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## The Chemkin Thermodynamic Data Base

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## THE CHEMKIN THERMODYNAMIC DATA BASE

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### Abstract

The Chemkin general-purpose chemical kinetics package uses a data base that contains polynomial fits to specific heats, standard state enthalpies, and standard state entropies. The fourteen coefficient fits are in the same form as used in the NASA Complex Chemical Equilibrium Program (Gordon and McBride, 1971). This report represents a compilation of the data that is currently in use at Sandia National Laboratories.

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## THE CHEMKIN THERMODYNAMIC DATA BASE

### Introduction

This report documents the thermodynamic property data base that is an integral part of the Chemkin<sup>1,2</sup> chemical kinetics computer code package. The codes are documented in user's manuals. However, a brief description of the package's structure may help put the role of the data base in perspective. Chemkin is composed of four important pieces: the Interpreter, the Thermodynamic Data Base, the Linking File, and the Gas-Phase Subroutine Library. The Interpreter is a program that first reads the user's symbolic description of the reaction mechanism. It then extracts thermodynamic information for the species involved from the Thermodynamic Data Base. The user may add to or modify the information in the data base by input to the Interpreter. In addition to printed output, the Interpreter writes a Linking File, which contains all the pertinent information on the elements, species, and reactions in the mechanism.

Once the Interpreter has been executed and the Linking File created, the user is ready to use the Gas-Phase Subroutine Library. These subroutines are called from the user's Fortran code. The Chemkin gas-phase subroutines, of which there are over 100, are called as needed to return information on the elements, species, reactions, equations of state, thermodynamic properties, chemical production rates, sensitivity parameters, derivatives of chemical production rates, and derivatives of thermodynamic properties. Generally the input to these routines is the state of the gas - pressure or density, temperature, and the species composition. The Chemkin documentation is designed to facilitate selection of the particular Chemkin subroutines that are needed for a given problem.

We developed the Chemkin package and its follow-on applications programs for use in our combustion research programs. Our combustion work concentrates on small molecule hydrocarbon systems, especially those involving the nitrogen chemistry responsible for producing nitrogen-oxygen based pollutants. Thus we have gathered thermodynamic properties for the species important in such systems. Moreover, because of our investigations of the chemical vapor deposition of silicon from silane, the data base includes several silicon-hydrogen compounds. It was not our intent to make wide distribution of these codes or data bases. However, over the past several years, the code package has found rather wide acceptance.

As part of the Chemkin code distribution process, we have supplied its associated thermodynamic data base. However, this was done in an unstructured way. That is, recipients of the data base had no way to tell where the data came from or any information about its validity. The data base was simply the one that was in use at Sandia at the time the tape was written. Since, a great many Chemkin simulations are finding their way into the literature, we decided that it would be a good idea to document the data base. However, our basic motivation remains unchanged. We maintain the data base for our own research programs, and we in no way see ourselves as a clearinghouse for property data or as competitors with JANAF or the National Bureau of Standards. Nevertheless, for certain classes of problems, we believe that sharing our thermodynamic data compilation could prove valuable in other research programs.

In this report, we first explain how the polynomial fits to the property data are generated. Then in three appendices we present the data itself in several formats. Appendix A lists the standard state heats of formation and entropies at 298K for each of the species in the data base. Appendix B is a listing of the data base in the form that Chemkin expects to find it. Finally, Appendix C presents a graphical account of the properties as a function of temperature. Where available, the actual data from which the fits were determined are also plotted to indicate the accuracy of the fit. Also in this section a reference to the source of the data is provided.

### The data sources

The data comes from three major sources. First is the JANAF<sup>3</sup> tables. Generally speaking, if available, JANAF is the preferred source of our data. The properties of many hydrocarbon species not included in the JANAF compilations come from the compilation of Burcat.<sup>4</sup> In this case, the data provided by Burcat is already fit in the form required for our data base. The third source of data is quantum chemistry computations.

Calculation of thermochemical data using high-quality *ab initio* electronic structure calculations has been a long-standing goal. However, the availability of supercomputers and new theoretical techniques now allow the calculation of thermochemical properties with chemical accuracy, i.e.,  $\Delta H_f$  to within  $\pm 3$  kcal/mole. A technique that has been applied to over 900 combustion-related chemical species and to our study of silicon-containing species is denoted the BAC-MP4 method.<sup>5-9</sup> It combines electronic structure calculations using fourth-order Møller-Plesset perturbation theory<sup>10-12</sup> (MP4) with empirically-derived bond additivity correction (BAC) factors to account for systematic error in the *ab initio* calculations due to truncated wave functions and incomplete basis sets.

### The fitting procedure

The data format used is a minor modification of that used by Gordon and McBride<sup>13</sup> for the thermodynamic data base in the NASA Chemical Equilibrium program. The thermodynamic data are stored as polynomial fits to specific heat  $c_p/R$ , enthalpy  $H^0/RT$ , and entropy  $S^0/R$ . There are seven coefficients for each of two temperature ranges.

$$\frac{c_p}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \quad (1)$$

$$\frac{H^0}{RT} = a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{T} \quad (2)$$

$$\frac{S^0}{R} = a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 + \frac{a_5}{4} T^4 + a_7 \quad (3)$$

Thus for each species there are 14 coefficients in all. In addition to the polynomial coefficients for each species, the Thermodynamic Data Base provides the species name, its elemental makeup, and the temperature ranges over which the fits are valid.

The essential input to the fitting procedure is a table of specific heat, enthalpy, and entropy as a function of temperature. In addition, since the fits span two temperature ranges, the temperature ranges have to be specified. Generally speaking, the common temperature connecting the two ranges is 1000K, but it may be different in some cases.

The constrained linear least squares fitting procedure<sup>14,15</sup> is a three stage process. The first step is to determine simultaneously  $a_1$  through  $a_5$  for both temperature ranges by fitting the specific heats Eq. (1). The fitting procedure is constrained such that at the common temperature both the specific heat and its first derivative are equal. The second step is to determine  $a_6$  for both temperature ranges by fitting the enthalpy data. In this stage,  $a_1 - a_5$  are held fixed, and as in the  $c_p$  fitting, equality constraints on the fit and its first derivative are imposed at the common temperature. Finally, the  $a_7$  coefficients are determined by fitting the entropy data. Again, the  $a_1 - a_5$  coefficients are held fixed and the equality constraints are imposed at the common temperature. We note that this fitting procedure is slightly different from the procedure followed by McBride and Gordon,<sup>16</sup> who fit all coefficients simultaneously.

### Data base management

The Chemkin data base requires a four card image fixed format representation of the properties for each species. This is consistent with other data bases, such as that used in the NASA Chemical Equilibrium Code.<sup>13</sup> However, while this format is complete enough to describe the properties, it contains only the bare minimum data needed. Therefore, we now maintain the data base using a relational data base manager program called DATA-TRIEVE, which is a proprietary product of the Digital Equipment Corporation (DEC).

The data base contains the following fields:

1. Identification - chemical symbol, species name, elemental composition, and phase;
2. Fit coefficients for the thermodynamic properties, and the temperature ranges for which they apply.
3. Data used to generate the fit, if available. These fields contain  $H^0(298)$ ,  $S^0(298)$ , and tables of  $c_p(T)$ ,  $S^0(T)$ ,  $H^0(T)$  as functions of temperature.
4. References - source of data, date, any relevant comments.

Using a relational data base manager provides considerably more flexibility in managing the data than the original Chemkin data base. Various types of reports can be produced from database manager program. The appendices in this report represent three examples of such reports. The data base that Chemkin uses is simply one of the reports from the DATATRIEVE system.

#### Acknowledgement

Our colleagues C. F. Melius, J. S. Binkley, P. Ho, R. E. Mitchell, and M. E. Coltrin have made and continue to make important contributions to this data base.

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APPENDIX A. STANDARD STATE ENTHALPIES AND ENTROPIES AT 298K

TABLE A1.

Species	H <sup>0</sup> (298) Kcal/mole	S <sup>0</sup> (298) cal/mole K	Species	H <sup>0</sup> (298) Kcal/mole	S <sup>0</sup> (298) cal/mole K
<i>Al</i>	78.77	39.29	<i>C<sub>2</sub>HCl</i>	51.08	57.80
<i>Al<sub>2</sub>H<sub>6</sub></i>	21.34	62.73	<i>C<sub>2</sub>N</i>	132.95	55.13
<i>Al<sub>2</sub>Me<sub>6</sub></i>	-61.17	131.01	<i>C<sub>2</sub>N<sub>2</sub></i>	73.84	57.69
<i>AlAs</i>	107.28	60.63	<i>C<sub>2</sub>O</i>	68.47	55.65
<i>AlH</i>	61.97	44.85	<i>C<sub>3</sub></i>	195.92	56.64
<i>AlH<sub>2</sub></i>	41.93	54.38	<i>C<sub>3</sub>H<sub>2</sub></i>	106.47	56.19
<i>AlH<sub>3</sub></i>	18.82	52.28	<i>C<sub>3</sub>H<sub>4</sub></i>	45.21	54.87
<i>AlMe</i>	19.74	60.65	<i>C<sub>3</sub>H<sub>4</sub>C</i>	66.17	58.16
<i>AlMe<sub>2</sub></i>	12.75	77.37	<i>C<sub>3</sub>H<sub>4</sub>P</i>	43.95	49.47
<i>AlMe<sub>3</sub></i>	-20.29	83.65	<i>C<sub>3</sub>H<sub>6</sub></i>	4.88	61.48
<i>Ar</i>	0.00	36.96	<i>C<sub>3</sub>H<sub>8</sub></i>	-24.81	64.53
<i>Ar<sup>+</sup></i>	364.76	39.73	<i>C<sub>3</sub>O<sub>2</sub></i>	-22.37	65.94
<i>As</i>	75.45	43.51	<i>C<sub>4</sub></i>	231.91	54.53
<i>As<sub>2</sub></i>	47.06	59.80	<i>C<sub>4</sub>H</i>	155.02	60.86
<i>As<sub>3</sub></i>	65.32	77.49	<i>C<sub>4</sub>H<sub>2</sub></i>	111.66	59.75
<i>As<sub>4</sub></i>	37.11	78.42	<i>C<sub>4</sub>H<sub>6</sub></i>	34.95	68.13
<i>AsAlMe</i>	69.97	81.57	<i>C<sub>4</sub>H<sub>8</sub></i>	-0.13	73.52
<i>AsAlMe<sub>2</sub></i>	63.23	90.97	<i>C<sub>5</sub></i>	233.91	57.80
<i>AsGaEt</i>	82.72	95.17	<i>C<sub>5</sub>H</i>	185.92	62.18
<i>AsGaEt<sub>2</sub></i>	69.52	109.79	<i>C<sub>5</sub>H<sub>12</sub></i>	-34.96	83.45
<i>AsGaMe</i>	83.47	85.72	<i>C<sub>5</sub>H<sub>2</sub></i>	165.17	63.66
<i>AsGaMe<sub>2</sub></i>	81.22	90.97	<i>C<sub>5</sub>H<sub>3</sub></i>	135.36	70.50
<i>AsGaMeH</i>	93.71	84.69	<i>C<sub>5</sub>H<sub>6</sub></i>	31.98	64.42
<i>AsH</i>	61.73	50.18	<i>C<sub>6</sub>H</i>	213.07	74.07
<i>AsH<sub>2</sub></i>	42.23	46.43	<i>C<sub>6</sub>H<sub>10</sub></i>	-1.00	74.72
<i>AsH<sub>3</sub></i>	16.62	55.63	<i>C<sub>6</sub>H<sub>14</sub></i>	-39.89	92.84
<i>AsMe</i>	59.18	63.78	<i>C<sub>6</sub>H<sub>2</sub></i>	169.59	70.89
<i>AsMe<sub>2</sub></i>	34.19	79.47	<i>C<sub>6</sub>H<sub>3</sub></i>	158.38	76.26
<i>AsMe<sub>3</sub></i>	2.92	85.74	<i>C<sub>6</sub>H<sub>4</sub></i>	121.72	69.51
<i>C</i>	171.22	37.74	<i>C<sub>6</sub>H<sub>5</sub></i>	79.40	69.79
<i>C(S)</i>	0.00	1.37	<i>C<sub>6</sub>H<sub>5</sub>(L)</i>	140.52	84.23
<i>C<sup>+</sup></i>	431.85	36.92	<i>C<sub>6</sub>H<sub>5</sub>O</i>	10.35	74.84
<i>C<sup>-</sup></i>	140.55	36.14	<i>C<sub>6</sub>H<sub>5</sub>OH</i>	-25.00	76.90
<i>C<sub>2</sub></i>	200.15	47.61	<i>C<sub>6</sub>H<sub>6</sub></i>	19.80	64.33
<i>C<sub>2</sub><sup>-</sup></i>	105.96	46.94	<i>C<sub>6</sub>H<sub>7</sub></i>	47.94	73.05
<i>C<sub>2</sub>F<sub>6</sub></i>	-321.07	79.35	<i>C<sub>8</sub>H</i>	288.74	78.35
<i>C<sub>2</sub>H</i>	133.95	49.54	<i>C<sub>8</sub>H<sub>2</sub></i>	226.06	75.91
<i>C<sub>2</sub>H<sub>2</sub></i>	54.17	47.99	<i>CCl</i>	119.95	53.61
<i>C<sub>2</sub>H<sub>3</sub></i>	68.38	55.30	<i>CCl<sub>2</sub></i>	56.98	63.36
<i>C<sub>2</sub>H<sub>4</sub></i>	12.53	52.35	<i>CCl<sub>3</sub></i>	18.99	70.90
<i>C<sub>2</sub>H<sub>5</sub></i>	28.00	60.11	<i>CCl<sub>4</sub></i>	-22.93	74.01
<i>C<sub>2</sub>H<sub>6</sub></i>	-20.03	54.69	<i>CH</i>	141.94	43.70

TABLE A1. (continued)

Species	H <sup>0</sup> (298) Kcal/mole	S <sup>0</sup> (298) cal/mole K	Species	H <sup>0</sup> (298) Kcal/mole	S <sup>0</sup> (298) cal/mole K
<i>CH</i> <sup>+</sup>	388.65	40.98	<i>CO</i> <sub>2</sub> <sup>-</sup>	-105.46	57.46
<i>CH</i> <sub>2</sub>	92.45	46.69	<i>COS</i>	-33.07	55.30
<i>CH</i> <sub>2</sub> ( <i>S</i> )	101.46	45.08	<i>CS</i>	66.97	50.27
<i>CH</i> <sub>2</sub> <i>CHCCH</i>	69.11	67.30	<i>CS</i> <sub>2</sub>	27.94	56.83
<i>CH</i> <sub>2</sub> <i>CHCCH</i> <sub>2</sub>	74.11	75.28	<i>E</i>	0.00	4.98
<i>CH</i> <sub>2</sub> <i>CHCH</i> <sub>2</sub>	38.62	64.71	<i>F</i>	18.85	37.90
<i>CH</i> <sub>2</sub> <i>CHCHCH</i>	86.06	73.04	<i>F</i> <sub>2</sub>	0.00	48.42
<i>CH</i> <sub>2</sub> <i>CHCHCH</i> <sub>2</sub>	28.28	70.41	<i>F</i> <sub>2</sub> <i>SiNH</i>	-146.87	70.89
<i>CH</i> <sub>2</sub> <i>Cl</i> <sub>2</sub>	-22.82	64.54	<i>F</i> <sub>3</sub> <i>SiN</i>	-199.94	73.84
<i>CH</i> <sub>2</sub> <i>CO</i>	-12.39	57.76	<i>FNNF</i>	17.87	63.44
<i>CH</i> <sub>2</sub> <i>F</i> <sub>2</sub>	-107.67	58.89	<i>FNO</i> <sub>3</sub>	2.50	69.96
<i>CH</i> <sub>2</sub> <i>HCO</i>	5.99	63.97	<i>FO</i>	25.99	51.74
<i>CH</i> <sub>2</sub> <i>O</i>	-27.69	52.22	<i>FO</i> <sub>2</sub>	3.00	61.88
<i>CH</i> <sub>2</sub> <i>OH</i>	-4.10	58.85	<i>FSiN</i>	54.35	63.64
<i>CH</i> <sub>3</sub>	34.80	46.35	<i>Ga</i>	68.50	43.81
<i>CH</i> <sub>3</sub> <i>CC</i>	123.77	60.25	<i>Ga</i> <sub>2</sub> <i>H</i> <sub>6</sub>	31.49	69.03
<i>CH</i> <sub>3</sub> <i>CCC</i> <sub>2</sub>	74.31	80.32	<i>GaAs</i>	88.37	63.20
<i>CH</i> <sub>3</sub> <i>CCCH</i> <sub>3</sub>	40.92	73.33	<i>GaAs</i> (3, <i>C</i> )	245.65	99.96
<i>CH</i> <sub>3</sub> <i>CCH</i> <sub>2</sub>	61.06	69.22	<i>GaAs</i> (3, <i>L</i> )	256.15	127.70
<i>CH</i> <sub>3</sub> <i>CH</i> <sub>2</sub> <i>CCH</i>	44.73	71.41	<i>GaAs</i> (5, <i>C</i> )	357.61	130.45
<i>CH</i> <sub>3</sub> <i>CHCH</i>	64.72	68.71	<i>GaAs</i> (5, <i>L</i> )	419.83	193.42
<i>CH</i> <sub>3</sub> <i>Cl</i>	-19.99	55.95	<i>GaEt</i>	17.74	81.57
<i>CH</i> <sub>3</sub> <i>CO</i>	-5.40	63.71	<i>GaEt</i> <sub>2</sub>	4.50	100.39
<i>CH</i> <sub>3</sub> <i>F</i>	-55.98	53.20	<i>GaEt</i> <sub>3</sub>	-17.04	112.94
<i>CH</i> <sub>3</sub> <i>HCO</i>	-39.49	63.02	<i>GaH</i>	54.78	49.16
<i>CH</i> <sub>3</sub> <i>O</i>	3.89	54.58	<i>GaH</i> <sub>2</sub>	40.98	55.98
<i>CH</i> <sub>3</sub> <i>OH</i>	-48.04	57.24	<i>GaH</i> <sub>3</sub>	26.99	54.48
<i>CH</i> <sub>3</sub> <i>SiCl</i> <sub>3</sub>	-126.35	83.85	<i>GaMe</i>	18.52	63.78
<i>CH</i> <sub>4</sub>	-17.89	44.44	<i>GaMe</i> <sub>2</sub>	16.42	80.52
<i>CHCl</i>	79.97	56.09	<i>GaMe</i> <sub>3</sub>	-10.87	87.84
<i>CHCl</i> <sub>3</sub>	-24.65	70.60	<i>H</i>	52.07	27.38
<i>CHF</i>	29.99	53.33	<i>H</i> <sup>+</sup>	367.01	26.00
<i>CHF</i> <sub>3</sub>	-166.54	62.00	<i>H</i> <sup>-</sup>	33.18	26.00
<i>Cl</i>	28.98	39.44	<i>H</i> <sub>2</sub>	0.00	31.19
<i>Cl</i> <sub>2</sub>	0.00	53.27	<i>H</i> <sub>2</sub> <i>AlMe</i>	6.00	61.70
<i>CN</i>	103.96	48.38	<i>H</i> <sub>2</sub> <i>AsMe</i>	24.04	64.83
<i>CN</i> <sup>+</sup>	430.70	50.96	<i>H</i> <sub>2</sub> <i>C</i> <sub>4</sub> <i>O</i>	54.57	66.40
<i>CN</i> <sup>-</sup>	14.49	46.79	<i>H</i> <sub>2</sub> <i>CCCC</i> <sub>2</sub>	111.27	72.91
<i>CN</i> <sub>2</sub>	112.95	54.01	<i>H</i> <sub>2</sub> <i>CCCC</i> <sub>2</sub>	75.46	65.10
<i>CNN</i>	139.64	55.33	<i>H</i> <sub>2</sub> <i>CCCH</i>	83.00	61.45
<i>CO</i>	-26.41	47.19	<i>H</i> <sub>2</sub> <i>CN</i>	59.08	53.57
<i>CO</i> <sub>2</sub>	-94.01	51.05	<i>H</i> <sub>2</sub> <i>CNH</i>	21.84	55.43

TABLE A1. (continued)

