.1592-6	6.3374-6	2.5108-5	1.0478-4	2.5578-4	4.5087-4	5.3601-4
C3H7	8.2027-7	1.2396-6	1.9174-6	7.2777-6	2.2628-5	3.5077-5	3.7346-5	3.6045-5
C3H8	2.3056-6	3.6442-6	5.4701-6	2.0741-5	8.0196-5	1.7877-4	2.9204-4	3.3893-4

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