Species	H <sup>0</sup> (298) Kcal/mole	S <sup>0</sup> (298) cal/mole K	Species	H <sup>0</sup> (298) Kcal/mole	S <sup>0</sup> (298) cal/mole K
H <sub>2</sub> CNNO <sub>2</sub>	33.63	73.03	HGaMe	28.99	65.88
H <sub>2</sub> GaEt	-2.30	83.65	HGaMe <sub>2</sub>	2.50	79.47
H <sub>2</sub> GaMe	14.99	64.83	HMeGaEt	4.00	88.87
H <sub>2</sub> NF	-6.49	54.70	HN <sub>3</sub>	71.84	57.12
H <sub>2</sub> O	-57.78	45.08	HNCO	-24.89	57.03
H <sub>2</sub> O(L)	-68.29	16.70	HNF	31.98	54.95
H <sub>2</sub> O(S)	-69.93	10.70	HNF <sub>2</sub>	-13.79	60.03
H <sub>2</sub> O <sub>2</sub>	-32.52	55.63	HNO	23.79	52.70
H <sub>2</sub> S	-4.90	49.12	HNO <sub>3</sub>	-32.09	63.64
H <sub>2</sub> Si(NH <sub>2</sub> ) <sub>2</sub>	-37.14	72.35	HO <sub>2</sub>	2.50	54.70
H <sub>2</sub> SiN	149.13	59.49	HOCN	-2.28	59.21
H <sub>2</sub> SiNH	40.94	60.07	HONO	-18.33	59.56
H <sub>2</sub> SiNH <sub>2</sub>	28.08	65.76	HSi(NH <sub>2</sub> ) <sub>2</sub>	5.76	73.35
H <sub>2</sub> SiNH <sub>3</sub>	23.84	66.76	HSi(NH <sub>2</sub> ) <sub>3</sub>	-64.65	79.49
H <sub>2</sub> SiSiH <sub>2</sub>	62.84	66.87	HSiCl	16.99	59.77
H <sub>3</sub> AsGaEt <sub>3</sub>	-10.99	124.43	HSiN	92.95	54.73
H <sub>3</sub> AsGaMe <sub>3</sub>	-4.70	102.46	HSiNH	84.75	60.66
H <sub>3</sub> SiN	234.51	56.91	HSiNH <sub>2</sub>	26.28	60.03
H <sub>3</sub> SiNH	51.32	66.19	I * C <sub>3</sub> H <sub>7</sub>	18.19	60.07
H <sub>3</sub> SiSiH	80.17	66.84	Me <sub>2</sub> GaEt	-5.25	97.24
H <sub>3</sub> SiSiH <sub>3</sub>	19.16	68.03	MeGaEt	14.25	89.92
HAlMe	27.24	62.75	MeGaEt <sub>2</sub>	-7.32	106.66
HAlMe <sub>2</sub>	-6.72	75.30	N	112.90	36.59
HAsAlMe	56.48	83.64	N * C <sub>3</sub> H <sub>7</sub>	22.59	64.10
HAsGaEt	69.12	97.24	N <sub>2</sub>	0.00	45.75
HAsGaMe	69.97	87.84	N <sub>2</sub> H <sub>2</sub>	50.88	52.18
HAsMe	42.56	65.88	N <sub>2</sub> H <sub>3</sub>	36.77	54.59
HAsMe <sub>2</sub>	18.09	78.42	N <sub>2</sub> H <sub>4</sub>	22.78	57.00
HCCCHCCH	129.83	69.03	N <sub>2</sub> H <sub>4</sub> (L)	12.09	29.02
HCCO	42.43	60.71	N <sub>2</sub> O	19.60	52.52
HCCOH	20.42	58.67	N <sub>2</sub> O <sup>+</sup>	318.56	55.84
HCl	-22.06	44.62	N <sub>2</sub> O <sub>4</sub>	2.17	72.70
HCN	32.29	48.19	N <sub>3</sub>	98.96	54.08
HCNH	66.08	55.87	NCO	38.08	55.45
HCNO	38.41	53.77	NF	59.47	51.40
HCO	10.39	53.63	NFO	-15.69	59.25
HCO <sup>+</sup>	199.02	48.57	NFO <sub>2</sub>	-25.99	62.15
He	0.00	30.11	NH	85.17	43.27
He <sup>+</sup>	568.23	31.48	NH <sub>2</sub>	45.48	46.48
HF	-65.12	41.49	NH <sub>3</sub>	-10.97	46.01
HGaEt	22.89	83.64	NNH	58.54	53.60
HGaEt <sub>2</sub>	-2.30	100.46	NO	21.57	50.32

TABLE A1. (continued)

Species	H <sup>0</sup> (298) Kcal/mole	S <sup>0</sup> (298) cal/mole K	Species	H <sup>0</sup> (298) Kcal/mole	S <sup>0</sup> (298) cal/mole K
<i>NO</i> <sup>+</sup>	236.57	47.32	<i>SiCl</i> <sub>3</sub> <i>H</i>	-118.55	74.87
<i>NO</i> <sub>2</sub>	7.91	57.31	<i>SiCl</i> <sub>4</sub>	-158.34	79.06
<i>NO</i> <sub>2</sub> <sup>-</sup>	-48.43	56.49	<i>SiClH</i> <sub>3</sub>	-32.19	59.77
<i>NO</i> <sub>3</sub>	16.99	60.33	<i>SiF</i>	-12.41	52.69
<i>O</i>	59.53	38.45	<i>SiF(NH</i> <sub>2</sub> ) <sub>2</sub>	-95.30	77.67
<i>O</i> <sup>+</sup>	374.80	36.99	<i>SiF(NH</i> <sub>2</sub> ) <sub>3</sub>	-170.48	87.88
<i>O</i> <sup>-</sup>	24.31	37.67	<i>SiF</i> <sub>2</sub>	-149.80	61.36
<i>O</i> <sub>2</sub>	0.00	48.98	<i>SiF</i> <sub>2</sub> ( <i>NH</i> <sub>2</sub> ) <sub>2</sub>	-247.09	82.74
<i>O</i> <sub>2</sub> <sup>-</sup>	-11.61	50.04	<i>SiF</i> <sub>2</sub> <i>N</i>	-63.08	70.48
<i>O</i> <sub>3</sub>	34.09	57.05	<i>SiF</i> <sub>2</sub> <i>NH</i> <sub>2</sub>	-167.14	77.45
<i>OH</i>	9.31	43.86	<i>SiF</i> <sub>3</sub> <i>NH</i>	-237.33	67.74
<i>OH</i> <sup>+</sup>	314.67	43.64	<i>SiF</i> <sub>3</sub> <i>NH</i> <sub>2</sub>	-249.55	83.66
<i>OH</i> <sup>-</sup>	-34.31	41.17	<i>SiF</i> <sub>3</sub> <i>NH</i> <sub>2</sub>	-317.76	81.00
<i>S</i>	66.17	40.07	<i>SiF</i> <sub>3</sub> <i>NHSiH</i> <sub>3</sub>	-320.04	96.84
<i>S(L)</i>	0.44	8.77	<i>SiF</i> <sub>3</sub> <i>NSiH</i> <sub>3</sub>	-252.73	99.30
<i>S(S)</i>	0.00	7.62	<i>SiF</i> <sub>4</sub>	-385.83	67.52
<i>S</i> <sup>+</sup>	306.35	39.06	<i>SiFH</i> <sub>3</sub>	-85.47	56.98
<i>S-Triazine</i>	56.35	64.46	<i>SiFNH</i>	-13.48	68.92
<i>S</i> <sub>2</sub>	30.70	54.48	<i>SiFNH</i> <sub>2</sub>	-80.01	64.59
<i>SH</i>	33.29	46.71	<i>SiH</i>	91.66	44.18
<i>Si</i>	107.66	40.10	<i>SiH</i> <sub>2</sub>	64.77	49.47
<i>Si(L)</i>	11.58	10.62	<i>SiH</i> <sub>2</sub> <i>Cl</i>	7.80	62.27
<i>Si(NH</i> <sub>2</sub> ) <sub>3</sub>	-18.62	84.24	<i>SiH</i> <sub>2</sub> <i>F</i>	-42.15	59.68
<i>Si(NH</i> <sub>2</sub> ) <sub>4</sub>	-92.63	85.34	<i>SiH</i> <sub>2</sub> <i>F</i> <sub>2</sub>	-186.31	62.78
<i>Si(S)</i>	0.00	4.50	<i>SiH</i> <sub>3</sub>	47.41	51.78
<i>Si</i> <sub>2</sub>	140.94	54.87	<i>SiH</i> <sub>3</sub> <i>NH</i> <sub>2</sub>	-11.39	65.64
<i>Si</i> <sub>2</sub> <i>C</i>	127.95	57.86	<i>SiH</i> <sub>3</sub> <i>NHSiH</i> <sub>3</sub>	-14.31	85.92
<i>Si</i> <sub>2</sub> <i>F</i> <sub>6</sub>	-569.38	97.12	<i>SiH</i> <sub>3</sub> <i>NSiH</i> <sub>3</sub>	48.88	86.66
<i>Si</i> <sub>2</sub> <i>H</i> <sub>2</sub>	83.46	58.53	<i>SiH</i> <sub>4</sub>	8.10	48.88
<i>Si</i> <sub>2</sub> <i>H</i> <sub>3</sub>	105.66	65.48	<i>SiHCl</i> <sub>2</sub>	-34.29	70.27
<i>Si</i> <sub>2</sub> <i>H</i> <sub>5</sub>	55.68	68.82	<i>SiHF</i>	-35.69	57.04
<i>Si</i> <sub>2</sub> <i>H</i> <sub>6</sub>	19.09	64.50	<i>SiHF</i> <sub>2</sub>	-139.51	65.03
<i>Si</i> <sub>3</sub>	151.94	63.98	<i>SiHF</i> <sub>3</sub>	-288.52	66.62
<i>Si</i> <sub>3</sub> <i>H</i> <sub>8</sub>	28.89	81.52	<i>SiN</i>	115.50	51.93
<i>Si</i> <sub>3</sub> <i>N</i> <sub>4</sub> ( <i>A</i> )	-177.93	26.98	<i>SiNH</i>	38.38	51.64
<i>SiC</i>	171.94	50.91	<i>SiNH</i> <sub>2</sub>	48.65	58.54
<i>SiC(B)</i>	-17.49	3.98	<i>SN</i>	62.97	53.02
<i>SiC</i> <sub>2</sub>	146.94	56.53	<i>SO</i>	1.19	52.99
<i>SiCl</i>	37.88	56.77	<i>SO</i> <sub>2</sub>	-70.92	59.27
<i>SiCl</i> <sub>2</sub>	-40.28	67.17	<i>SO</i> <sub>3</sub>	-94.55	61.32
<i>SiCl</i> <sub>2</sub> <i>H</i> <sub>2</sub>	-74.47	68.37			
<i>SiCl</i> <sub>3</sub>	-76.47	75.47			

## APPENDIX B. DATA BASE LISTING IN THE CHEMKIN FORMAT

Chemkin expects the thermodynamic data in a specific format, which is essentially the same as that used by the NASA Complex Chemical Equilibrium Program.<sup>13</sup> In addition to the fourteen fit coefficients, the data base also contains the species' name, its elemental composition, its electronic charge, and an indication of its phase (gas, liquid or solid). The data for each species requires four formatted 80 column card images. Table B1 provides the data format specification.

**TABLE B1.**  
**FORMAT FOR THERMODYNAMIC DATA**

Card Number	Contents	Format	Card Column
1	Species name (must start in Column 1)	18A1	1 to 18
	Date (not used in the code)	6A1	19 to 24
	Atomic symbols and formula	4(2A1,I3)	25 to 44
	Phase of species (S, L, or G for solid, liquid, or gas, respectively)	A1	45
	Low temperature	E10.0	46 to 55
	High temperature	E10.0	56 to 65
	Common temperature (if needed) (blank for default)	E8.0	66 to 73
	Atomic symbols and formula (if needed) (blank for default)	2A1,I3	74 to 78
	The integer "1"	I1	80
2	Coefficients $a_1 - a_5$ in Eqs. (1-3), for upper temperature interval	5(E15.0)	1 to 75
	The integer "2"	I1	80
3	Coefficients $a_6, a_7$ for upper temperature interval, and $a_1, a_2$ , and $a_3$ for lower	5(E15.0)	1 to 75
	The integer "3"	I1	80
4	Coefficients $a_4, a_5, a_6, a_7$ for lower temperature interval	4(E15.0)	1 to 60
	The integer "4"	I1	80

## THERMO

	300.000	1000.000	5000.000					
AL	62987AL	1		G	0300.00	5000.00	0600.00	
0.02559589E+02	-0.10632239E-03	0.07202828E-06	-0.02121105E-09	0.02289429E-13	1	2		
0.03890214E+06	0.05234522E+02	0.02736825E+02	-0.05912374E-02	-0.04033937E-05	3			
0.02322343E-07	-0.01705599E-10	0.03886794E+06	0.04363879E+02		4			
AL2H6	62987AL	2H	6	G	0300.00	1500.00	0600.00	
0.02634884E+02	0.02135952E+00	0.03154151E-05	-0.07684674E-07	0.02335831E-10	2			
0.08871346E+05	0.09827515E+02	0.06800681E+02	0.05080744E+00	0.10397471E-04	3			
-0.11195819E-06	0.08459155E-09	0.10605371E+05	0.05554526E+03		4			
AL2ME6	62987AL	2C	6H	18	G	0300.00	1500.00	0600.00
0.01773147E+03	0.04935747E+00	0.11968535E-05	-0.16398263E-07	0.04890867E-10	2			
-0.03855560E+06	-0.05053298E+03	-0.07159750E+01	0.10671087E+00	0.02117604E-03	3			
-0.02193211E-05	0.16441438E-09	-0.03515546E+06	0.03890762E+03		4			
ALAS	62987AL	1AS	1	G	0300.00	1500.00	0600.00	
0.04790026E+02	-0.01908225E-03	-0.01983390E-05	0.02239358E-08	-0.06904706E-12	2			
0.05259290E+06	0.03259703E+02	0.05047764E+02	-0.06419947E-02	-0.14320714E-05	3			
0.04754390E-07	-0.03297621E-10	0.05254264E+06	0.01985205E+02		4			
ALH	62987AL	1H	1	G	0300.00	5000.00	1000.00	
0.03392644E+02	0.12153990E-02	-0.04676595E-05	0.08691624E-09	-0.06022668E-13	2			
0.03006845E+06	0.02758899E+02	0.03071503E+02	0.02165549E-01	-0.03275638E-04	3			
0.04136983E-07	-0.01877120E-10	0.03021221E+06	0.04548855E+02		4			
ALH2	62987AL	1H	2	G	0300.00	1500.00	0600.00	
0.04486543E+02	0.03128831E-01	-0.01969438E-05	-0.10160304E-08	0.03497468E-11	2			
0.01960959E+06	0.08167897E+01	0.02442136E+02	0.09915913E-01	0.02471082E-05	3			
-0.02119583E-06	0.01710233E-09	0.01997587E+06	0.10652699E+02		4			
ALH3	62987AL	1H	3	G	0300.00	1500.00	0600.00	
0.04186837E+02	0.06159249E-01	-0.03877593E-06	-0.02061928E-07	0.06600276E-11	2			
0.07908078E+05	0.05134396E+01	0.10083231E+01	0.16403245E-01	0.01976746E-04	3			
-0.03528558E-06	0.02753377E-09	0.08484656E+05	0.15858377E+02		4			
ALME	62987AL	1C	1H	3	G	0300.00	1500.00	0600.00
0.04662737E+02	0.07097939E-01	0.02520013E-05	-0.02114863E-07	0.06097489E-11	2			
0.08203227E+05	0.01769244E+02	0.02664176E+02	0.13249141E-01	0.02525847E-04	3			
-0.02394396E-06	0.01761854E-09	0.08574173E+05	0.11474494E+02		4			
ALME2	62987AL	1C	2H	6	G	0300.00	1500.00	0600.00
0.06481282E+02	0.14746049E-01	0.05816529E-05	-0.04621347E-07	0.13960405E-11	2			
0.03745072E+05	-0.02603325E+02	0.09494573E+01	0.03206353E+00	0.06134020E-04	3			
-0.06500042E-06	0.04911485E-09	0.04761408E+05	0.02419465E+03		4			
ALME3	62987AL	1C	3H	9	G	0300.00	1500.00	0600.00
0.06654948E+02	0.02455144E+00	0.11765745E-05	-0.07815023E-07	0.02255622E-10	2			
-0.13409524E+05	-0.03454481E+02	-0.07027567E+01	0.04682764E+00	0.11499028E-04	3			
-0.09160441E-06	0.06687293E-09	-0.12037989E+05	0.03232771E+03		4			
AR	120186AR	1		G	0300.00	5000.00	1000.00	
0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	2			
-0.07453750E+04	0.04366000E+02	0.02500000E+02	0.00000000E+00	0.00000000E+00	3			
0.00000000E+00	0.00000000E+00	-0.07453750E+04	0.04366000E+02		4			
AR+	121286AR	1E	-1	G	0300.00	5000.00	1000.00	
0.02864864E+02	-0.12035732E-03	-0.10651992E-07	0.09074839E-10	-0.09623876E-14	2			
0.01827230E+07	0.03543584E+02	0.02301341E+02	0.08035528E-02	-0.01758805E-05	3			
-0.01781093E-08	-0.08937268E-13	0.01829281E+07	0.06659358E+02		4			

AS	62987AS	1	G	0300.00	1500.00	0600.00	1		
0.02617010E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2		
0.03720454E+06	0.06995524E+02	0.02617010E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00		3		
0.00000000E+00	0.00000000E+00	0.03720454E+06	0.06995524E+02				4		
AS2	62987AS	2	G	0300.00	1500.00	0600.00	1		
0.04394201E+02	0.05389968E-02	-0.02379401E-05	-0.06541924E-09	0.05184186E-12			2		
0.02235093E+06	0.04897918E+02	0.03682891E+02	0.03121811E-01	-0.10740519E-05			3		
-0.05629472E-07	0.05178811E-10	0.02247355E+06	0.08283423E+02				4		
AS3	62987AS	3	G	0300.00	1500.00	0600.00	1		
0.07404036E+02	0.07818425E-02	-0.03918297E-05	-0.05203629E-09	0.06291907E-12			2		
0.03063825E+06	-0.03417323E+02	0.06403142E+02	0.04477098E-01	-0.01866642E-04			3		
-0.07394750E-07	0.07012752E-10	0.03080965E+06	0.13371355E+01				4		
AS4	62987AS	4	G	0300.00	1500.00	0600.00	1		
0.09695766E+02	0.13062585E-02	-0.05519564E-05	-0.02150873E-08	0.14579349E-12			2		
0.15717321E+05	-0.16188696E+02	0.07853760E+02	0.07916509E-01	-0.02329820E-04			3		
-0.15263119E-07	0.13774348E-10	0.16036290E+05	-0.07409755E+02				4		
ASALME	62987AS	1AL	1C	1H	3G	0300.00	1500.00	0600.00	1
0.07127107E+02	0.07357863E-01	0.02300796E-06	-0.02226398E-07	0.06927227E-11			2		
0.03273438E+06	-0.01847179E+02	0.04053423E+02	0.01726125E+00	0.01833498E-04			3		
-0.03386952E-06	0.02626980E-09	0.03329309E+06	0.12996653E+02				4		
ASALME2	62987AS	1AL	1C	2H	6G	0300.00	1500.00	0600.00	1
0.09909938E+02	0.14638499E-01	0.04118730E-05	-0.04444657E-07	0.13295010E-11			2		
0.02815111E+06	-0.15235312E+02	0.04808530E+02	0.03067687E+00	0.05048000E-04			3		
-0.05908099E-06	0.04462290E-09	0.02908816E+06	0.09471621E+02				4		
ASGAET	62987AS	1GA	1C	2H	5G	0300.00	1500.00	0600.00	1
0.09081073E+02	0.16746316E-01	0.12831301E-06	-0.05590435E-07	0.01781314E-10			2		
0.03807443E+06	-0.09142782E+02	0.06364698E+01	0.04382467E+00	0.06144686E-04			3		
-0.09491641E-06	0.07374197E-09	0.03960893E+06	0.03164673E+03				4		
ASGAET2	62987AS	1GA	1C	4H	10G	0300.00	1500.00	0600.00	1
0.10324288E+02	0.03073570E+00	0.10863354E-05	-0.09971948E-07	0.02945979E-10			2		
0.03039490E+06	-0.13164016E+02	-0.03539248E+01	0.06369772E+00	0.13597417E-04			3		
-0.12861423E-06	0.09572181E-09	0.03236903E+06	0.03865086E+03				4		
ASGAME	62987AS	1GA	1C	1H	3G	0300.00	1500.00	0600.00	1
0.07322183E+02	0.06995478E-01	0.10693509E-06	-0.01995283E-07	0.06040446E-11			2		
0.03949448E+06	-0.07416680E+01	0.04877266E+02	0.14825589E-01	0.16521240E-05			3		
-0.02712058E-06	0.02080195E-09	0.03994071E+06	0.11076703E+02				4		
ASGAME2	62987AS	1GA	1C	2H	6G	0300.00	1500.00	0600.00	1
0.09352436E+02	0.15048197E-01	0.05157975E-05	-0.04553518E-07	0.13487630E-11			2		
0.03735855E+06	-0.12181144E+02	0.04382076E+02	0.03056344E+00	0.05477067E-04			3		
-0.05834108E-06	0.04373509E-09	0.03827434E+06	0.11911109E+02				4		
ASGAMEH	62987AS	1GA	1C	1H	4G	0300.00	1500.00	0600.00	1
0.07842794E+02	0.09682097E-01	0.10603061E-06	-0.02991402E-07	0.09382673E-11			2		
0.04435297E+06	-0.05093455E+02	0.03585119E+02	0.02336317E+00	0.02873356E-04			3		
-0.04737894E-06	0.03674461E-09	0.04512702E+06	0.15471604E+02				4		
ASH	62987AS	1H	1		G	0300.00	1500.00	0600.00	1
0.03219848E+02	0.10012498E-02	-0.04874997E-08	-0.11076533E-09	-0.09254321E-13			2		
0.03008175E+06	0.06647311E+02	0.03865843E+02	-0.11575710E-02	-0.03494371E-05			3		
0.07079686E-07	-0.06014027E-10	0.02996829E+06	0.03549869E+02				4		

ASH2	62987AS	1H	2	G	0300.00	1500.00	0600.00	1	
	0.03428307E+02	0.03181140E-01	0.14604843E-06-0.07937145E-08	0.01694413E-11				2	
	0.02010282E+06	0.02904703E+02	0.03778945E+02	0.01759233E-01	0.08070806E-05			3	
	0.02358763E-07-0.03043521E-10	0.02004861E+06	0.12729740E+01					4	
ASH3	62987AS	1H	3	G	0300.00	1500.00	0600.00	1	
	0.04172022E+02	0.04371322E-01	0.02177574E-05-0.11832641E-08	0.04536373E-11				2	
	0.06882915E+05	0.02803476E+02	0.09446356E+01	0.15084686E-01	0.12016960E-05			3	
	-0.03397465E-06	0.02767656E-09	0.07459168E+05	0.01832267E+03				4	
ASME	62987AS	1C	1H	3	G	0300.00	1500.00	0600.00	1
	0.04657260E+02	0.06976297E-01	0.02147556E-05-0.02101159E-07	0.06082149E-11				2	
	0.02806422E+06	0.03409834E+02	0.02625270E+02	0.13252423E-01	0.02441628E-04			3	
	-0.02419566E-06	0.01786943E-09	0.02844080E+06	0.13273359E+02				4	
ASME2	62987AS	1C	2H	6	G	0300.00	1500.00	0600.00	1
	0.05981395E+02	0.15212837E-01	0.06993355E-05-0.04721619E-07	0.13699115E-11				2	
	0.14679847E+05	0.11927411E+01	0.13903998E+01	0.02923331E+00	0.06598870E-04			3	
	-0.05620559E-06	0.04130367E-09	0.15533022E+05	0.02349980E+03				4	
ASME3	62987AS	1C	3H	9	G	0300.00	1500.00	0600.00	1
	0.06347764E+02	0.02466454E+00	0.11546286E-05-0.07877435E-07	0.02202225E-10				2	
	-0.16173225E+04-0.06316786E+01	0.02667388E+01	0.04253171E+00	0.11651064E-04				3	
	-0.07914706E-06	0.05603126E-09-0.04685539E+04	0.02904590E+03					4	
C	121086C	1			G	0300.00	5000.00	1000.00	1
	0.02602087E+02-0.01787081E-02	0.09087041E-06-0.11499333E-10	0.03310844E-14					2	
	0.08542154E+06	0.04195177E+02	0.02498584E+02	0.08085776E-03-0.02697697E-05				3	
	0.03040729E-08-0.11066518E-12	0.08545878E+06	0.04753459E+02					4	
C(S)	121286C	1			S	0300.00	5000.00	1000.00	1
	0.14901664E+01	0.16621256E-02-0.06687204E-05	0.12908796E-09-0.09205334E-13					2	
	-0.07074018E+04-0.08717785E+02-0.06705661E+01	0.07181499E-01-0.05632921E-04					3		
	0.02142298E-07-0.04168562E-11-0.07339498E+03	0.02601595E+02						4	
C+	120186C	1E	-1		G	0300.00	5000.00	1000.00	1
	0.02511827E+02-0.01735978E-03	0.09504267E-07-0.02218851E-10	0.01862189E-14					2	
	0.02166772E+07	0.04286130E+02	0.02595384E+02-0.04068664E-02	0.06892366E-05				3	
	-0.05266488E-08	0.15083378E-12	0.02166628E+07	0.03895729E+02				4	
C-	121686C	1E	1		G	0300.00	5000.00	1000.00	1
	0.02990221E+02-0.09184596E-02	0.05055560E-05-0.07703410E-09	0.03163271E-13					2	
	0.06983931E+06	0.12594533E+01	0.02783902E+02-0.01774287E-01	0.03696760E-04				3	
	-0.03066693E-07	0.08637622E-11	0.06998511E+06	0.02726281E+02				4	
C2	121286C	2			G	0300.00	5000.00	1000.00	1
	0.04135978E+02	0.06531618E-03	0.01837099E-05-0.05295085E-09	0.04712137E-13				2	
	0.09967272E+06	0.07472923E+01	0.06996045E+02-0.07400601E-01	0.03234703E-04				3	
	0.04802535E-07-0.03295917E-10	0.09897487E+06-0.13862268E+02						4	
C2-	121286C	2E	1		G	0300.00	5000.00	1000.00	1
	0.03796891E+02	0.02530049E-02	0.09709118E-06-0.16148038E-10-0.03212893E-15					2	
	0.05207981E+06	0.16581468E+01	0.03468011E+02-0.02352874E-02	0.12439123E-05				3	
	0.04705960E-08-0.08164274E-11	0.05231215E+06	0.03886699E+02					4	
C2F6	82489C	2F	6		G	0300.00	5000.00	1000.00	1
	0.16020573E+02	0.06273007E-01-0.02797778E-04	0.05517547E-08-0.04004651E-12					2	
	-0.16756543E+06-0.05519459E+03	0.03577448E+02	0.03913670E+00-0.02714862E-03					3	
	0.04348459E-08	0.04007135E-10-0.16421741E+06	0.09098384E+02					4	

C2H	20387C	2H	1	G	0300.00	5000.00	1000.00	1	
	0.04427688E+02	0.02216268E-01	-0.06048952E-05	0.09882517E-09	-0.07351179E-13			2	
	0.06590415E+06	-0.11994418E+01	0.03050667E+02	0.06051674E-01	-0.04956634E-04			3	
	0.02804159E-07	-0.08193332E-11	0.06630011E+06	0.05954361E+02				4	
C2H2	121386C	2H	2	G	0300.00	5000.00	1000.00	1	
	0.04436770E+02	0.05376039E-01	-0.01912816E-04	0.03286379E-08	-0.02156709E-12			2	
	0.02566766E+06	-0.02800338E+02	0.02013562E+02	0.15190446E-01	-0.16163189E-04			3	
	0.09078992E-07	-0.01912746E-10	0.02612444E+06	0.08805378E+02				4	
C2H3	12787C	2H	3	G	0300.00	5000.00	1000.00	1	
	0.05933468E+02	0.04017745E-01	-0.03966739E-05	-0.14412666E-09	0.02378643E-12			2	
	0.03185434E+06	-0.08530313E+02	0.02459276E+02	0.07371476E-01	0.02109872E-04			3	
	-0.13216421E-08	-0.11847838E-11	0.03335225E+06	0.11556202E+02				4	
C2H4	121286C	2H	4	G	0300.00	5000.00	1000.00	1	
	0.03528418E+02	0.11485185E-01	-0.04418385E-04	0.07844600E-08	-0.05266848E-12			2	
	0.04428288E+05	0.02230389E+02	-0.08614880E+01	0.02796162E+00	-0.03388677E-03			3	
	0.02785152E-06	-0.09737879E-10	0.05573046E+05	0.02421148E+03				4	
C2H5	12387C	2H	5	G	0300.00	5000.00	1000.00	1	
	0.07190480E+02	0.06484077E-01	-0.06428064E-05	-0.02347879E-08	0.03880877E-12			2	
	0.10674549E+05	-0.14780892E+02	0.02690701E+02	0.08719133E-01	0.04419838E-04			3	
	0.09338703E-08	-0.03927773E-10	0.12870404E+05	0.12138195E+02				4	
C2H6	121686C	2H	6	G	0300.00	4000.00	1000.00	1	
	0.04825938E+02	0.13840429E-01	-0.04557258E-04	0.06724967E-08	-0.03598161E-12			2	
	-0.12717793E+05	-0.05239506E+02	0.14625388E+01	0.15494667E-01	0.05780507E-04			3	
	-0.12578319E-07	0.04586267E-10	-0.11239176E+05	0.14432295E+02				4	
C2HCl	112989C	2H	1CL	1	G	0300.00	5000.00	1000.00	1
	0.06295372E+02	0.03883113E-01	-0.15060494E-05	0.02700003E-08	-0.01830213E-12			2	
	0.02357278E+06	-0.08137063E+02	0.03618443E+02	0.13319791E-01	-0.13218222E-04			3	
	0.06092023E-07	-0.08879026E-11	0.02415385E+06	0.05050645E+02				4	
C2N	121286C	2N	1	G	0300.00	5000.00	1000.00	1	
	0.06151561E+02	0.15116498E-02	-0.06629362E-05	0.12861485E-09	-0.09160830E-13			2	
	0.06484318E+06	-0.08177850E+02	0.03498544E+02	0.08554433E-01	-0.06288697E-04			3	
	0.08638478E-08	0.04915996E-11	0.06556611E+06	0.05548374E+02				4	
C2N2	121286C	2N	2	G	0300.00	5000.00	1000.00	1	
	0.06548002E+02	0.03984707E-01	-0.16342164E-05	0.03038596E-08	-0.02111069E-12			2	
	0.03490716E+06	-0.09735790E+02	0.04265459E+02	0.11922569E-01	-0.13420142E-04			3	
	0.09192297E-07	-0.02778941E-10	0.03547887E+06	0.01713212E+02				4	
C2O	121286C	20	1	G	0300.00	5000.00	1000.00	1	
	0.04849809E+02	0.02947585E-01	-0.10907286E-05	0.01792562E-08	-0.11157585E-13			2	
	0.03282055E+06	-0.06453225E+01	0.03368850E+02	0.08241803E-01	-0.08765145E-04			3	
	0.05569262E-07	-0.15400086E-11	0.03317081E+06	0.06713314E+02				4	
C3	121286C	3		G	0300.00	5000.00	1000.00	1	
	0.03803709E+02	0.02253566E-01	-0.07704534E-05	0.13162939E-09	-0.08694264E-13			2	
	0.09736135E+06	0.06128062E+02	0.04345527E+02	0.12644661E-02	-0.04652557E-04			3	
	0.08695855E-07	-0.04243535E-10	0.09731403E+06	0.03519437E+02				4	
C3H2	121686C	3H	2	G	0300.00	5000.00	1000.00	1	
	0.06530853E+02	0.05870316E-01	-0.01720776E-04	0.02127498E-08	-0.08291910E-13			2	
	0.05115213E+06	-0.11227278E+02	0.02691077E+02	0.14803664E-01	-0.03250551E-04			3	
	-0.08644363E-07	0.05284877E-10	0.05219072E+06	0.08757391E+02				4	

C3H4	40687C	3H	4	G	0300.00	5000.00	1000.00	1
0.05729144E+02	0.12368045E-01	-0.04805626E-04	0.08601364E-08	-0.05812802E-12				2
0.02012984E+06	-0.09448668E+02	-0.02131968E+01	0.03358713E+00	-0.03804870E-03				3
0.02745838E-06	-0.08690044E-10	0.02162048E+06	0.02029392E+03					4
C3H4C	121686C	3H	4	G	0300.00	5000.00	1000.00	1
0.06699993E+02	0.10357372E-01	-0.03455116E-04	0.05065295E-08	-0.02668227E-12				2
0.03019905E+06	-0.13391933E+02	-0.02462104E+00	0.02319721E+00	-0.01847435E-04				3
-0.15927594E-07	0.08684615E-10	0.03233413E+06	0.02271659E+03					4
C3H4P	40687C	3H	4	G	0300.00	5000.00	1000.00	1
0.05511034E+02	0.12469562E-01	-0.04814164E-04	0.08573770E-08	-0.05771561E-12				2
0.01961967E+06	-0.10794748E+02	0.06271447E+01	0.03116179E+00	-0.03747663E-03				3
0.02964117E-06	-0.09987381E-10	0.02083492E+06	0.13468796E+02					4
C3H6	120186C	3H	6	G	0300.00	5000.00	1000.00	1
0.06732257E+02	0.14908336E-01	-0.04949899E-04	0.07212022E-08	-0.03766204E-12				2
-0.09235703E+04	-0.13313348E+02	0.14933071E+01	0.02092517E+00	0.04486794E-04				3
-0.16689121E-07	0.07158146E-10	0.10748264E+04	0.16145340E+02					4
C3H8	120186C	3H	8	G	0300.00	5000.00	1000.00	1
0.07525217E+02	0.01889034E+00	-0.06283924E-04	0.09179373E-08	-0.04812410E-12				2
-0.16464548E+05	-0.01784390E+03	0.08969208E+01	0.02668986E+00	0.05431425E-04				3
-0.02126000E-06	0.09243330E-10	-0.13954918E+05	0.01935533E+03					4
C3O2	121286C	30	2	G	0300.00	5000.00	1000.00	1
0.08098897E+02	0.05560039E-01	-0.02312264E-04	0.04340709E-08	-0.03036387E-12				2
-0.14214353E+05	-0.15219745E+02	0.04018127E+02	0.01836660E+00	-0.01907148E-03				3
0.11855871E-07	-0.03418747E-10	-0.13128236E+05	0.05582083E+02					4
C4	121286C	4		G	0300.00	5000.00	1000.00	1
0.06500180E+02	0.04228632E-01	-0.01790717E-04	0.03404812E-08	-0.02403978E-12				2
0.11434008E+06	-0.11488894E+02	0.02343028E+02	0.16429811E-01	-0.15279858E-04				3
0.07343826E-07	-0.15822743E-11	0.11545384E+06	0.09826204E+02					4
C4H	121686C	4H	1	G	0300.00	5000.00	1000.00	1
0.06242882E+02	0.06193682E-01	-0.02085931E-04	0.03082203E-08	-0.16364826E-13				2
0.07568019E+06	-0.07210806E+02	0.05023247E+02	0.07092375E-01	-0.06073762E-07				3
-0.02275752E-07	0.08086994E-11	0.07623812E+06	-0.06942594E+00					4
C4H2	121686C	4H	2	G	0300.00	5000.00	1000.00	1
0.09031407E+02	0.06047252E-01	-0.01948788E-04	0.02754863E-08	-0.13856080E-13				2
0.05294735E+06	-0.02385067E+03	0.04005191E+02	0.01981000E+00	-0.09865877E-04				3
-0.06635158E-07	0.06077413E-10	0.05424065E+06	0.01845736E+02					4
C4H6	120186C	4H	6	G	0300.00	5000.00	1000.00	1
0.08046583E+02	0.16485251E-01	-0.05522227E-04	0.08123593E-08	-0.04295078E-12				2
0.13701305E+05	-0.01800457E+03	0.03197108E+02	0.02025591E+00	0.06510192E-04				3
-0.16584423E-07	0.06400282E-10	0.15715203E+05	0.09895660E+02					4
C4H8	120386C	4H	8	G	0300.00	5000.00	1000.00	1
0.02053584E+02	0.03435050E+00	-0.15883196E-04	0.03308966E-07	-0.02536104E-11				2
-0.02139723E+05	0.15543201E+02	0.11811380E+01	0.03085338E+00	0.05086524E-04				3
-0.02465488E-06	0.11110192E-10	-0.01790400E+05	0.02106247E+03					4
C5	121286C	5		G	0300.00	5000.00	1000.00	1
0.08078081E+02	0.05743464E-01	-0.02436405E-04	0.04638916E-08	-0.03278909E-12				2
0.11470216E+06	-0.01953023E+03	0.02115273E+02	0.02326331E+00	-0.02109499E-03				3
0.09072734E-07	-0.15400926E-11	0.11627381E+06	0.10976027E+02					4

C5H	20387C	5H	1	G	0300.00	5000.00	1000.00	1
	0.08695749E+02	0.06054301E-01	-0.02016010E-04	0.02892892E-08	-0.14700996E-13			2
	0.09031069E+06	-0.02101594E+03	0.16348248E+01	0.02509538E+00	-0.12066364E-04			3
	-0.10465110E-07	0.08809988E-10	0.09212488E+06	0.15121937E+02				4
C5H12	20387C	5H	12	G	0300.00	4000.00	1000.00	1
	0.16677979E+02	0.02114483E+00	-0.03533321E-04	-0.05742202E-08	0.15159483E-12			2
	-0.02553670E+06	-0.06372940E+03	0.01877907E+02	0.04121645E+00	0.12532337E-04			3
	-0.03701536E-06	0.15255685E-10	-0.02003815E+06	0.01877256E+03				4
C5H2	20587C	5H	2	G	0300.00	5000.00	1000.00	1
	0.11329175E+02	0.07424056E-01	-0.02628188E-04	0.04082541E-08	-0.02301332E-12			2
	0.07878706E+06	-0.03617117E+03	0.03062321E+02	0.02709998E+00	-0.10091697E-04			3
	-0.12727451E-07	0.09167219E-10	0.08114969E+06	0.07071078E+02				4
C5H3	20387C	5H	3	G	0300.00	5000.00	1000.00	1
	0.10787622E+02	0.09539619E-01	-0.03206744E-04	0.04733323E-08	-0.02512135E-12			2
	0.06392904E+06	-0.03005444E+03	0.04328720E+02	0.02352480E+00	-0.05856723E-04			3
	-0.12154494E-07	0.07726478E-10	0.06588531E+06	0.04173258E+02				4
C5H6	20387C	5H	6	G	0300.00	5000.00	1000.00	1
	0.09689815E+02	0.01838262E+00	-0.06264884E-04	0.09393377E-08	-0.05087708E-12			2
	0.11021242E+05	-0.03122908E+03	-0.03196739E+02	0.04081361E+00	0.06816505E-05			3
	-0.03137459E-06	0.15772230E-10	0.15290676E+05	0.03869938E+03				4
C6H	121686C	6H	1	G	0300.00	5000.00	1000.00	1
	0.11587352E+02	0.07295362E-01	-0.02466008E-04	0.03407045E-08	-0.14981855E-13			2
	0.10314481E+06	-0.03172578E+03	0.04769848E+02	0.02457279E+00	-0.07561252E-04			3
	-0.14806908E-07	0.09768053E-10	0.10485231E+06	0.03241530E+02				4
C6H10	20387C	6H	10	G	0300.00	5000.00	1000.00	1
	0.15927771E+02	0.02374412E+00	-0.06908672E-04	0.08109777E-08	-0.02683122E-12			2
	-0.08642656E+05	-0.06525186E+03	-0.13942280E+01	0.04720693E+00	0.11960419E-04			3
	-0.04162895E-06	0.01740335E-09	-0.02217790E+05	0.03129603E+03				4
C6H14	20387C	6H	14	G	0300.00	4000.00	1000.00	1
	0.02280471E+03	0.02097989E+00	-0.03530674E-04	-0.05466245E-08	0.14789499E-12			2
	-0.03073756E+06	-0.09583162E+03	0.01836174E+02	0.05098461E+00	0.12595857E-04			3
	-0.04428362E-06	0.01872237E-09	-0.02292749E+06	0.02088145E+03				4
C6H2	121686C	6H	2	G	0300.00	5000.00	1000.00	1
	0.12756519E+02	0.08034381E-01	-0.02618215E-04	0.03725060E-08	-0.01878850E-12			2
	0.08075469E+06	-0.04041262E+03	0.05751085E+02	0.02636719E+00	-0.11667596E-04			3
	-0.10714498E-07	0.08790297E-10	0.08262012E+06	-0.04335532E+02				4
C6H3	20387C	6H	3	G	0300.00	5000.00	1000.00	1
	0.12761181E+02	0.10385573E-01	-0.03479192E-04	0.05109733E-08	-0.02690965E-12			2
	0.07477706E+06	-0.03891745E+03	0.05007089E+02	0.02692851E+00	-0.05919865E-04			3
	-0.15272335E-07	0.09408310E-10	0.07713200E+06	0.02225621E+02				4
C6H4	20387C	6H	4	G	0300.00	5000.00	1000.00	1
	0.10062741E+02	0.01690304E+00	-0.06473045E-04	0.11240806E-08	-0.07307566E-12			2
	0.05645373E+06	-0.02969310E+03	-0.13004846E+01	0.03866476E+00	-0.03643944E-04			3
	-0.02668580E-06	0.14509357E-10	0.06002907E+06	0.03124939E+03				4
C6H5	82489C	6H	5	G	0300.00	4000.00	1000.00	1
	0.15775887E+02	0.09651109E-01	-0.09429416E-05	-0.05469111E-08	0.10265216E-12			2
	0.03302698E+06	-0.06176280E+03	0.11435567E+00	0.03627324E+00	0.11582856E-05			3
	-0.02196964E-06	0.08463556E-10	0.03836054E+06	0.02380117E+03				4

C6H5(L)	82489C	6H	5	G	0300.00	4000.00	1000.00	1	
	0.01721540E+03	0.08621068E-01	-0.08221340E-05	-0.04752164E-08	0.08844086E-12			2	
	0.06385819E+06	-0.06139128E+03	0.04854268E+02	0.03031659E+00	0.01742892E-05			3	
	-0.01811010E-06	0.07392511E-10	0.06798733E+06	0.05854934E+02				4	
C6H5O	82489C	6H	50	1	G	0300.00	4000.00	1000.00	1
	0.01822638E+03	0.10039851E-01	-0.09915668E-05	-0.05672804E-08	0.10683716E-12			2	
	-0.02620846E+05	-0.07361390E+03	0.11074965E+01	0.03956945E+00	0.08497295E-05			3	
	-0.02436311E-06	0.09650659E-10	0.03159672E+05	0.01973496E+03				4	
C6H5OH	82489C	6H	60	1	G	0300.00	4000.00	1000.00	1
	0.01821632E+03	0.11424269E-01	-0.10966843E-05	-0.06427442E-08	0.11988930E-12			2	
	-0.02053664E+06	-0.07304233E+03	0.13914556E+01	0.03931957E+00	0.01777096E-04			3	
	-0.02277673E-06	0.08309659E-10	-0.14721809E+05	0.01917813E+03				4	
C6H6	20387C	6H	6		G	0300.00	5000.00	1000.00	1
	0.12910740E+02	0.01723296E+00	-0.05024210E-04	0.05893497E-08	-0.01947521E-12			2	
	0.03664511E+05	-0.05002699E+03	-0.03138012E+02	0.04723103E+00	-0.02962207E-04			3	
	-0.03262819E-06	0.01718691E-09	0.08890031E+05	0.03657573E+03				4	
C6H7	82489C	6H	7		G	0300.00	4000.00	1000.00	1
	0.01755221E+03	0.12270795E-01	-0.11857424E-05	-0.06959661E-08	0.13013259E-12			2	
	0.16245813E+05	-0.07166588E+03	0.04639166E+01	0.03975928E+00	0.02529095E-04			3	
	-0.02223792E-06	0.07557053E-10	0.02225169E+06	0.02235387E+03				4	
C8H	121686C	8H	1		G	0300.00	5000.00	1000.00	1
	0.14749907E+02	0.09931501E-01	-0.03374841E-04	0.04687592E-08	-0.02073536E-12			2	
	0.13994481E+06	-0.04892689E+03	0.04489507E+02	0.03521521E+00	-0.10193898E-04			3	
	-0.02197024E-06	0.14214164E-10	0.14259919E+06	0.03996225E+02				4	
C8H2	121686C	8H	2		G	0300.00	5000.00	1000.00	1
	0.15680213E+02	0.11154614E-01	-0.03724372E-04	0.05197891E-08	-0.02375550E-12			2	
	0.10811225E+06	-0.05571437E+03	0.04630427E+02	0.03937080E+00	-0.11480348E-04			3	
	-0.02562213E-06	0.16707913E-10	0.11082850E+06	0.08077425E+01				4	
CCL	112989C	1CL	1		G	0300.00	5000.00	1000.00	1
	0.04072804E+02	0.05508787E-02	-0.02319334E-05	0.04669038E-09	-0.03236856E-13			2	
	0.05909198E+06	0.03481073E+02	0.03188782E+02	0.02965197E-01	-0.02305370E-04			3	
	0.04866913E-08	0.0990141E-12	0.05932937E+06	0.08037628E+02				4	
CCL2	112989C	1CL	2		G	0300.00	5000.00	1000.00	1
	0.03501741E+02	0.05749397E-01	-0.02589721E-04	0.04783950E-08	-0.03188271E-12			2	
	0.02763633E+06	0.10829469E+02	0.02651916E+02	0.15169552E-01	-0.02230162E-03			3	
	0.15041039E-07	-0.03452951E-10	0.02739027E+06	0.13136703E+02				4	
CCL3	112989C	1CL	3		G	0300.00	5000.00	1000.00	1
	0.08639372E+02	0.15880909E-02	-0.07176410E-05	0.14271238E-09	-0.10407368E-13			2	
	0.06701065E+05	-0.14518221E+02	0.04866162E+02	0.11903691E-01	-0.07849049E-04			3	
	-0.14484371E-08	0.02169760E-10	0.07655364E+05	0.04781636E+02				4	
CCL4	112989C	1CL	4		G	0300.00	5000.00	1000.00	1
	0.11369968E+02	0.01933276E-01	-0.08832003E-05	0.01770067E-08	-0.12982896E-13			2	
	-0.15283466E+05	-0.02874324E+03	0.06286815E+02	0.15997799E-01	-0.10203526E-04			3	
	-0.03043311E-07	0.03546287E-10	-0.14032573E+05	-0.02850812E+02				4	
CH	121286C	1H	1		G	0300.00	5000.00	1000.00	1
	0.02196223E+02	0.02340381E-01	-0.07058201E-05	0.09007582E-09	-0.03855040E-13			2	
	0.07086723E+06	0.09178373E+02	0.03200202E+02	0.02072875E-01	-0.05134431E-04			3	
	0.05733890E-07	-0.01955533E-10	0.07045259E+06	0.03331587E+02				4	

CH+	121286C	1H	1E	-1	G	0300.00	5000.00	1000.00	1
	0.02753358E+02	0.15528998E-02	-0.05368453E-05	0.08921772E-09	-0.05416801E-13				2
	0.01948467E+07	0.04654892E+02	0.03327207E+02	0.13470505E-02	-0.03895861E-04				3
	0.05129390E-07	-0.02054575E-10	0.01946452E+07	0.14084738E+01					4
CH2	120186C	1H	2		G	0250.00	4000.00	1000.00	1
	0.03636407E+02	0.01933056E-01	-0.01687016E-05	-0.10098994E-09	0.01808255E-12				2
	0.04534134E+06	0.02156560E+02	0.03762237E+02	0.11598191E-02	0.02489585E-05				3
	0.08800836E-08	-0.07332435E-11	0.04536790E+06	0.01712577E+02					4
CH2(S)	31287C	1H	2		G	0300.00	4000.00	1000.00	1
	0.03552888E+02	0.02066788E-01	-0.01914116E-05	-0.11046733E-09	0.02021349E-12				2
	0.04984975E+06	0.01686570E+02	0.03971265E+02	-0.01699088E-02	0.10253689E-05				3
	0.02492550E-07	-0.01981266E-10	0.04989367E+06	0.05753207E+00					4
CH2CHCCH	82489C	4H	4		G	0300.00	4000.00	1000.00	1
	0.10697773E+02	0.06982014E-01	-0.06567747E-05	-0.03884517E-08	0.07200946E-12				2
	0.03034803E+06	-0.03128430E+03	0.03233893E+02	0.01865634E+00	0.12703205E-05				3
	-0.09410096E-07	0.02956110E-10	0.03301097E+06	0.09922676E+02					4
CH2CHCCH2	82489C	4H	5		G	0300.00	4000.00	1000.00	1
	0.11997762E+02	0.07990580E-01	-0.08098172E-05	-0.04568733E-08	0.08636911E-12				2
	0.03228493E+06	-0.03528494E+03	0.03879443E+02	0.01997663E+00	0.01872777E-04				3
	-0.09306953E-07	0.02386116E-10	0.03526859E+06	0.09842152E+02					4
CH2CHCH2	82489C	3H	5		G	0300.00	4000.00	1000.00	1
	0.09651539E+02	0.08075596E-01	-0.07965424E-05	-0.04650696E-08	0.08603281E-12				2
	0.15300955E+05	-0.02686773E+03	0.02276486E+02	0.01985564E+00	0.11238421E-05				3
	-0.10145757E-07	0.03441342E-10	0.01789496E+06	0.13725151E+02					4
CH2CHCHCH	82489C	4H	5		G	0300.00	4000.00	1000.00	1
	0.12865971E+02	0.07943369E-01	-0.08626466E-05	-0.04655635E-08	0.08951131E-12				2
	0.03783552E+06	-0.04182502E+03	0.02995240E+02	0.02288456E+00	0.01975471E-04				3
	-0.11482454E-07	0.03197823E-10	0.04142218E+06	0.12894539E+02					4
CH2CHCHCH2	120189C	4H	6		G	0300.00	4000.00	1000.00	1
	0.12544366E+02	0.09596525E-01	-0.09187012E-05	-0.05429640E-08	0.10053636E-12				2
	0.08597330E+05	-0.04217450E+03	0.01931624E+02	0.02479030E+00	0.03018071E-04				3
	-0.11546856E-07	0.02586623E-10	0.12554682E+05	0.01701999E+03					4
CH2CL2	112989C	1H	2CL	2	G	0300.00	5000.00	1000.00	1
	0.05917327E+02	0.06762395E-01	-0.02676163E-04	0.04856687E-08	-0.03316973E-12				2
	-0.13859256E+05	-0.03877739E+02	0.14232844E+01	0.02116658E+00	-0.02178088E-03				3
	0.13458726E-07	-0.03811649E-10	-0.12686636E+05	0.01893445E+03					4
CH2CO	121686C	2H	20	1	G	0300.00	5000.00	1000.00	1
	0.06038817E+02	0.05804840E-01	-0.01920953E-04	0.02794484E-08	-0.14588676E-13				2
	-0.08583402E+05	-0.07657581E+02	0.02974970E+02	0.12118712E-01	-0.02345045E-04				3
	-0.06466685E-07	0.03905649E-10	-0.07632636E+05	0.08673553E+02					4
CH2F2	82489C	1H	2F	2	G	0300.00	5000.00	1000.00	1
	0.04730052E+02	0.07997300E-01	-0.03186045E-04	0.05801159E-08	-0.03967925E-12				2
	-0.05637288E+06	-0.04954843E+01	0.03669433E+01	0.02168917E+00	-0.02441912E-03				3
	0.01942310E-06	-0.06978343E-10	-0.05510102E+06	0.02202214E+03					4
CH2HCO	1201860	1H	3C	2	G	0300.00	5000.00	1000.00	1
	0.05975670E+02	0.08130591E-01	-0.02743624E-04	0.04070304E-08	-0.02176017E-12				2
	0.04903218E+04	-0.05045251E+02	0.03409062E+02	0.10738574E-01	0.01891492E-04				3
	-0.07158583E-07	0.02867385E-10	0.15214766E+04	0.09558290E+02					4

CH2O	121286C	1H	20	1	G	0300.00	5000.00	1000.00	1
	0.02995606E+02	0.06681321E-01	-0.02628954E-04	0.04737153E-08	-0.03212517E-12				2
-0.15320369E+05	0.06912572E+02	0.16527311E+01	0.12631439E-01	-0.01888168E-03					3
0.02050031E-06	-0.08413237E-10	-0.14865404E+05	0.13784820E+02						4
CH2OH	120186H	3C	10	1	G	0250.00	4000.00	1000.00	1
	0.06327520E+02	0.03608270E-01	-0.03201547E-05	-0.01938750E-08	0.03509704E-12				2
-0.04474509E+05	-0.08329365E+02	0.02862628E+02	0.10015273E-01	-0.05285435E-05					3
-0.05138539E-07	0.02246041E-10	-0.03349678E+05	0.10397938E+02						4
CH3	121286C	1H	3		G	0300.00	5000.00	1000.00	1
	0.02844051E+02	0.06137974E-01	-0.02230345E-04	0.03785161E-08	-0.02452159E-12				2
0.16437809E+05	0.05452697E+02	0.02430442E+02	0.11124099E-01	-0.01680220E-03					3
0.16218288E-07	-0.05864952E-10	0.16423781E+05	0.06789794E+02						4
CH3CC	82489C	3H	3		G	0300.00	4000.00	1000.00	1
	0.07640221E+02	0.05233556E-01	-0.05053635E-05	-0.02919772E-08	0.05445700E-12				2
0.05909763E+06	-0.16295735E+02	0.03798751E+02	0.08749062E-01	0.02523014E-04					3
-0.15293730E-08	-0.14105619E-11	0.06077425E+06	0.05989223E+02						4
CH3CCCH2	82489C	4H	5		G	0300.00	4000.00	1000.00	1
	0.11565059E+02	0.08030297E-01	-0.07649450E-05	-0.04476533E-08	0.08313260E-12				2
0.03256813E+06	-0.03014066E+03	0.05068450E+02	0.15717475E-01	0.02968975E-04					3
-0.04990586E-07	-0.02984224E-11	0.03518855E+06	0.06791893E+02						4
CH3CCCH3	120189C	4H	6		G	0300.00	4000.00	1000.00	1
	0.11336582E+02	0.10057637E-01	-0.09511323E-05	-0.05660496E-08	0.10494509E-12				2
0.15476594E+05	-0.03350866E+03	0.04077105E+02	0.01703158E+00	0.04707490E-04					3
-0.03767239E-07	-0.02066962E-10	0.01859756E+06	0.08444801E+02						4
CH3CCH2	82489C	3H	5		G	0300.00	4000.00	1000.00	1
	0.09101018E+02	0.07964167E-01	-0.07884945E-05	-0.04562036E-08	0.08529212E-12				2
0.02670680E+06	-0.02150559E+03	0.03385811E+02	0.14045337E-01	0.03204127E-04					3
-0.03824120E-07	-0.09053742E-11	0.02909066E+06	0.11266487E+02						4
CH3CH2CCH	120189C	4H	6		G	0300.00	4000.00	1000.00	1
	0.12006946E+02	0.09576069E-01	-0.08995018E-05	-0.05369808E-08	0.09934174E-12				2
0.01729419E+06	-0.03802692E+03	0.03726043E+02	0.02053492E+00	0.03021439E-04					3
-0.08131812E-07	0.10952799E-11	0.02048821E+06	0.08538826E+02						4
CH3CHCH	82489C	3H	5		G	0300.00	4000.00	1000.00	1
	0.09209764E+02	0.07871412E-01	-0.07724522E-05	-0.04497357E-08	0.08377272E-12				2
0.02853967E+06	-0.02232369E+03	0.03161863E+02	0.15180997E-01	0.02722659E-04					3
-0.05177112E-07	0.05435286E-12	0.03095547E+06	0.11979733E+02						4
CH3CL	112989C	1H	3CL	1	G	0300.00	5000.00	1000.00	1
	0.03633875E+02	0.08664625E-01	-0.03343871E-04	0.05950130E-08	-0.04001401E-12				2
-0.11776588E+05	0.04430651E+02	0.04621901E+01	0.02068247E+00	-0.02553133E-03					3
0.02160310E-06	-0.07706816E-10	-0.10936672E+05	0.02032976E+03						4
CH3CO	120186C	2H	30	1	G	0300.00	5000.00	1000.00	1
	0.05612279E+02	0.08449886E-01	-0.02854147E-04	0.04238376E-08	-0.02268403E-12				2
-0.05187863E+05	-0.03274949E+02	0.03125278E+02	0.09778220E-01	0.04521448E-04					3
-0.09009462E-07	0.03193717E-10	-0.04108507E+05	0.11228854E+02						4
CH3F	82489C	1H	3F	1	G	0300.00	5000.00	1000.00	1
	0.03014978E+02	0.09314397E-01	-0.03611697E-04	0.06443728E-08	-0.04339594E-12				2
-0.02977838E+06	0.06323815E+02	0.02600910E+01	0.02000787E+00	-0.02662584E-03					3
0.02561176E-06	-0.09935237E-10	-0.02896232E+06	0.02031799E+03						4

CH3HCO	120186C	20	1H	4	G	0300.00	5000.00	1000.00	1
	0.05868650E+02	0.10794241E-01	-0.03645530E-04	0.05412912E-08	-0.02896844E-12				2
-0.02264568E+06	-0.06012946E+02	0.02505695E+02	0.13369907E-01	0.04671953E-04					3
-0.11281401E-07	0.04263566E-10	-0.02124588E+06	0.13350887E+02						4
CH3O	121686C	1H	30	1	G	0300.00	3000.00	1000.00	1
	0.03770799E+02	0.07871497E-01	-0.02656384E-04	0.03944431E-08	-0.02112616E-12				2
0.12783252E+03	0.02929575E+02	0.02106204E+02	0.07216595E-01	0.05338472E-04					3
-0.07377636E-07	0.02075610E-10	0.09786011E+04	0.13152177E+02						4
CH3OH	121686C	1H	40	1	G	0300.00	5000.00	1000.00	1
	0.04029061E+02	0.09376593E-01	-0.03050254E-04	0.04358793E-08	-0.02224723E-12				2
-0.02615791E+06	0.02378195E+02	0.02660115E+02	0.07341508E-01	0.07170050E-04					3
-0.08793194E-07	0.02390570E-10	-0.02535348E+06	0.11232631E+02						4
CH3SICL3	112989C	1H	3CL	3SI	1G	0300.00	1500.00	1000.00	1
	0.11803988E+02	0.07642902E-01	-0.09493348E-06	-0.01852654E-07	0.05302190E-11				2
-0.06773651E+06	-0.02794492E+03	0.04637712E+02	0.03733016E+00	-0.04798528E-03					3
0.03353132E-06	-0.09484405E-10	-0.06629348E+06	0.06524867E+02						4
CH4	121286C	1H	4		G	0300.00	5000.00	1000.00	1
	0.01683478E+02	0.10237236E-01	-0.03875128E-04	0.06785585E-08	-0.04503423E-12				2
-0.10080787E+05	0.09623395E+02	0.07787415E+01	0.01747668E+00	-0.02783409E-03					3
0.03049708E-06	-0.12239307E-10	-0.09825229E+05	0.13722195E+02						4
CHCL	112989C	1H	1CL	1	G	0300.00	5000.00	1200.00	1
	0.03216518E+02	0.05976969E-01	-0.02918238E-04	0.05912801E-08	-0.04297945E-12				2
0.03879839E+06	0.07793842E+02	0.02781262E+02	0.07805384E-01	-0.10637111E-04					3
0.10654407E-07	-0.03916796E-10	0.03916144E+06	0.10455153E+02						4
CHCL3	112989C	1H	1CL	3	G	0300.00	5000.00	1000.00	1
	0.08523544E+02	0.04480142E-01	-0.01837282E-04	0.03424891E-08	-0.02387283E-12				2
-0.15461167E+05	-0.15056193E+02	0.03437633E+02	0.01941496E+00	-0.16494730E-04					3
0.05196545E-07	-0.06939614E-12	-0.14161262E+05	0.10863299E+02						4
CHF	82489C	1H	1F	1	G	0300.00	5000.00	1000.00	1
	0.04242812E+02	0.02066316E-01	-0.06527951E-05	0.13887000E-09	-0.12133360E-13				2
0.13559817E+05	0.01680196E+02	0.03029060E+02	0.04850873E-01	-0.04971678E-04					3
0.05277968E-07	-0.02403154E-10	0.14014348E+05	0.08324101E+02						4
CHF3	82489C	1H	1F	3	G	0300.00	5000.00	1000.00	1
	0.06834333E+02	0.06248730E-01	-0.02575750E-04	0.04809112E-08	-0.03352074E-12				2
-0.08663771E+06	-0.10627405E+02	0.08725142E+01	0.02308431E+00	-0.02123718E-03					3
0.11144284E-07	-0.02909229E-10	-0.08496391E+06	0.02021498E+03						4
CL	42189CL	1			G	0300.00	5000.00	1000.00	1
	0.02920236E+02	-0.03597985E-02	0.12942943E-06	-0.02162776E-09	0.13765171E-14				2
0.13713381E+05	0.03262690E+02	0.02381576E+02	0.08891079E-02	0.04070475E-05					3
-0.02168943E-07	0.11608274E-11	0.13839987E+05	0.06021817E+02						4
CL2	42189CL	2			G	0300.00	5000.00	1000.00	1
	0.04274586E+02	0.03717336E-02	-0.01893489E-05	0.05337465E-09	-0.05057602E-13				2
-0.13311486E+04	0.02256946E+02	0.03439587E+02	0.02870774E-01	-0.02385870E-04					3
0.02892918E-08	0.02915057E-11	-0.11317875E+04	0.06471359E+02						4
CN	121286C	1N	1		G	0300.00	5000.00	1000.00	1
	0.03720119E+02	0.15183506E-03	0.01987381E-05	-0.03798371E-09	0.13282296E-14				2
0.05111626E+06	0.02888597E+02	0.03663204E+02	-0.11565290E-02	0.02163409E-04					3
0.01854208E-08	-0.08214695E-11	0.05128118E+06	0.03739015E+02						4

CN+	121286C	1N	1E	-1	G	0300.00	5000.00	1000.00	1
	0.03701463E+02	0.07482931E-02	-0.01790173E-05	0.02366368E-09	-0.14370368E-14				2
	0.02155966E+07	0.04108678E+02	0.03118657E+02	0.15532581E-02	-0.09487764E-05				3
	0.14795005E-08	-0.09096763E-11	0.02158512E+07	0.07456254E+02					4
CN-	121286C	1N	1E	1	G	0300.00	5000.00	1000.00	1
	0.02981276E+02	0.14647728E-02	-0.05672737E-05	0.10176226E-09	-0.06870930E-13				2
	0.06346098E+05	0.06171693E+02	0.03278995E+02	0.14641916E-02	-0.03925899E-04				3
	0.05629874E-07	-0.02473496E-10	0.06279509E+05	0.04568972E+02					4
CN2	121686C	1N	2		G	0300.00	5000.00	1000.00	1
	0.05567064E+02	0.02100501E-01	-0.09010517E-05	0.01718571E-08	-0.12062552E-13				2
	0.05489968E+06	-0.05630054E+02	0.03039963E+02	0.08812105E-01	-0.07605508E-04				3
	0.03554357E-07	-0.08746100E-11	0.05563268E+06	0.07555298E+02					4
CNN	121286C	1N	2		G	0300.00	5000.00	1000.00	1
	0.04785930E+02	0.02559553E-01	-0.10031326E-05	0.01807148E-08	-0.12273827E-13				2
	0.06870411E+06	-0.02953957E+01	0.03524436E+02	0.07271923E-01	-0.08272698E-04				3
	0.05628704E-07	-0.16415759E-11	0.06899647E+06	0.05932444E+02					4
CO	121286C	10	1		G	0300.00	5000.00	1000.00	1
	0.03025078E+02	0.14426885E-02	-0.05630827E-05	0.10185813E-09	-0.06910951E-13				2
	-0.14268350E+05	0.06108217E+02	0.03262451E+02	0.15119409E-02	-0.03881755E-04				3
	0.05581944E-07	-0.02474951E-10	-0.14310539E+05	0.04848897E+02					4
C02	121286C	10	2		G	0300.00	5000.00	1000.00	1
	0.04453623E+02	0.03140168E-01	-0.12784105E-05	0.02393996E-08	-0.16690333E-13				2
	-0.04896696E+06	-0.09553959E+01	0.02275724E+02	0.09922072E-01	-0.10409113E-04				3
	0.06866686E-07	-0.02117280E-10	-0.04837314E+06	0.10188488E+02					4
C02-	121286C	10	2E	1	G	0300.00	5000.00	1000.00	1
	0.04610574E+02	0.02532962E-01	-0.10701653E-05	0.02026770E-08	-0.14249581E-13				2
	-0.05479881E+06	0.14496295E+01	0.02637077E+02	0.07803230E-01	-0.08196187E-04				3
	0.06537897E-07	-0.02520220E-10	-0.05416772E+06	0.11889549E+02					4
COS	121286C	10	1S	1	G	0300.00	5000.00	1000.00	1
	0.05191924E+02	0.02506123E-01	-0.10243963E-05	0.01943914E-08	-0.13707999E-13				2
	-0.01846210E+06	-0.02825755E+02	0.02858530E+02	0.09515458E-01	-0.08884915E-04				3
	0.04220994E-07	-0.08557340E-11	-0.01785144E+06	0.09081989E+02					4
CS	121686C	1S	1		G	0300.00	5000.00	1000.00	1
	0.03737430E+02	0.08180451E-02	-0.03178918E-05	0.05356801E-09	-0.02886194E-13				2
	0.03247725E+06	0.03576556E+02	0.02938623E+02	0.02724351E-01	-0.02397706E-04				3
	0.01689500E-07	-0.06665050E-11	0.03273992E+06	0.07848720E+02					4
CS2	121286C	1S	2		G	0300.00	5000.00	1000.00	1
	0.05930515E+02	0.01813645E-01	-0.07492172E-05	0.14458920E-09	-0.10326380E-13				2
	0.12051166E+05	-0.06093909E+02	0.03566139E+02	0.08374927E-01	-0.06835704E-04				3
	0.02091214E-07	-0.06737193E-12	0.12688482E+05	0.06085967E+02					4
E	120186E	1			G	0300.00	5000.00	1000.00	1
	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2
	-0.07453749E+04	-0.11734026E+02	0.02500000E+02	0.00000000E+00	0.00000000E+00				3
	0.00000000E+00	0.00000000E+00	-0.07453750E+04	-0.11734026E+02					4
F	121286F	1			G	0300.00	5000.00	1000.00	1
	0.02687459E+02	-0.02010358E-02	0.08597957E-06	-0.16449738E-10	0.11661605E-14				2
	0.08722883E+05	0.03882212E+02	0.02913904E+02	-0.07336339E-02	0.05571015E-05				3
	-0.02666871E-08	0.08643255E-12	0.08651201E+05	0.02677115E+02					4

F2	121286F	2	G	0300.00	5000.00	1000.00	1		
0.04018308E+02	0.06221479E-02	-0.02420845E-05	0.04742076E-09	-0.03418141E-13			2		
-0.13007128E+04	0.11263273E+01	0.02940287E+02	0.03491491E-01	-0.02458207E-04			3		
0.01837073E-08	0.02850916E-11	-0.10104296E+04	0.06694194E+02				4		
F2SINH	42489SI	1N	1F	2H	1G	0300.00	3000.00	1000.00	1
0.10048301E+02	0.01983144E-01	-0.02703168E-05	-0.01767852E-08	0.04444367E-12			2		
-0.07739741E+06	-0.02303888E+03	0.04951547E+02	0.13296361E-01	-0.02098648E-04			3		
-0.10072757E-07	0.05552285E-10	-0.07597540E+06	0.03690891E+02				4		
F3SIN	22790F	3SI	1N	1	G	0300.00	4000.00	1000.00	1
0.11512423E+02	0.11150295E-02	-0.16054655E-06	-0.05271933E-09	0.11608998E-13			2		
-0.10459191E+06	-0.02981224E+03	0.06028419E+02	0.12786807E-01	-0.01878856E-04			3		
-0.09695426E-07	0.05184847E-10	-0.10299499E+06	-0.08217830E+01				4		
FNNF	42489F	2N	2		G	0300.00	3000.00	1000.00	1
0.07255211E+02	0.02274409E-01	-0.02793346E-05	-0.02203843E-08	0.05359234E-12			2		
0.06360352E+05	-0.10942477E+02	0.03127143E+02	0.10571342E-01	-0.09746113E-05			3		
-0.07208357E-07	0.03567978E-10	0.07615830E+05	0.11074648E+02				4		
FN03	121286F	1N	10	3	G	0300.00	5000.00	1000.00	1
0.09176275E+02	0.04219072E-01	-0.01835575E-04	0.03553717E-08	-0.02541078E-12			2		
-0.02118638E+05	-0.01934397E+03	0.02985786E+02	0.02094642E+00	-0.16527329E-04			3		
0.04318770E-07	0.16607836E-12	-0.04237215E+04	0.12667929E+02				4		
F0	121286F	10	1		G	0300.00	5000.00	1000.00	1
0.03913735E+02	0.07210714E-02	-0.02796614E-05	0.05337821E-09	-0.03720183E-13			2		
0.11801406E+05	0.03346367E+02	0.02879578E+02	0.03399121E-01	-0.02572854E-04			3		
0.07422381E-08	-0.04328053E-12	0.12096633E+05	0.08738887E+02				4		
F02	121286F	10	2		G	0300.00	5000.00	1000.00	1
0.05678971E+02	0.14424551E-02	-0.06229546E-05	0.11996118E-09	-0.08543416E-13			2		
-0.03861836E+04	-0.01941811E+02	0.03872542E+02	0.06409974E-01	-0.05517784E-04			3		
0.02232770E-07	-0.03876157E-11	0.11570760E+03	0.07406949E+02				4		
FSIN	42489SI	1N	1F	1	G	0300.00	3000.00	1000.00	1
0.06269572E+02	0.06747867E-02	-0.12419759E-06	-0.04970158E-09	0.14244521E-13			2		
0.02533350E+06	-0.04201141E+02	0.04269969E+02	0.05298358E-01	-0.11038015E-05			3		
-0.03962805E-07	0.02282982E-10	0.02587238E+06	0.06215038E+02				4		
GA	62987GA	1			G	0300.00	1500.00	0600.00	1
0.02679919E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			2		
0.03368804E+06	0.06788109E+02	0.02679919E+02	0.00000000E+00	0.00000000E+00			3		
0.00000000E+00	0.00000000E+00	0.03368803E+06	0.06788109E+02				4		
GA2H6	62987GA	2H	6		G	0300.00	1500.00	0600.00	1
0.06016247E+02	0.01788370E+00	-0.12042288E-06	-0.06487881E-07	0.02075367E-10			2		
0.13125479E+05	-0.05228029E+02	-0.03914560E+02	0.04965434E+00	0.07401903E-04			3		
-0.11241373E-06	0.08726339E-09	0.14930795E+05	0.04274882E+03				4		
GAAS	62987GA	1AS	1		G	0300.00	1500.00	0600.00	1
0.04471149E+02	0.04238449E-02	-0.02279404E-05	-0.04441172E-10	0.02618952E-12			2		
0.04313359E+06	0.06212470E+02	0.03967473E+02	0.02318966E-01	-0.11454521E-05			3		
-0.03411430E-07	0.03365821E-10	0.04321919E+06	0.08599628E+02				4		
GAAS(3,C)	62987GA	3AS	3		G	0300.00	1500.00	0600.00	1
0.14852467E+02	0.02959435E-01	-0.07124246E-05	-0.05316048E-08	0.12873211E-12			2		
0.11912617E+06	-0.03514144E+03	0.14701892E+02	0.03827728E-01	-0.02945747E-04			3		
0.02465370E-07	-0.15205979E-11	0.11914958E+06	-0.03445955E+03				4		

GAAS(3,L)	62987GA	3AS	3	G	0300.00	1500.00	0600.00	1	
0.13568498E+02	0.02802435E-01	-0.07969918E-05	-0.06437098E-08	0.15602546E-12				2	
0.12480055E+06	-0.13810628E+02	0.13412763E+02	0.03617689E-01	-0.02726208E-04				3	
0.01877183E-07	-0.12591780E-11	0.12482649E+06	-0.13091947E+02					4	
GAAS(5,C)	62987GA	5AS	5	G	0300.00	1500.00	0600.00	1	
0.02573672E+03	0.05523956E-01	-0.12034680E-05	-0.10437431E-08	0.02528930E-11				2	
0.01721381E+07	-0.08254488E+03	0.02546511E+03	0.07014337E-01	-0.04881356E-04				3	
0.03825484E-07	-0.02450420E-10	0.01721819E+07	-0.08130267E+03					4	
GAAS(5,L)	62987GA	5AS	5	G	0300.00	1500.00	0600.00	1	
0.03045793E+03	0.05403151E-01	-0.16494765E-05	-0.09968843E-08	0.02413154E-11				2	
0.02020691E+07	-0.07768010E+03	0.03015255E+03	0.07234394E-01	-0.06497993E-04				3	
0.05559584E-07	-0.03339653E-10	0.02021150E+07	-0.07630866E+03					4	
GAET	62987GA	1C	2H	5	G	0300.00	1500.00	0600.00	1
0.05932970E+02	0.13424544E-01	0.04110518E-05	-0.04286069E-07	0.12387095E-11				2	
0.06504863E+05	0.03090838E+02	0.01846399E+02	0.02592050E+00	0.05522393E-04				3	
-0.04977960E-06	0.03654361E-09	0.07264445E+05	0.02294638E+03					4	
GAET2	62987GA	1C	4H	10	G	0300.00	1500.00	0600.00	1
0.07213832E+02	0.03055227E+00	0.12494508E-05	-0.09990274E-07	0.02881965E-10				2	
-0.13921194E+04	-0.07795098E+00	-0.02162930E+02	0.05892512E+00	0.14471449E-04				3	
-0.11686023E-06	0.08526654E-09	0.03561840E+04	0.04552626E+03					4	
GAET3	62987GA	1C	6H	15	G	0300.00	1500.00	0600.00	1
0.08436453E+02	0.04804950E+00	0.02119157E-04	-0.15816849E-07	0.04571178E-10				2	
-0.13469963E+05	-0.06196490E+02	-0.06544288E+02	0.09332246E+00	0.02364121E-03				3	
-0.01874104E-05	0.13677210E-09	-0.10676594E+05	0.06666796E+03					4	
GAH	62987GA	1H	1	G	0300.00	1500.00	0600.00	1	
0.03232142E+02	0.13432469E-02	-0.04325498E-06	-0.02791841E-08	0.04973590E-12				2	
0.02656059E+06	0.05947896E+02	0.03524579E+02	0.03386213E-02	-0.02064013E-05				3	
0.03220998E-07	-0.02936132E-10	0.02651074E+06	0.04554066E+02					4	
GAH2	62987GA	1H	2	G	0300.00	1500.00	0600.00	1	
0.03762384E+02	0.03210792E-01	0.02180096E-06	-0.08908394E-08	0.02219062E-11				2	
0.01936646E+06	0.05783398E+02	0.03559710E+02	0.03676741E-01	0.06484499E-05				3	
-0.03109349E-07	0.15854136E-11	0.01940976E+06	0.06803081E+02					4	
GAH3	62987GA	1H	3	G	0300.00	1500.00	0600.00	1	
0.03345475E+02	0.06399313E-01	0.11229964E-06	-0.02065899E-07	0.05780202E-11				2	
0.12281851E+05	0.06394841E+02	0.01726153E+02	0.11247386E-01	0.02447526E-04				3	
-0.02026314E-06	0.14470000E-10	0.12586196E+05	0.14284450E+02					4	
GAME	62987GA	1C	1H	3	G	0300.00	1500.00	0600.00	1
0.04809857E+02	0.06824206E-01	0.02258235E-05	-0.02018341E-07	0.05736453E-11				2	
0.07558677E+05	0.02595904E+02	0.03054536E+02	0.12186402E-01	0.02332213E-04				3	
-0.02121866E-06	0.15442261E-10	0.07885868E+05	0.11128781E+02					4	
GAME2	62987GA	1C	2H	6	G	0300.00	1500.00	0600.00	1
0.07068372E+02	0.14216021E-01	0.05120694E-05	-0.04421986E-07	0.13096413E-11				2	
0.05453790E+05	-0.04173960E+02	0.02257655E+02	0.02916445E+00	0.05669861E-04				3	
-0.05709755E-06	0.04268905E-09	0.06341297E+05	0.01915435E+03					4	
GAME3	62987GA	1C	3H	9	G	0300.00	1500.00	0600.00	1
0.08410636E+02	0.02262803E+00	0.10430190E-05	-0.07049610E-07	0.02015307E-10				2	
-0.09087271E+05	-0.10722496E+02	0.02120238E+02	0.04161029E+00	0.09959505E-04				3	
-0.07846792E-06	0.05693396E-09	-0.07911968E+05	0.01988516E+03					4	

H	120186H	1		G	0300.00	5000.00	1000.00	1	
	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			2	
	0.02547162E+06	-0.04601176E+01	0.02500000E+02	0.00000000E+00	0.00000000E+00			3	
	0.00000000E+00	0.00000000E+00	0.02547162E+06	-0.04601176E+01				4	
H+	120186H	1E	-1	G	0300.00	5000.00	1000.00	1	
	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			2	
	0.01840334E+07	-0.11538620E+01	0.02500000E+02	0.00000000E+00	0.00000000E+00			3	
	0.00000000E+00	0.00000000E+00	0.01840334E+07	-0.11538621E+01				4	
H-	120186H	1E	1	G	0300.00	5000.00	1000.00	1	
	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			2	
	0.15961045E+05	-0.11524488E+01	0.02500000E+02	0.00000000E+00	0.00000000E+00			3	
	0.00000000E+00	0.00000000E+00	0.15961045E+05	-0.11524486E+01				4	
H2	121286H	2		G	0300.00	5000.00	1000.00	1	
	0.02991423E+02	0.07000644E-02	-0.05633828E-06	-0.09231578E-10	0.15827519E-14			2	
	-0.08350340E+04	-0.13551101E+01	0.03298124E+02	0.08249441E-02	-0.08143015E-05			3	
	-0.09475434E-09	0.04134872E-11	-0.10125209E+04	-0.03294094E+02				4	
H2ALME	62987AL	1C	1H	5	G	0300.00	1500.00	0600.00	1
	0.04898410E+02	0.13582233E-01	0.02611458E-05	-0.04575170E-07	0.13848023E-11			2	
	0.08743072E+04	-0.11131169E+01	-0.06283259E+01	0.03089530E+00	0.05774090E-04			3	
	-0.06488033E-06	0.04907111E-09	0.01889333E+05	0.02565779E+03				4	
H2ASME	62987AS	1C	1H	5	G	0300.00	1500.00	0600.00	1
	0.05686213E+02	0.02154421E+00	0.08185247E-05	-0.07069951E-07	0.02101522E-10			2	
	0.09331084E+05	-0.06513957E+02	-0.02113506E+02	0.04564229E+00	0.09983227E-04			3	
	-0.09399697E-06	0.07014021E-09	0.10771701E+05	0.03132610E+03				4	
H2C40	120189H	2C	40	1	G	0300.00	4000.00	1000.00	1
	0.10268878E+02	0.04896164E-01	-0.04885080E-05	-0.02708566E-08	0.05107013E-12			2	
	0.02346902E+06	-0.02815985E+03	0.04810971E+02	0.13139988E-01	0.09865073E-05			3	
	-0.06120720E-07	0.16400028E-11	0.02545803E+06	0.02113424E+02				4	
H2CCCCH	82489C	4H	3		G	0300.00	4000.00	1000.00	1
	0.11314095E+02	0.05014414E-01	-0.05350444E-05	-0.02825309E-08	0.05403279E-12			2	
	0.05181211E+06	-0.03062434E+03	0.06545799E+02	0.12424768E-01	0.05603226E-05			3	
	-0.05631141E-07	0.16652183E-11	0.05352502E+06	-0.04264082E+02				4	
H2CCCCH2	82489C	4H	4		G	0300.00	4000.00	1000.00	1
	0.10620828E+02	0.07199370E-01	-0.06806234E-05	-0.04021185E-08	0.07378498E-12			2	
	0.03358797E+06	-0.03193583E+03	0.03849007E+02	0.01713169E+00	0.16442703E-05			3	
	-0.07761590E-07	0.01947859E-10	0.03608372E+06	0.05732120E+02				4	
H2CCCH	82489C	3H	3		G	0300.00	4000.00	1000.00	1
	0.08831047E+02	0.04357194E-01	-0.04109066E-05	-0.02368723E-08	0.04376520E-12			2	
	0.03847419E+06	-0.02177919E+03	0.04754199E+02	0.11080277E-01	0.02793323E-05			3	
	-0.05479212E-07	0.01949629E-10	0.03988883E+06	0.05854549E+01				4	
H2CN	41687H	2C	1N	1	G	0300.00	4000.00	1000.00	1
	0.05209703E+02	0.02969291E-01	-0.02855589E-05	-0.16355504E-09	0.03043259E-12			2	
	0.02767711E+06	-0.04444478E+02	0.02851661E+02	0.05695233E-01	0.10711403E-05			3	
	-0.16226120E-08	-0.02351108E-11	0.02863782E+06	0.08992751E+02				4	
H2CNH	41687C	1H	3N	1	G	0300.00	4000.00	1000.00	1
	0.05221589E+02	0.04748525E-01	-0.04179158E-05	-0.02606612E-08	0.04703140E-12			2	
	0.08657219E+05	-0.04500776E+02	0.02365878E+02	0.06780570E-01	0.02422999E-04			3	
	-0.06157824E-08	-0.16150971E-11	0.09971141E+05	0.12307176E+02				4	

H2CNN02	41687H	2C	1N	20	2G	0300.00	4000.00	1000.00	1
	0.11407942E+02	0.04564542E-01	-0.04600304E-05	-0.02513538E-08	0.04782211E-12				2
	0.12421422E+05	-0.03165237E+03	0.03534316E+02	0.01811271E+00	0.02394017E-05				3
	-0.10800240E-07	0.04222725E-10	0.15090057E+05	0.11311378E+02					4
H2GAET	62987GA	1C	2H	7	G	0300.00	1500.00	0600.00	1
	0.07187273E+02	0.01867211E+00	0.06156157E-05	-0.06027763E-07	0.01797524E-10				2
	-0.04232757E+05	-0.04686699E+02	0.04124020E+01	0.03972971E+00	0.07979140E-04				3
	-0.08059233E-06	0.06040387E-09	-0.02983932E+05	0.02816147E+03					4
H2GAME	62987GA	1C	1H	5	G	0300.00	1500.00	0600.00	1
	0.05831604E+02	0.12228715E-01	0.03033669E-05	-0.03956941E-07	0.12254516E-11				2
	0.05189255E+05	-0.04446614E+02	0.05251130E+01	0.02904695E+00	0.04844148E-04				3
	-0.06097646E-06	0.04672763E-09	0.06158712E+05	0.02122148E+03					4
H2NF	42489H	2N	1F	1	G	0300.00	3000.00	1000.00	1
	0.04143658E+02	0.03805135E-01	-0.02771153E-05	-0.03589717E-08	0.07589549E-12				2
	-0.04891486E+05	0.02309362E+02	0.02597862E+02	0.05882104E-01	0.04938351E-05				3
	-0.01948600E-07	0.03634002E-11	-0.04301253E+05	0.10982895E+02					4
H2O	20387H	20	1		G	0300.00	5000.00	1000.00	1
	0.02672145E+02	0.03056293E-01	-0.08730260E-05	0.12009964E-09	-0.06391618E-13				2
	-0.02989921E+06	0.06862817E+02	0.03386842E+02	0.03474982E-01	-0.06354696E-04				3
	0.06968581E-07	-0.02506588E-10	-0.03020811E+06	0.02590232E+02					4
H2O(L)	120186H	20	1		L	0273.15	1000.00	1000.00	1
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2
	0.00000000E+00	0.00000000E+00	0.12712782E+02	-0.01766279E+00	-0.02255666E-03				3
	0.02082090E-05	-0.02407861E-08	-0.03748320E+06	-0.05911534E+03					4
H2O(S)	120186H	20	1		S	0200.00	0273.15	1000.00	1
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2
	0.00000000E+00	0.00000000E+00	-0.03926933E+00	0.01692042E+00	0.00000000E+00				3
	0.00000000E+00	0.00000000E+00	-0.03594958E+06	0.05693378E+01					4
H2O2	120186H	20	2		G	0300.00	5000.00	1000.00	1
	0.04573167E+02	0.04336136E-01	-0.14746888E-05	0.02348903E-08	-0.14316536E-13				2
	-0.01800696E+06	0.05011369E+01	0.03388753E+02	0.06569226E-01	-0.14850125E-06				3
	-0.04625805E-07	0.02471514E-10	-0.01766314E+06	0.06785363E+02					4
H2S	121286H	2S	1		G	0300.00	5000.00	1000.00	1
	0.02883147E+02	0.03827835E-01	-0.14233978E-05	0.02497998E-08	-0.16602733E-13				2
	-0.03480742E+05	0.07258161E+02	0.03071029E+02	0.05578261E-01	-0.10309669E-04				3
	0.12019529E-07	-0.04838369E-10	-0.03559826E+05	0.05935226E+02					4
H2SI(NH2)2	22790SI	1H	6N	2	G	0300.00	4000.00	1000.00	1
	0.13021791E+02	0.06465444E-01	-0.05816746E-05	-0.03484493E-08	0.06340675E-12				2
	-0.02357070E+06	-0.04132569E+03	0.05615307E+02	0.02079854E+00	-0.09999531E-05				3
	-0.12885246E-07	0.06091865E-10	-0.02126283E+06	0.16156578E+01					4
H2SIN	22790H	2SI	1N	1	G	0300.00	4000.00	1000.00	1
	0.06826533E+02	0.02125460E-01	-0.02343131E-05	-0.11663394E-09	0.02277273E-12				2
	0.07253672E+06	-0.10521624E+02	0.03549344E+02	0.07311004E-01	0.03249025E-05				3
	-0.03682945E-07	0.11215113E-11	0.07370656E+06	0.07565328E+02					4
H2SINH	42489SI	1N	1H	3	G	0300.00	3000.00	1000.00	1
	0.06588295E+02	0.04903194E-01	-0.04944719E-05	-0.05014630E-08	0.11394698E-12				2
	0.01809794E+06	-0.09522970E+02	0.02822195E+02	0.12455182E-01	-0.08350819E-05				3
	-0.07411813E-07	0.03579019E-10	0.01923616E+06	0.10547831E+02					4

H2SINH2	42489SI	1N	1H	4	G	0300.00	3000.00	1000.00	1
0.07392047E+02	0.05476841E-01	-0.04453276E-05	-0.05236661E-08	0.11383899E-12					2
0.11368581E+05	-0.11380495E+02	0.04053222E+02	0.11822311E-01	-0.04348128E-05					3
-0.06225818E-07	0.02798829E-10	0.12419705E+05	0.06562032E+02						4
H2SINH3	121386SI	1H	5N	1	G	0300.00	4000.00	1000.00	1
0.08711392E+02	0.05909106E-01	-0.05436615E-05	-0.03248350E-08	0.05960257E-12					2
0.08441694E+05	-0.01933470E+03	0.04269729E+02	0.11252245E-01	0.01951721E-04					3
-0.03578372E-07	-0.08372202E-12	0.10222041E+05	0.05876735E+02						4
H2SISIH2	42489SI	2H	4		G	0300.00	3000.00	1000.00	1
0.08986817E+02	0.05405047E-01	-0.05214021E-05	-0.05313742E-08	0.11887266E-12					2
0.02832747E+06	-0.02004478E+03	0.05133186E+02	0.12528548E-01	-0.04620421E-05					3
-0.06606075E-07	0.02864344E-10	0.02956915E+06	0.07605133E+01						4
H3ASGAET3	62987AS	1GA	1C	6H	18G	0300.00	1500.00	0600.00	1
0.08508501E+02	0.05632369E+00	0.02524140E-04	-0.01861451E-06	0.05372402E-10					2
-0.10855169E+05	-0.03399857E+02	-0.08974745E+02	0.10905161E+00	0.02811457E-03					3
-0.02195513E-05	0.15997339E-09	-0.07592761E+05	0.08165459E+03						4
H3ASGAME3	62987AS	1GA	1C	3H	12G	0300.00	1500.00	0600.00	1
0.11254990E+02	0.03159752E+00	0.11779036E-05	-0.10133524E-07	0.02947355E-10					2
-0.07280344E+05	-0.02238729E+03	0.12671606E+01	0.06214586E+00	0.13856307E-04					3
-0.12200444E-06	0.08982019E-09	-0.05425619E+05	0.02613306E+03						4
H3SIN	22790H	3SI	1N	1	G	0300.00	4000.00	1000.00	1
0.07964213E+02	0.03355633E-01	-0.03579695E-05	-0.01889818E-08	0.03650912E-12					2
0.11486972E+06	-0.01924110E+03	0.02790628E+02	0.11345662E-01	0.08321879E-05					3
-0.05845045E-07	0.01685969E-10	0.11673571E+06	0.09384630E+02						4
H3SINH	42489SI	1N	1H	4	G	0300.00	3000.00	1000.00	1
0.07697340E+02	0.05657943E-01	-0.05209306E-05	-0.05617966E-08	0.12635020E-12					2
0.02282005E+06	-0.13303793E+02	0.02778390E+02	0.15107111E-01	-0.06734260E-05					3
-0.08928515E-07	0.04115347E-10	0.02435913E+06	0.13093859E+02						4
H3SISIH	90589SI	2H	4		G	0300.00	2000.00	1000.00	1
0.07778291E+02	0.07255418E-01	-0.08123265E-05	-0.11682818E-08	0.03425139E-11					2
0.03742600E+06	-0.13484629E+02	0.02774192E+02	0.02555302E+00	-0.02883836E-03					3
0.02000737E-06	-0.06100616E-10	0.03861801E+06	0.11350098E+02						4
H3SISIH3	42489SI	2H	6		G	0300.00	3000.00	1000.00	1
0.10682729E+02	0.08221416E-01	-0.08096035E-05	-0.08337975E-08	0.01908205E-11					2
0.05316920E+05	-0.03082188E+03	0.03898289E+02	0.01977415E+00	0.01791014E-05					3
-0.10331682E-07	0.03931698E-10	0.07621719E+05	0.06227022E+02						4
HALME	62987AL	1C	1H	4	G	0300.00	1500.00	0600.00	1
0.04812273E+02	0.10296448E-01	0.02582807E-05	-0.03323596E-07	0.09884584E-11					2
0.11766730E+05	0.09557062E+01	0.11187894E+01	0.02180038E+00	0.04120785E-04					3
-0.04366690E-06	0.03273825E-09	0.12447363E+05	0.01886107E+03						4
HALME2	62987AL	1C	2H	7	G	0300.00	1500.00	0600.00	1
0.05705171E+02	0.01924317E+00	0.06377855E-05	-0.06346800E-07	0.01896799E-10					2
-0.06049864E+05	-0.06331378E+01	-0.14942614E+01	0.04158567E+00	0.08686772E-04					3
-0.08604142E-06	0.06447652E-09	-0.04722516E+05	0.03427724E+03						4
HASALME	62987AS	1AL	1C	1H	4G	0300.00	1500.00	0600.00	1
0.06956538E+02	0.10612781E-01	0.02440153E-05	-0.03297737E-07	0.10200039E-11					2
0.02582505E+06	-0.08625792E+01	0.02544858E+02	0.02465794E+00	0.03677807E-04					3
-0.05008893E-06	0.03848383E-09	0.02663010E+06	0.02046858E+03						4

HASGAET	62987AS	1GA	1C	2H	6G	0300.00	1500.00	0600.00	1
	0.06336445E+02	0.02340603E+00	0.09066638E-05	-0.07519059E-07	0.01828115E-10				2
	0.03184605E+06	0.05812180E+02	0.05642723E+02	0.02296738E+00	0.10948674E-04				3
	-0.02449038E-06	0.09602700E-10	0.03204717E+06	0.09675533E+02					4
HASGAME	62987AS	1GA	1C	1H	4G	0300.00	1500.00	0600.00	1
	0.07507970E+02	0.09277900E-01	0.01891931E-05	-0.02769886E-07	0.07996069E-11				2
	0.03253907E+06	-0.14226081E+01	0.04859126E+02	0.01750423E+00	0.02831995E-04				3
	-0.03107936E-06	0.02299468E-09	0.03302941E+06	0.11429521E+02					4
HASME	62987AS	1C	1H	4	G	0300.00	1500.00	0600.00	1
	0.05753261E+02	0.01841813E+00	0.07493312E-05	-0.05919916E-07	0.01726246E-10				2
	0.01880057E+06	-0.05360325E+02	-0.15750948E+00	0.03649094E+00	0.08332939E-04				3
	-0.07234666E-06	0.05330928E-09	0.01989791E+06	0.02335316E+03					4
HASME2	62987AS	1C	2H	7	G	0300.00	1500.00	0600.00	1
	0.05850436E+02	0.01841765E+00	0.08066844E-05	-0.05868715E-07	0.01726428E-10				2
	0.06450535E+05	0.03909152E+01	-0.02908405E+01	0.03729576E+00	0.08335854E-04				3
	-0.07455611E-06	0.05527881E-09	0.07587765E+05	0.03020451E+03					4
HCCHCCH	82489C	4H	3		G	0300.00	4000.00	1000.00	1
	0.10752738E+02	0.05381153E-01	-0.05549637E-05	-0.03052266E-08	0.05761740E-12				2
	0.06121419E+06	-0.02973025E+03	0.04153881E+02	0.01726287E+00	-0.02389374E-05				3
	-0.10187000E-07	0.04340504E-10	0.06338070E+06	0.06036506E+02					4
HCCO	32387H	1C	20	1	G	0300.00	4000.00	1000.00	1
	0.06758073E+02	0.02000400E-01	-0.02027607E-05	-0.10411318E-09	0.01965164E-12				2
	0.01901513E+06	-0.09071262E+02	0.05047965E+02	0.04453478E-01	0.02268282E-05				3
	-0.14820945E-08	0.02250741E-11	0.01965891E+06	0.04818439E+01					4
HCCOH	32387H	2C	20	1	G	0300.00	4000.00	1000.00	1
	0.07328324E+02	0.03336416E-01	-0.03024705E-05	-0.01781106E-08	0.03245168E-12				2
	0.07598258E+05	-0.14012140E+02	0.03899465E+02	0.09701075E-01	-0.03119309E-05				3
	-0.05537732E-07	0.02465732E-10	0.08701190E+05	0.04491874E+02					4
HCL	42189CL	1H	1		G	0300.00	5000.00	1000.00	1
	0.02755335E+02	0.14735811E-02	-0.04971254E-05	0.08108658E-09	-0.05072063E-13				2
	-0.11918058E+05	0.06515116E+02	0.03338534E+02	0.12682066E-02	-0.03666916E-04				3
	0.04703992E-07	-0.01836011E-10	-0.12131511E+05	0.03193555E+02					4
HCN	121286H	1C	1N	1	G	0300.00	5000.00	1000.00	1
	0.03650077E+02	0.03460998E-01	-0.12742788E-05	0.02217655E-08	-0.14771774E-13				2
	0.14983916E+05	0.02393220E+02	0.02490462E+02	0.08611280E-01	-0.10310342E-04				3
	0.07481498E-07	-0.02229109E-10	0.15208344E+05	0.07904981E+02					4
HCNH	41687C	1H	2N	1	G	0300.00	4000.00	1000.00	1
	0.04923292E+02	0.03332897E-01	-0.03370896E-05	-0.01901619E-08	0.03531825E-12				2
	0.03132669E+06	-0.16325088E+01	0.02759456E+02	0.06103386E-01	0.07713149E-05				3
	-0.02063093E-07	0.01931919E-11	0.03217247E+06	0.10574895E+02					4
HCNO	120186H	1C	1N	10	1G	0250.00	4000.00	1000.00	1
	0.06692412E+02	0.02368360E-01	-0.02371510E-05	-0.12755033E-09	0.02407137E-12				2
	0.01694736E+06	-0.12454345E+02	0.03184858E+02	0.09752316E-01	-0.12802028E-05				3
	-0.06163104E-07	0.03226275E-10	0.01797907E+06	0.06123843E+02					4
HCO	121286H	1C	10	1	G	0300.00	5000.00	1000.00	1
	0.03557271E+02	0.03345572E-01	-0.13350060E-05	0.02470572E-08	-0.01713850E-12				2
	0.03916324E+05	0.05552299E+02	0.02898329E+02	0.06199146E-01	-0.09623084E-04				3
	0.10898249E-07	-0.04574885E-10	0.04159922E+05	0.08983614E+02					4

HCO+	121286H	1C	10	1E	-1G	0300.00	5000.00	1000.00	1
	0.03692074E+02	0.03454732E-01	-0.13165244E-05	0.02323551E-08	-0.15541321E-13				2
	0.09890941E+06	0.02330722E+02	0.02496483E+02	0.08690658E-01	-0.10604453E-04				3
	0.07882791E-07	-0.02418385E-10	0.09915097E+06	0.08048177E+02					4
HE	120186HE	1			G	0300.00	5000.00	1000.00	1
	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2
	-0.07453750E+04	0.09153489E+01	0.02500000E+02	0.00000000E+00	0.00000000E+00				3
	0.00000000E+00	0.00000000E+00	-0.07453750E+04	0.09153488E+01					4
HE+	120186HE	1E	-1		G	0300.00	5000.00	1000.00	1
	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2
	0.02853426E+07	0.16084045E+01	0.02500000E+02	0.00000000E+00	0.00000000E+00				3
	0.00000000E+00	0.00000000E+00	0.02853426E+07	0.16084046E+01					4
HF	121286H	1F	1		G	0300.00	5000.00	1000.00	1
	0.02956767E+02	0.07721015E-02	-0.09899834E-06	-0.04993520E-10	0.14293306E-14				2
	-0.03361061E+06	0.04011673E+02	0.03431841E+02	0.04404165E-02	-0.08828452E-05				3
	0.06574516E-08	-0.02055909E-12	-0.03381977E+06	0.12382699E+01					4
HGAET	62987GA	1C	2H	6	G	0300.00	1500.00	0600.00	1
	0.06580151E+02	0.16101323E-01	0.05009545E-05	-0.05185148E-07	0.15240853E-11				2
	0.08765131E+05	-0.04046067E+01	0.11632838E+01	0.03282212E+00	0.06765717E-04				3
	-0.06509541E-06	0.04835806E-09	0.09767174E+05	0.02588269E+03					4
HGAET2	62987GA	1C	4H	11	G	0300.00	1500.00	0600.00	1
	0.06511306E+02	0.02819753E+00	0.14187506E-05	-0.09000947E-07	0.02572894E-10				2
	-0.04482180E+05	0.04709021E+02	-0.14865759E+01	0.05217640E+00	0.13563420E-04				3
	-0.10119820E-06	0.07319853E-09	-0.02985242E+05	0.04364749E+03					4
HGAME	62987GA	1C	1H	4	G	0300.00	1500.00	0600.00	1
	0.05318279E+02	0.09490931E-01	0.02277164E-05	-0.03005070E-07	0.09037830E-11				2
	0.12535338E+05	-0.10657105E+00	0.01784749E+02	0.02058861E+00	0.03548509E-04				3
	-0.04111927E-06	0.03108978E-09	0.13184225E+05	0.01700701E+03					4
HGAME2	62987GA	1C	2H	7	G	0300.00	1500.00	0600.00	1
	0.06759397E+02	0.14261030E-01	-0.11740239E-06	-0.05001401E-07	0.15027851E-11				2
	-0.14732646E+04	-0.02967135E+02	0.09039155E+01	0.03264779E+00	0.05389243E-04				3
	-0.06814504E-06	0.05150323E-09	-0.03978242E+04	0.02539304E+03					4
HMEGAET	62987GA	1C	3H	9	G	0300.00	1500.00	0600.00	1
	0.07025463E+02	0.02564787E+00	0.09619100E-05	-0.08403699E-07	0.02488960E-10				2
	-0.13613768E+04	-0.03319484E+02	-0.02079142E+02	0.05373076E+00	0.11810364E-04				3
	-0.10998548E-06	0.08189554E-09	0.03216961E+04	0.04086070E+03					4
HN3	82687H	1N	3		G	0300.00	4000.00	1000.00	1
	0.06023015E+02	0.02454362E-01	-0.02404279E-05	-0.13229726E-09	0.02474146E-12				2
	0.03394051E+06	-0.07015537E+02	0.03621003E+02	0.06030785E-01	0.04054460E-05				3
	-0.02545270E-07	0.06174280E-11	0.03482373E+06	0.06333769E+02					4
HNCO	31287H	1N	1C	10	1G	0300.00	4000.00	1000.00	1
	0.06211867E+02	0.02297137E-01	-0.02216128E-05	-0.12220438E-09	0.02272406E-12				2
	-0.14770725E+05	-0.08016633E+02	0.03694059E+02	0.06657236E-01	-0.05054468E-06				3
	-0.03473411E-07	0.13605694E-11	-0.13919758E+05	0.05712742E+02					4
HNF	42489H	1N	1F	1	G	0300.00	3000.00	1000.00	1
	0.04133219E+02	0.01912056E-01	-0.16253301E-06	-0.01726461E-08	0.03743691E-12				2
	0.14670521E+05	0.03292122E+02	0.03249760E+02	0.03261817E-01	0.04355642E-06				3
	-0.11002765E-08	0.02926757E-11	0.14991264E+05	0.08187434E+02					4

HNF2	42489H	1N	1F	2	G	0300.00	3000.00	1000.00	1
	0.05704866E+02	0.03049897E-01	-0.02826802E-05	-0.02923184E-08	0.06551055E-12				2
	-0.09107488E+05	-0.03941331E+02	0.02572812E+02	0.08762144E-01	-0.02326921E-05				3
	-0.05000826E-07	0.02143837E-10	-0.08086760E+05	0.13006810E+02					4
HNO	121286H	1N	10	1	G	0300.00	5000.00	1000.00	1
	0.03615144E+02	0.03212485E-01	-0.12603370E-05	0.02267297E-08	-0.15362358E-13				2
	0.10661911E+05	0.04810263E+02	0.02784402E+02	0.06609646E-01	-0.09300223E-04				3
	0.09437980E-07	-0.03753146E-10	0.10918779E+05	0.09035629E+02					4
HN03	121286H	1N	10	3	G	0300.00	5000.00	1000.00	1
	0.07003844E+02	0.05811493E-01	-0.02333788E-04	0.04288814E-08	-0.02959385E-12				2
	-0.01889952E+06	-0.10478628E+02	0.13531850E+01	0.02220024E+00	-0.01978811E-03				3
	0.08773908E-07	-0.16583844E-11	-0.01738562E+06	0.01851868E+03					4
H02	20387H	10	2		G	0300.00	5000.00	1000.00	1
	0.04072191E+02	0.02131296E-01	-0.05308145E-05	0.06112269E-09	-0.02841164E-13				2
	-0.15797270E+03	0.03476029E+02	0.02979963E+02	0.04996697E-01	-0.03790997E-04				3
	0.02354192E-07	-0.08089024E-11	0.01762273E+04	0.09222724E+02					4
HOCN	120186H	10	1C	1N	1G	0250.00	4000.00	1000.00	1
	0.05645607E+02	0.02298206E-01	-0.02162629E-05	-0.12148014E-09	0.02238636E-12				2
	-0.03178109E+05	-0.03590263E+02	0.03628292E+02	0.05664184E-01	-0.11702056E-06				3
	-0.02348638E-07	0.08016402E-11	-0.02475925E+05	0.07476825E+02					4
HONO	31787H	1N	10	2	G	0300.00	5000.00	1000.00	1
	0.05486892E+02	0.04218064E-01	-0.16491426E-05	0.02971876E-08	-0.02021148E-12				2
	-0.11268646E+05	-0.02997002E+02	0.02290413E+02	0.14099223E-01	-0.13678717E-04				3
	0.07498780E-07	-0.01876905E-10	-0.10431945E+05	0.13280769E+02					4
HSI(NH2)2	22790SI	1H	5N	2	G	0300.00	4000.00	1000.00	1
	0.11716773E+02	0.05339021E-01	-0.04667823E-05	-0.02824087E-08	0.05080915E-12				2
	-0.12641686E+04	-0.03245117E+03	0.06289698E+02	0.16750596E-01	-0.15208775E-05				3
	-0.10700650E-07	0.05538640E-10	0.03154770E+04	-0.03746008E+02					4
HSI(NH2)3	22790SI	1H	7N	3	G	0300.00	4000.00	1000.00	1
	0.16614058E+02	0.07395874E-01	-0.06440009E-05	-0.03918887E-08	0.07045959E-12				2
	-0.03859547E+06	-0.05865317E+03	0.07070983E+02	0.02754435E+00	-0.02603669E-04				3
	-0.01874567E-06	0.09778511E-10	-0.03582658E+06	-0.08209675E+02					4
HSICL	121986SI	1H	1CL	1	G	0300.00	2000.00	1000.00	1
	0.04900627E+02	0.01981752E-01	-0.03634646E-05	-0.02285211E-08	0.07633527E-12				2
	0.06914634E+05	0.13770041E+01	0.03072747E+02	0.09057843E-01	-0.11591338E-04				3
	0.08310476E-07	-0.02482999E-10	0.07324210E+05	0.10334904E+02					4
HSIN	22790H	1SI	1N	1	G	0300.00	4000.00	1000.00	1
	0.05746590E+02	0.11671186E-02	-0.13607424E-06	-0.05908616E-09	0.11746961E-13				2
	0.04484671E+06	-0.05931788E+02	0.04865176E+02	0.01775119E-01	0.04890869E-05				3
	0.03922382E-08	-0.07913276E-11	0.04526352E+06	-0.07134509E+01					4
HSINH	42489SI	1H	2N	1	G	0300.00	3000.00	1000.00	1
	0.06493435E+02	0.02567980E-01	-0.03126526E-05	-0.02577467E-08	0.06216479E-12				2
	0.04035934E+06	-0.07830112E+02	0.03566343E+02	0.08446736E-01	-0.07699952E-05				3
	-0.05270970E-07	0.02581065E-10	0.04124903E+06	0.07780791E+02					4
HSINH2	42489SI	1N	1H	3	G	0300.00	3000.00	1000.00	1
	0.06177894E+02	0.04689964E-01	-0.03583293E-05	-0.04457980E-08	0.09379187E-12				2
	0.10912773E+05	-0.07006672E+02	0.02716144E+02	0.12042781E-01	-0.09827195E-05				3
	-0.07408477E-07	0.03789792E-10	0.11907715E+05	0.11262523E+02					4

I*C3H7	120186C	3H	7	G	0300.00	5000.00	1000.00	1	
0.08063369E+02	0.15744876E-01	-0.05182391E-04	0.07477245E-08	-0.03854422E-12				2	
0.05313871E+05	-0.02192646E+03	0.01713299E+02	0.02542616E+00	0.15808083E-05				3	
-0.01821286E-06	0.08827710E-10	0.07535808E+05	0.12979008E+02					4	
ME2GAET	62987GA	1C	4H	11	G	0300.00	1500.00	0600.00	1
0.07174541E+02	0.03235532E+00	0.14951986E-05	-0.10482260E-07	0.03053961E-10				2	
-0.06383914E+05	-0.02026765E+02	-0.03218207E+02	0.06398884E+00	0.15545521E-04				3	
-0.12847095E-06	0.09441259E-09	-0.04451897E+05	0.04848091E+03					4	
MEGAET	62987GA	1C	3H	8	G	0300.00	1500.00	0600.00	1
0.06600990E+02	0.02284791E+00	0.10133754E-05	-0.07318045E-07	0.02140196E-10				2	
0.04071592E+05	0.05239051E+01	-0.08169937E+01	0.04554296E+00	0.10531326E-04				3	
-0.09079987E-06	0.06700563E-09	0.05448005E+05	0.03655501E+03					4	
MEGAET2	62987GA	1C	5H	13	G	0300.00	1500.00	0600.00	1
0.08123155E+02	0.03978908E+00	0.01690979E-04	-0.13084149E-07	0.03852598E-10				2	
-0.08091056E+05	-0.05039992E+02	-0.05607498E+02	0.08187357E+00	0.01920530E-03				3	
-0.01678978E-05	0.12433538E-09	-0.05546687E+05	0.06163371E+03					4	
N	120186N	1			G	0300.00	5000.00	1000.00	1
0.02450268E+02	0.10661458E-03	-0.07465337E-06	0.01879652E-09	-0.10259839E-14				2	
0.05611604E+06	0.04448758E+02	0.02503071E+02	-0.02180018E-03	0.05420529E-06				3	
-0.05647560E-09	0.02099904E-12	0.05609890E+06	0.04167566E+02					4	
N*C3H7	120186C	3H	7	G	0300.00	5000.00	1000.00	1	
0.07978290E+02	0.15761134E-01	-0.05173243E-04	0.07443892E-08	-0.03824978E-12				2	
0.07579402E+05	-0.01935611E+03	0.01922536E+02	0.02478927E+00	0.01810249E-04				3	
-0.01783265E-06	0.08582996E-10	0.09713281E+05	0.13992715E+02					4	
N2	121286N	2			G	0300.00	5000.00	1000.00	1
0.02926640E+02	0.14879768E-02	-0.05684760E-05	0.10097038E-09	-0.06753351E-13				2	
-0.09227977E+04	0.05980528E+02	0.03298677E+02	0.14082404E-02	-0.03963222E-04				3	
0.05641515E-07	-0.02444854E-10	-0.10208999E+04	0.03950372E+02					4	
N2H2	121286N	2H	2		G	0300.00	5000.00	1000.00	1
0.03371185E+02	0.06039968E-01	-0.02303853E-04	0.04062789E-08	-0.02713144E-12				2	
0.02418172E+06	0.04980585E+02	0.16179994E+01	0.13063122E-01	-0.01715711E-03				3	
0.16056079E-07	-0.06093638E-10	0.02467526E+06	0.13794670E+02					4	
N2H3	120186N	2H	3		G	0300.00	5000.00	1000.00	1
0.04441846E+02	0.07214270E-01	-0.02495684E-04	0.03920564E-08	-0.02298949E-12				2	
0.16642211E+05	-0.04275204E+01	0.03174203E+02	0.04715907E-01	0.13348671E-04				3	
-0.01919684E-06	0.07487563E-10	0.01727269E+06	0.07557224E+02					4	
N2H4	121286N	2H	4		G	0300.00	5000.00	1000.00	1
0.04977317E+02	0.09595519E-01	-0.03547639E-04	0.06124299E-08	-0.04029795E-12				2	
0.09341219E+05	-0.02962989E+02	0.06442605E+00	0.02749729E+00	-0.02899451E-03				3	
0.01745239E-06	-0.04422282E-10	0.10451917E+05	0.02127789E+03					4	
N2H4(L)	90589H	4N	2		L	0300.00	0600.00	0450.00	1
0.08890683E+02	0.08330343E-01	0.04945549E-04	-0.04909251E-08	-0.03355824E-10				2	
0.03032250E+05	-0.03871433E+03	0.09047444E+02	0.09241592E-01	0.02263547E-04				3	
-0.08952247E-07	0.14868629E-10	0.02970392E+05	-0.03974033E+03					4	
N2O	121286N	20	1		G	0300.00	5000.00	1000.00	1
0.04718977E+02	0.02873713E-01	-0.11974958E-05	0.02250551E-08	-0.15753370E-13				2	
0.08165811E+05	-0.16572504E+01	0.02543057E+02	0.09492193E-01	-0.09792775E-04				3	
0.06263844E-07	-0.01901825E-10	0.08765100E+05	0.09511222E+02					4	

N20+	121286N	20	1E	-1	G	0300.00	5000.00	1000.00	1
	0.05398516E+02	0.02249478E-01	-0.09577056E-05	0.01823192E-08	-0.12844222E-13				2
	0.15848513E+06	-0.03733146E+02	0.03187228E+02	0.08350714E-01	-0.07894548E-04				3
	0.04597444E-07	-0.13810748E-11	0.15912794E+06	0.07779425E+02					4
N204	121286N	20	4		G	0300.00	5000.00	1000.00	1
	0.10482201E+02	0.05972272E-01	-0.02564043E-04	0.04916885E-08	-0.03490969E-12				2
	-0.02849988E+05	-0.02612289E+03	0.03624592E+02	0.02474708E+00	-0.02172874E-03				3
	0.09927103E-07	-0.02222817E-10	-0.09128241E+04	0.09457174E+02					4
N3	121286N	3			G	0300.00	5000.00	1000.00	1
	0.05208505E+02	0.02444507E-01	-0.10389415E-05	0.01977416E-08	-0.13956436E-13				2
	0.04796178E+06	-0.03612755E+02	0.02882218E+02	0.08930338E-01	-0.08539038E-04				3
	0.05045585E-07	-0.15212480E-11	0.04863468E+06	0.08481757E+02					4
NCO	121286N	1C	10	1	G	0300.00	5000.00	1000.00	1
	0.05012045E+02	0.02626773E-01	-0.11082433E-05	0.02093860E-08	-0.14603470E-13				2
	0.01737185E+06	-0.01830075E+02	0.02830320E+02	0.08871490E-01	-0.08945636E-04				3
	0.05876918E-07	-0.01907734E-10	0.01800543E+06	0.09498831E+02					4
NF	121286N	1F	1		G	0300.00	5000.00	1000.00	1
	0.03862176E+02	0.07551806E-02	-0.03044942E-05	0.05874447E-09	-0.04187479E-13				2
	0.02867242E+06	0.03457232E+02	0.02871947E+02	0.03312192E-01	-0.02691158E-04				3
	0.11219514E-08	-0.02475130E-11	0.02896257E+06	0.08640247E+02					4
NFO	121286N	1F	10	1	G	0300.00	5000.00	1000.00	1
	0.05174520E+02	0.01938472E-01	-0.08222701E-05	0.15642909E-09	-0.11044974E-13				2
	-0.09670935E+05	-0.05352460E+01	0.03352307E+02	0.07229966E-01	-0.06951136E-04				3
	0.03828526E-07	-0.10235582E-11	-0.09167035E+05	0.08854189E+02					4
NF02	121286N	1F	10	2	G	0300.00	5000.00	1000.00	1
	0.06816857E+02	0.03462639E-01	-0.14922156E-05	0.02869665E-08	-0.02041856E-12				2
	-0.15602619E+05	-0.09320129E+02	0.02447528E+02	0.15441095E-01	-0.13005952E-04				3
	0.04856383E-07	-0.06852266E-11	-0.14393999E+05	0.13283604E+02					4
NH	31387H	1N	1		G	0300.00	5000.00	1000.00	1
	0.02760249E+02	0.13753463E-02	-0.04451914E-05	0.07692791E-09	-0.05017592E-13				2
	0.04207828E+06	0.05857199E+02	0.03339758E+02	0.12530086E-02	-0.03491645E-04				3
	0.04218812E-07	-0.15576179E-11	0.04185047E+06	0.02507180E+02					4
NH2	121686N	1H	2		G	0300.00	5000.00	1000.00	1
	0.02961311E+02	0.02932699E-01	-0.09063600E-05	0.16172575E-09	-0.12042003E-13				2
	0.02191976E+06	0.05777878E+02	0.03432493E+02	0.03299540E-01	-0.06613600E-04				3
	0.08590947E-07	-0.03572046E-10	0.02177227E+06	0.03090110E+02					4
NH3	121386N	1H	3		G	0300.00	5000.00	1000.00	1
	0.02461904E+02	0.06059166E-01	-0.02004976E-04	0.03136003E-08	-0.01938317E-12				2
	-0.06493269E+05	0.07472097E+02	0.02204351E+02	0.10114765E-01	-0.14652648E-04				3
	0.14472350E-07	-0.05328509E-10	-0.06525488E+05	0.08127138E+02					4
NNH	120186N	2H	1		G	0250.00	4000.00	1000.00	1
	0.04415342E+02	0.16143879E-02	-0.16328943E-06	-0.08559846E-09	0.16147909E-13				2
	0.02788029E+06	0.09042888E+01	0.03501344E+02	0.02053586E-01	0.07170409E-05				3
	0.04921348E-08	-0.09671170E-11	0.02833347E+06	0.06391837E+02					4
NO	121286N	10	1		G	0300.00	5000.00	1000.00	1
	0.03245435E+02	0.12691383E-02	-0.05015890E-05	0.09169283E-09	-0.06275419E-13				2
	0.09800840E+05	0.06417293E+02	0.03376541E+02	0.12530634E-02	-0.03302750E-04				3
	0.05217810E-07	-0.02446262E-10	0.09817961E+05	0.05829590E+02					4

N0+	121286N	10	1E	-1	G	0300.00	5000.00	1000.00	1
0.02914888E+02	0.14993349E-02	-0.05727972E-05	0.10177767E-09	-0.06825390E-13					2
0.11818688E+06	0.06844346E+02	0.03297349E+02	0.14228899E-02	-0.04007441E-04					3
0.05670551E-07	-0.02446971E-10	0.11808338E+06	0.04749948E+02						4
N02	121286N	10	2		G	0300.00	5000.00	1000.00	1
0.04682859E+02	0.02462429E-01	-0.10422585E-05	0.01976902E-08	-0.13917168E-13					2
0.02261292E+05	0.09885985E+01	0.02670600E+02	0.07838500E-01	-0.08063864E-04					3
0.06161714E-07	-0.02320150E-10	0.02896290E+05	0.11612071E+02						4
N02-	121286N	10	2E	1	G	0300.00	5000.00	1000.00	1
0.05043114E+02	0.02166427E-01	-0.09455454E-05	0.01816313E-08	-0.12383945E-13					2
-0.02621553E+06	-0.14459051E+01	0.02448586E+02	0.08982507E-01	-0.07853431E-04					3
0.03927276E-07	-0.10716939E-11	-0.02545097E+06	0.12130600E+02						4
N03	121286N	10	3		G	0300.00	5000.00	1000.00	1
0.07120307E+02	0.03246228E-01	-0.14316134E-05	0.02797053E-08	-0.02013007E-12					2
0.05864479E+05	-0.12137301E+02	0.12210763E+01	0.01878797E+00	-0.13443212E-04					3
0.12746013E-08	0.13540601E-11	0.07473144E+05	0.01840202E+03						4
O	1201860	1			G	0300.00	5000.00	1000.00	1
0.02542059E+02	-0.02755061E-03	-0.03102803E-07	0.04551067E-10	-0.04368051E-14					2
0.02923080E+06	0.04920308E+02	0.02946428E+02	-0.16381665E-02	0.02421031E-04					3
-0.16028431E-08	0.03890696E-11	0.02914764E+06	0.02963995E+02						4
O+	1212860	1E	-1		G	0300.00	5000.00	1000.00	1
0.02501869E+02	-0.06107262E-04	0.07324307E-07	-0.03438353E-10	0.05506407E-14					2
0.01879552E+07	0.04372826E+02	0.02499272E+02	0.05820598E-04	-0.11209219E-07					3
0.08232108E-10	-0.01916378E-13	0.01879556E+07	0.04384825E+02						4
O-	905890	1E	1		G	0300.00	5000.00	1000.00	1
0.02559580E+02	-0.07147887E-03	0.03301804E-06	-0.06660944E-10	0.04900726E-14					2
0.11489346E+05	0.04426186E+02	0.02747263E+02	-0.05724860E-02	0.02712548E-05					3
0.02691511E-08	-0.02002357E-11	0.11443947E+05	0.03469852E+02						4
O2	1213860	2			G	0300.00	5000.00	1000.00	1
0.03697578E+02	0.06135197E-02	-0.12588420E-06	0.01775281E-09	-0.11364354E-14					2
-0.12339301E+04	0.03189165E+02	0.03212936E+02	0.11274864E-02	-0.05756150E-05					3
0.13138773E-08	-0.08768554E-11	-0.10052490E+04	0.06034737E+02						4
O2-	1212860	2E	1		G	0300.00	5000.00	1000.00	1
0.03883013E+02	0.07407872E-02	-0.02961776E-05	0.05724304E-09	-0.04086547E-13					2
-0.07121644E+05	0.02658211E+02	0.02872291E+02	0.03359716E-01	-0.02664886E-04					3
0.09807524E-08	-0.16709571E-12	-0.06829094E+05	0.07938372E+02						4
O3	1212860	3			G	0300.00	5000.00	1000.00	1
0.05429371E+02	0.01820380E-01	-0.07705607E-05	0.14992929E-09	-0.10755629E-13					2
0.15235267E+05	-0.03266386E+02	0.02462608E+02	0.09582781E-01	-0.07087359E-04					3
0.13633683E-08	0.02969647E-11	0.16061522E+05	0.12141870E+02						4
OH	1212860	1H	1		G	0300.00	5000.00	1000.00	1
0.02882730E+02	0.10139743E-02	-0.02276877E-05	0.02174683E-09	-0.05126305E-14					2
0.03886888E+05	0.05595712E+02	0.03637266E+02	0.01850910E-02	-0.16761646E-05					3
0.02387202E-07	-0.08431442E-11	0.03606781E+05	0.13588605E+01						4
OH+	1212860	1H	1E	-1	G	0300.00	5000.00	1000.00	1
0.02719058E+02	0.15085714E-02	-0.05029369E-05	0.08261951E-09	-0.04947452E-13					2
0.15763414E+06	0.06234536E+02	0.03326978E+02	0.13457859E-02	-0.03777167E-04					3
0.04687749E-07	-0.01780982E-10	0.15740294E+06	0.02744042E+02						4

OH-	1212860	1H	1E	1	G	0300.00	5000.00	1000.00	1
	0.02846204E+02	0.10418347E-02	-0.02416850E-05	0.02483215E-09	-0.07775605E-14				2
	-0.01807280E+06	0.04422712E+02	0.03390037E+02	0.07922381E-02	-0.01943429E-04				3
	0.02001769E-07	-0.05702087E-11	-0.01830493E+06	0.12498923E+01					4
S	121286S	1			G	0300.00	5000.00	1000.00	1
	0.02902148E+02	-0.05484546E-02	0.02764576E-05	-0.05017114E-09	0.03150684E-13				2
	0.03249423E+06	0.03838471E+02	0.03187329E+02	-0.15957763E-02	0.02005531E-04				3
	-0.15070814E-08	0.04931282E-11	0.03242259E+06	0.02414441E+02					4
S(L)	120186S	1			L	0388.36	2000.00	1000.00	1
	0.03603667E+02	0.09903341E-02	-0.10114410E-05	0.04053632E-08	-0.05667913E-12				2
	-0.08453839E+04	-0.16344708E+02	0.12706310E+02	0.09072521E+00	-0.01695178E-02				3
	0.13070636E-06	-0.03527615E-09	0.12346069E+04	0.05621016E+03					4
S(S)	120186S	1			S	0300.00	0388.36	1000.00	1
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2
	0.00000000E+00	0.00000000E+00	-0.05063702E+02	0.02881935E-01	-0.02133020E-03				3
	0.08478786E-05	-0.01734496E-07	0.07148263E+04	0.02871407E+03					4
S+	121286S	1E	-1		G	0300.00	5000.00	1000.00	1
	0.02404600E+02	0.02410908E-02	-0.02041779E-05	0.06592945E-09	-0.05756939E-13				2
	0.15352225E+06	0.05924256E+02	0.02366100E+02	0.09130767E-02	-0.02140283E-04				3
	0.02076177E-07	-0.07133859E-11	0.15350910E+06	0.05993094E+02					4
S-TRIAZINE	41687C	3N	3H	3	G	0300.00	4000.00	1000.00	1
	0.13036170E+02	0.07711820E-01	-0.07724374E-05	-0.04385191E-08	0.08298992E-12				2
	0.02251663E+06	-0.04777676E+03	0.04493492E+01	0.02728306E+00	0.02309304E-04				3
	-0.14968443E-07	0.04546753E-10	0.02703032E+06	0.02178518E+03					4
S2	121386S	1			G	0300.00	5000.00	1000.00	1
	0.03904443E+02	0.06925733E-02	-0.12330970E-06	0.08783809E-11	0.13746621E-14				2
	0.14256933E+05	0.04956834E+02	0.03157672E+02	0.03099480E-01	-0.15607465E-05				3
	-0.13578905E-08	0.11374435E-11	0.14391873E+05	0.08596062E+02					4
SH	121286S	1H	1		G	0300.00	5000.00	1000.00	1
	0.03053810E+02	0.12588843E-02	-0.04249169E-05	0.06929591E-09	-0.04281691E-13				2
	0.15882250E+05	0.05973551E+02	0.04133326E+02	-0.03787893E-02	-0.02777854E-04				3
	0.05370112E-07	-0.02394006E-10	0.15558623E+05	0.16115348E+00					4
SI	32989SI	1			G	0300.00	4000.00	1000.00	1
	0.02775845E+02	-0.06213257E-02	0.04843696E-05	-0.12756146E-09	0.11344818E-13				2
	0.05339790E+06	0.04543298E+02	0.03113515E+02	-0.02330991E-01	0.03518530E-04				3
	-0.02417573E-07	0.06391902E-11	0.05335061E+06	0.03009718E+02					4
SI(L)	90589SI	1			L	0300.00	4500.00	1000.00	1
	0.03271263E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2
	0.04855057E+05	-0.13290542E+02	0.03271263E+02	0.00000000E+00	0.00000000E+00				3
	0.00000000E+00	0.00000000E+00	0.04855058E+05	-0.13290542E+02					4
SI(NH2)3	42489SI	1N	3H	6	G	0300.00	3000.00	1000.00	1
	0.14065501E+02	0.07581744E-01	-0.05168510E-05	-0.06743626E-08	0.13979258E-12				2
	-0.14144028E+05	-0.04063873E+03	0.07598413E+02	0.02435266E+00	-0.04296202E-04				3
	-0.01756006E-06	0.10501017E-10	-0.12653434E+05	-0.07808647E+02					4
SI(NH2)4	22790SI	1N	4H	8	G	0300.00	4000.00	1000.00	1
	0.02032107E+03	0.08289798E-01	-0.07077612E-05	-0.04340724E-08	0.07747068E-12				2
	-0.05389855E+06	-0.07730464E+03	0.08454529E+02	0.03465772E+00	-0.04266782E-04				3
	-0.02495363E-06	0.13654663E-10	-0.05061518E+06	-0.15143013E+02					4

SI(S)	90589SI	1	S	0300.00	2500.00	1000.00	1	
0.02530275E+02	0.08522433E-02	-0.03223468E-05	0.12808208E-09	-0.01850849E-12			2	
-0.08395197E+04	-0.12514782E+02	0.05746418E+01	0.10264855E-01	-0.01775345E-03			3	
0.14575000E-07	-0.04491292E-10	-0.04969951E+04	-0.03400242E+02				4	
SI2	90589SI	2	G	0300.00	2000.00	1000.00	1	
0.04232196E+02	0.04315355E-02	-0.02964833E-05	0.09823294E-09	-0.12962688E-13			2	
0.06964651E+06	0.03308527E+02	0.02993750E+02	0.06053689E-01	-0.10158575E-04			3	
0.07909737E-07	-0.02346083E-10	0.06987498E+06	0.09151741E+02				4	
SI2C	112989C	1SI	2	G	0300.00	5000.00	1000.00	1
0.06334110E+02	0.12102520E-02	-0.06798289E-05	0.02244432E-08	-0.02280177E-12			2	
0.06227189E+06	-0.07770097E+02	0.04157246E+02	0.07031825E-01	-0.07263033E-04			3	
0.04633583E-07	-0.14934475E-11	0.06292421E+06	0.03635125E+02				4	
SI2F6	42489SI	2F	6	G	0300.00	3000.00	1000.00	1
0.01830047E+03	0.02868752E-01	-0.04545576E-05	-0.02497900E-08	0.06630658E-12			2	
-0.02928185E+07	-0.05760425E+03	0.09998134E+02	0.02170313E+00	-0.03875091E-04			3	
-0.16702523E-07	0.09407529E-10	-0.02905482E+07	-0.14228863E+02				4	
SI2H2	90589SI	2H	2	G	0300.00	2000.00	1000.00	1
0.05778180E+02	0.04070596E-01	-0.04259125E-05	-0.07920228E-08	0.02379752E-11			2	
0.03980520E+06	-0.05392375E+02	0.16247229E+01	0.14871029E-01	-0.08707160E-04			3	
-0.01699554E-09	0.10972211E-11	0.04095325E+06	0.16165730E+02				4	
SI2H3	90589SI	2H	3	G	0300.00	2000.00	1000.00	1
0.07257627E+02	0.05123859E-01	-0.07633465E-05	-0.06662471E-08	0.02053052E-11			2	
0.05062055E+06	-0.10314127E+02	0.03335404E+02	0.02155614E+00	-0.02933937E-03			3	
0.02287784E-06	-0.07272827E-10	0.05146157E+06	0.08656853E+02				4	
SI2H5	90589SI	2H	5	G	0300.00	2000.00	1000.00	1
0.08451010E+02	0.09286371E-01	-0.10911831E-05	-0.14423673E-08	0.04250824E-11			2	
0.02472718E+06	-0.01710331E+03	0.15788481E+01	0.03549382E+00	-0.04267511E-03			3	
0.03059177E-06	-0.09360425E-10	0.02630549E+06	0.16720734E+02				4	
SI2H6	90589SI	2H	6	G	0300.00	2000.00	1000.00	1
0.08882090E+02	0.11513955E-01	-0.12162159E-05	-0.01905085E-07	0.05542379E-11			2	
0.05967241E+05	-0.02265611E+03	0.05301921E+01	0.04184055E+00	-0.04685249E-03			3	
0.03179525E-06	-0.09484526E-10	0.07950597E+05	0.01880453E+03				4	
SI3	32989SI	3		G	0300.00	4000.00	1000.00	1
0.07021584E+02	0.06981538E-02	-0.04818729E-05	0.01720754E-08	-0.01927024E-12			2	
0.07429956E+06	-0.08179232E+02	0.05312161E+02	0.05920180E-01	-0.05075224E-04			3	
0.05303866E-08	0.07031630E-11	0.07469501E+06	0.04036452E+01				4	
SI3H8	90589SI	3H	8	G	0300.00	2000.00	1000.00	1
0.13422770E+02	0.15636323E-01	-0.01936565E-04	-0.02388329E-07	0.07120030E-11			2	
0.09165887E+05	-0.04163000E+03	0.06319791E+01	0.06412995E+00	-0.07772444E-03			3	
0.05486969E-06	-0.16460971E-10	0.12092580E+05	0.02133318E+03				4	
SI3N4(A)	42589N	4SI	3	S	0300.00	3000.00	1000.00	1
0.09667453E+02	0.11927212E-01	-0.01709281E-04	-0.10846074E-08	0.02713018E-11			2	
-0.09324734E+06	-0.04556492E+03	0.06631384E+02	0.02293928E+00	-0.02152875E-03			3	
0.01766237E-06	-0.06632214E-10	-0.09241684E+06	-0.03021795E+03				4	
SIC	112989C	1SI	1	G	0300.00	5000.00	1000.00	1
0.05024270E+02	-0.04920894E-02	0.03109315E-05	-0.06901344E-09	0.05215735E-13			2	
0.08531026E+06	-0.02478798E+02	0.02427812E+02	0.09551934E-01	-0.02796633E-04			3	
-0.13600122E-07	0.09196322E-10	0.08546512E+06	0.09179253E+02				4	

SIC(B)	112989C	1SI	1	S	0300.00	4000.00	1000.00	1	
0.03548056E+02	0.03636817E-01	-0.01734872E-04	0.03912869E-08	-0.03337952E-12				2	
-0.10188585E+05	-0.01967253E+03	-0.03551395E+01	0.15998806E-01	-0.13933268E-04				3	
0.03314914E-07	0.07825957E-11	-0.09294352E+05	-0.15153885E+00					4	
SIC2	112989C	2SI	1	G	0300.00	5000.00	1000.00	1	
0.05753725E+02	0.02067546E-01	-0.11325346E-05	0.03106456E-08	-0.02799936E-12				2	
0.07200461E+06	-0.05294926E+02	0.03647724E+02	0.08765100E-01	-0.10798686E-04				3	
0.07974287E-07	-0.02617042E-10	0.07258578E+06	0.05481049E+02					4	
SICL	121986SI	1CL	1	G	0300.00	2000.00	1000.00	1	
0.04258459E+02	0.04020317E-02	-0.02888145E-05	0.10097771E-09	-0.14110117E-13				2	
0.01775613E+06	0.04134521E+02	0.03096406E+02	0.05738623E-01	-0.09740903E-04				3	
0.07643597E-07	-0.02279178E-10	0.01796794E+06	0.09603212E+02					4	
SICL2	121986SI	1CL	2	G	0300.00	2000.00	1000.00	1	
0.06491204E+02	0.08242384E-02	-0.05767737E-05	0.01972405E-08	-0.02713757E-12				2	
-0.02232408E+06	-0.03570531E+02	0.03826666E+02	0.13082964E-01	-0.02234087E-03				3	
0.01760741E-06	-0.05267404E-10	-0.02183869E+06	0.08965448E+02					4	
SICL2H2	121986SI	1H	2CL	2	G	0300.00	2000.00	1000.00	1
0.07727079E+02	0.05034188E-01	-0.10957459E-05	-0.04419587E-08	0.16311241E-12				2	
-0.04028605E+06	-0.11708156E+02	0.11002086E+01	0.03262361E+00	-0.04691994E-03				3	
0.03494565E-06	-0.10362847E-10	-0.03892086E+06	0.02022693E+03					4	
SICL3	121986SI	1CL	3	G	0300.00	2000.00	1000.00	1	
0.09098097E+02	0.14053526E-02	-0.09317005E-05	0.02982296E-08	-0.03822010E-12				2	
-0.04140193E+06	-0.14550117E+02	0.04485690E+02	0.02241754E+00	-0.03794196E-03				3	
0.02973183E-06	-0.08861335E-10	-0.04055264E+06	0.07198771E+02					4	
SICL3H	121986SI	1H	1CL	3	G	0300.00	2000.00	1000.00	1
0.09663121E+02	0.03563367E-01	-0.12149114E-05	-0.16090094E-10	0.05641710E-12				2	
-0.06295557E+06	-0.01894777E+03	0.02883769E+02	0.03308240E+00	-0.05169241E-03				3	
0.03949918E-06	-0.11721043E-10	-0.06163323E+06	0.13374664E+02					4	
SICL4	121986SI	1CL	4	G	0300.00	2000.00	1000.00	1	
0.11709377E+02	0.01972091E-01	-0.12690771E-05	0.03900188E-08	-0.04756468E-12				2	
-0.08347808E+06	-0.02791153E+03	0.05252110E+02	0.03122067E+00	-0.05254593E-03				3	
0.04102707E-06	-0.12199071E-10	-0.08228177E+06	0.02575727E+02					4	
SICLH3	121986SI	1H	3CL	1	G	0300.00	2000.00	1000.00	1
0.05964237E+02	0.06278087E-01	-0.08205634E-05	-0.09280558E-08	0.02796642E-11				2	
-0.01854309E+06	-0.06395305E+02	0.05057173E+01	0.02703377E+00	-0.03301474E-03				3	
0.02302732E-06	-0.06778703E-10	-0.01730819E+06	0.02043167E+03					4	
SIF	42489SI	1F	1	G	0300.00	3000.00	1000.00	1	
0.04120066E+02	0.03548820E-02	-0.07200222E-06	-0.02190434E-09	0.06764591E-13				2	
-0.07561378E+05	0.02784246E+02	0.03144947E+02	0.02588557E-01	-0.05795912E-05				3	
-0.01807278E-07	0.10411718E-11	-0.07294439E+05	0.07876774E+02					4	
SIF(NH2)2	22790SI	1F	1N	2H	4G	0300.00	4000.00	1000.00	1
0.12879436E+02	0.04598535E-01	-0.04004440E-05	-0.02374189E-08	0.04255211E-12				2	
-0.05238278E+06	-0.03653418E+03	0.07210094E+02	0.01764697E+00	-0.02542059E-04				3	
-0.12422138E-07	0.06989787E-10	-0.05086706E+06	-0.07024622E+02					4	
SIF(NH2)3	42489SI	1N	3H	6F	1G	0300.00	3000.00	1000.00	1
0.16111795E+02	0.08329222E-01	-0.06023787E-05	-0.07470125E-08	0.15707311E-12				2	
-0.09137007E+06	-0.05098123E+03	0.08388268E+02	0.02746622E+00	-0.04455674E-04				3	
-0.01955732E-06	0.11407210E-10	-0.08947806E+06	-0.11381777E+02					4	

SIF2	42489SI	1F	2	G	0300.00	3000.00	1000.00	1	
0.06142470E+02	0.07807974E-02	-0.13393119E-06	-0.06264839E-09	0.01725138E-12				2	
-0.07744042E+06	-0.04712327E+02	0.03845345E+02	0.06038465E-01	-0.11677323E-05				3	
-0.04579553E-07	0.02607414E-10	-0.07681633E+06	0.07272983E+02					4	
SIF2(NH2)2	42489SI	1N	2H	4F	2G	0300.00	3000.00	1000.00	1
0.14414775E+02	0.06110646E-01	-0.04871145E-05	-0.05455935E-08	0.11727140E-12				2	
-0.12927572E+06	-0.04308682E+03	0.07634268E+02	0.02315843E+00	-0.04193827E-04				3	
-0.01715350E-06	0.10164619E-10	-0.12764102E+06	-0.08419031E+02					4	
SIF2N	42489SI	1N	1F	2	G	0300.00	3000.00	1000.00	1
0.08687337E+02	0.11934885E-02	-0.01992660E-05	-0.09951333E-09	0.02704383E-12				2	
-0.03463832E+06	-0.14940526E+02	0.05102583E+02	0.09456606E-01	-0.01819383E-04				3	
-0.07309616E-07	0.04178902E-10	-0.03367293E+06	0.03734423E+02					4	
SIF2NH2	42489SI	1N	1F	2H	2G	0300.00	3000.00	1000.00	1
0.09872415E+02	0.03722112E-01	-0.03271338E-05	-0.03321674E-08	0.07293692E-12				2	
-0.08751628E+06	-0.01899095E+03	0.05890444E+02	0.12851282E-01	-0.01863556E-04				3	
-0.08718963E-07	0.04848951E-10	-0.08644527E+06	0.01756162E+02					4	
SIF3	42489SI	1F	3		G	0300.00	3000.00	1000.00	1
0.08524790E+02	0.13237924E-02	-0.02104278E-05	-0.11495040E-09	0.03055301E-12				2	
-0.12235223E+06	-0.15502343E+02	0.04662868E+02	0.10087878E-01	-0.01805544E-04				3	
-0.07769299E-07	0.04377851E-10	-0.12129652E+06	0.04672966E+02					4	
SIF3NH	42489SI	1N	1F	3H	1G	0300.00	3000.00	1000.00	1
0.11637665E+02	0.02880768E-01	-0.03357310E-05	-0.02584594E-08	0.06162371E-12				2	
-0.12958909E+06	-0.02590717E+03	0.06013822E+02	0.15977294E-01	-0.02791466E-04				3	
-0.12141200E-07	0.06927415E-10	-0.12809741E+06	0.03316770E+02					4	
SIF3NH2	42489SI	1N	1F	3H	2G	0300.00	3000.00	1000.00	1
0.12109636E+02	0.04383282E-01	-0.04142245E-05	-0.03989090E-08	0.08958954E-12				2	
-0.16417679E+06	-0.03046928E+03	0.06229403E+02	0.01778015E+00	-0.02612304E-04				3	
-0.12672434E-07	0.07044556E-10	-0.16258489E+06	0.02045440E+01					4	
SIF3NHSIH3	42489SI	2N	1H	4F	3G	0300.00	3000.00	1000.00	1
0.16699406E+02	0.07789784E-01	-0.08110570E-05	-0.07650199E-08	0.01773956E-11				2	
-0.16734123E+06	-0.05080007E+03	0.06216046E+02	0.02939330E+00	-0.02717745E-04				3	
-0.01982877E-06	0.10027676E-10	-0.16422818E+06	0.04858261E+02					4	
SIF3NSIH3	42489SI	2N	1H	3F	3G	0300.00	3000.00	1000.00	1
0.15991462E+02	0.06371085E-01	-0.07256823E-05	-0.06292690E-08	0.14951566E-12				2	
-0.13311576E+06	-0.04495265E+03	0.06404371E+02	0.02601982E+00	-0.02491543E-04				3	
-0.01769542E-06	0.08919883E-10	-0.13025197E+06	0.06002945E+02					4	
SIF4	41389F	4SI	1		G	0300.00	2000.00	1000.00	1
0.09985301E+02	0.03532637E-01	-0.11973776E-05	-0.10365486E-09	0.08661585E-12				2	
-0.01977199E+07	-0.02472643E+03	0.02147416E+02	0.03402219E+00	-0.04756873E-03				3	
0.03252196E-06	0.08819304E-10	-0.01960449E+07	0.13463150E+02					4	
SIFH3	42489SI	1F	1H	3	G	0300.00	3000.00	1000.00	1
0.06799678E+02	0.04747086E-01	-0.04767066E-05	-0.04814665E-08	0.11077613E-12				2	
-0.04577024E+06	-0.12614326E+02	0.02032189E+02	0.13413632E-01	-0.02806381E-05				3	
-0.07803291E-07	0.03337474E-10	-0.04421627E+06	0.13187677E+02					4	
SIFNH	42489SI	1N	1F	1H	1G	0300.00	3000.00	1000.00	1
0.07163298E+02	0.15213245E-02	-0.15363371E-06	-0.11959331E-09	0.02684099E-12				2	
-0.09065496E+05	-0.06764144E+02	0.05390691E+02	0.06071319E-01	-0.13594903E-05				3	
-0.04267435E-07	0.02603153E-10	-0.08644237E+05	0.02272064E+02					4	

SIFNH2	22790F	1SI	1N	1H	2G	0300.00	4000.00	1000.00	1
	0.08017582E+02	0.03209103E-01	-0.03361364E-05	-0.01796536E-08	0.03385552E-12				2
	-0.04313426E+06	-0.14870236E+02	0.04214050E+02	0.11054231E-01	-0.10147254E-05				3
	-0.07143728E-07	0.03634922E-10	-0.04200629E+06	0.05318889E+02					4
SIH	121986SI	1H	1		G	0300.00	2000.00	1000.00	1
	0.03110430E+02	0.10949460E-02	0.02898628E-06	-0.02745104E-08	0.07051799E-12				2
	0.04516897E+06	0.04193487E+02	0.03836009E+02	-0.02702656E-01	0.06849070E-04				3
	-0.05424184E-07	0.14721313E-11	0.04507593E+06	0.09350778E+01					4
SIH2	42489SI	1H	2		G	0300.00	3000.00	1000.00	1
	0.04142390E+02	0.02150191E-01	-0.02190730E-05	-0.02073725E-08	0.04741018E-12				2
	0.03110483E+06	0.02930745E+01	0.03475092E+02	0.02139338E-01	0.07672305E-05				3
	0.05217668E-08	-0.09898824E-11	0.03147397E+06	0.04436585E+02					4
SIH2CL	121986SI	1H	2CL	1	G	0300.00	2000.00	1000.00	1
	0.05555901E+02	0.04046479E-01	-0.06581751E-05	-0.05027548E-08	0.15991101E-12				2
	0.01912428E+05	-0.01906889E+02	0.01699256E+02	0.01961407E+00	-0.02622973E-03				3
	0.01936416E-06	-0.05846399E-10	0.02743661E+05	0.01683132E+03					4
SIH2F	42489SI	1F	1H	2	G	0300.00	3000.00	1000.00	1
	0.06020398E+02	0.03074039E-01	-0.03248886E-05	-0.03052243E-08	0.07098090E-12				2
	-0.02347670E+06	-0.05919595E+02	0.02782566E+02	0.09148257E-01	-0.04186787E-05				3
	-0.05388971E-07	0.02412133E-10	-0.02244201E+06	0.11528536E+02					4
SIH2F2	42489SI	1H	2F	2	G	0300.00	3000.00	1000.00	1
	0.07997762E+02	0.03911538E-01	-0.04222679E-05	-0.03913812E-08	0.09171569E-12				2
	-0.09682880E+06	-0.16223999E+02	0.02701455E+02	0.14565451E-01	-0.11633003E-05				3
	-0.09685830E-07	0.04769590E-10	-0.09522440E+06	0.12006887E+02					4
SIH3	42489SI	1H	3		G	0300.00	3000.00	1000.00	1
	0.05015906E+02	0.03732750E-01	-0.03609053E-05	-0.03729193E-08	0.08468491E-12				2
	0.02190233E+06	-0.04291368E+02	0.02946733E+02	0.06466763E-01	0.05991653E-05				3
	-0.02218413E-07	0.03052669E-11	0.02270173E+06	0.07347948E+02					4
SIH3NH2	42489SI	1N	1H	5	G	0300.00	3000.00	1000.00	1
	0.08109945E+02	0.07215752E-01	-0.06052251E-05	-0.07086088E-08	0.15578638E-12				2
	-0.08999782E+05	-0.16516504E+02	0.02936348E+02	0.16747041E-01	-0.03232858E-05				3
	-0.09171970E-07	0.03979516E-10	-0.07334716E+05	0.11414373E+02					4
SIH3NSIHI3	42489SI	2N	1H	7	G	0300.00	3000.00	1000.00	1
	0.12652963E+02	0.10667481E-01	-0.10073358E-05	-0.10812221E-08	0.02452363E-11				2
	-0.12497210E+05	-0.03441428E+03	0.02468749E+02	0.02940254E+00	-0.06248179E-05				3
	-0.01731461E-06	0.07545261E-10	-0.09209690E+05	0.02059559E+03					4
SIH3NSIHI3	42489SI	2N	1H	6	G	0300.00	3000.00	1000.00	1
	0.12014620E+02	0.09187517E-01	-0.09159516E-05	-0.09380967E-08	0.02156435E-11				2
	0.01965065E+06	-0.02978185E+03	0.02827574E+02	0.02580646E+00	-0.04200477E-05				3
	-0.15038588E-07	0.06388324E-10	0.02265351E+06	0.01997012E+03					4
SIH4	121386SI	1H	4		G	0300.00	4000.00	1000.00	1
	0.06893873E+02	0.04030500E-01	-0.04183314E-05	-0.02291394E-08	0.04384766E-12				2
	0.11070374E+04	-0.01749116E+03	0.02475166E+02	0.09003721E-01	0.02185394E-04				3
	-0.02681423E-07	-0.06621080E-11	0.02925488E+05	0.07751014E+02					4
SIHCL2	121986SI	1H	1CL	2	G	0300.00	2000.00	1000.00	1
	0.07229734E+02	0.02869205E-01	-0.08849876E-05	-0.07495865E-09	0.05752338E-12				2
	-0.01971399E+06	-0.07052663E+02	0.02368353E+02	0.02401088E+00	-0.03717219E-03				3
	0.02851997E-06	-0.08530494E-10	-0.01875884E+06	0.16145866E+02					4

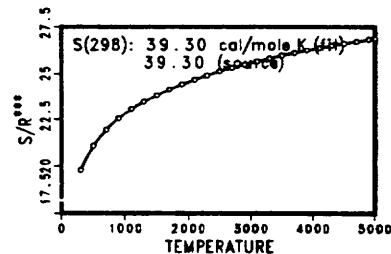
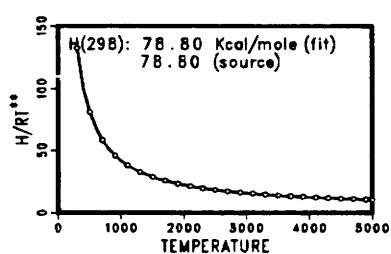
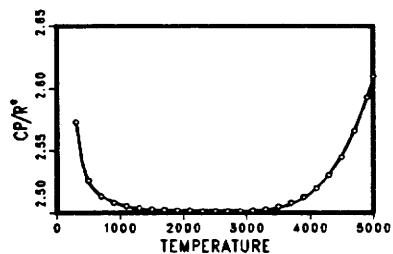
SIHF	42489SI	1F	1H	1	G	0300.00	3000.00	1000.00	1
	0.05073508E+02	0.15332789E-02	-0.01840658E-05	-0.14400376E-09	0.03452517E-12				2
	-0.01973879E+06	-0.10795069E+01	0.03223727E+02	0.04981220E-01	-0.03173051E-05				3
	-0.02822231E-07	0.12478316E-11	-0.01914167E+06	0.08906423E+02					4
SIHF2	42489SI	1H	1F	2	G	0300.00	3000.00	1000.00	1
	0.07216536E+02	0.02253240E-01	-0.02737472E-05	-0.02173460E-08	0.05255331E-12				2
	-0.07280241E+06	-0.09783487E+02	0.03377237E+02	0.10366072E-01	-0.12390823E-05				3
	-0.07267981E-07	0.03794989E-10	-0.07168358E+06	0.10521894E+02					4
SIHF3	42489SI	1H	1F	3	G	0300.00	3000.00	1000.00	1
	0.09363567E+02	0.02947555E-01	-0.03577633E-05	-0.02858224E-08	0.06915728E-12				2
	-0.14860736E+06	-0.02169452E+03	0.03918053E+02	0.14639172E-01	-0.01856069E-04				3
	-0.10582003E-07	0.05617543E-10	-0.14704386E+06	0.07024261E+02					4
SIN	42489SI	1N	1		G	0300.00	3000.00	1000.00	1
	0.04122909E+02	0.03521457E-02	-0.07161080E-06	-0.02154956E-09	0.06667570E-13				2
	0.05683927E+06	0.02389837E+02	0.03149181E+02	0.02584376E-01	-0.05804624E-05				3
	-0.01805626E-07	0.10410949E-11	0.05710563E+06	0.07474389E+02					4
SINH	42489SI	1N	1H	1	G	0300.00	3000.00	1000.00	1
	0.04928800E+02	0.16286244E-02	-0.13671971E-06	-0.13904604E-09	0.02998968E-12				2
	0.01767789E+06	-0.02823472E+02	0.03166974E+02	0.05805822E-01	-0.09524443E-05				3
	-0.03991892E-07	0.02283188E-10	0.01813560E+06	0.06298439E+02					4
SINH2	42489SI	1N	1H	2	G	0300.00	3000.00	1000.00	1
	0.05186435E+02	0.03016656E-01	-0.02165476E-05	-0.02722658E-08	0.05706182E-12				2
	0.02270507E+06	-0.12421399E+01	0.03362769E+02	0.07261175E-01	-0.08721233E-05				3
	-0.04400014E-07	0.02419532E-10	0.02318445E+06	0.08223867E+02					4
SN	121286S	1N	1		G	0300.00	5000.00	1000.00	1
	0.03888286E+02	0.06778427E-02	-0.02725308E-05	0.05135927E-09	-0.03593836E-13				2
	0.03044496E+06	0.04194291E+02	0.03407345E+02	0.01797887E-01	-0.02018969E-04				3
	0.02107857E-07	-0.09527593E-11	0.03062373E+06	0.06821481E+02					4
S0	121286S	10	1		G	0300.00	5000.00	1000.00	1
	0.04021077E+02	0.02584856E-02	0.08948142E-06	-0.03580144E-09	0.03228430E-13				2
	-0.07119620E+04	0.03452522E+02	0.03080401E+02	0.01803105E-01	0.06705022E-05				3
	-0.02069005E-07	0.08514657E-11	-0.03986163E+04	0.08581028E+02					4
S02	121286S	10	2		G	0300.00	5000.00	1000.00	1
	0.05254498E+02	0.01978545E-01	-0.08204226E-05	0.15763830E-09	-0.11204512E-13				2
	-0.03756885E+06	-0.11460563E+01	0.02911438E+02	0.08103022E-01	-0.06906710E-04				3
	0.03329015E-07	-0.08777121E-11	-0.03687881E+06	0.11117403E+02					4
S03	121286S	10	3		G	0300.00	5000.00	1000.00	1
	0.07050668E+02	0.03246560E-01	-0.14088974E-05	0.02721535E-08	-0.01942364E-12				2
	-0.05020667E+06	-0.11064426E+02	0.02575282E+02	0.15150916E-01	-0.12298717E-04				3
	0.04240257E-07	-0.05266812E-11	-0.04894410E+06	0.12195116E+02					4

## APPENDIX C. GRAPHICAL REPRESENTATION OF DATA BASE

Species: AL ALUMINUM, MONATOMIC GAS As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.02736825E+02	-0.05912374E-02	-0.04033937E-05	0.02322343E-07	-0.01705599E-10	0.03886794E+06	0.04363879E+02
0600-5000K	0.02559589E+02	-0.10632239E-03	0.07202828E-06	-0.02121105E-09	0.02289429E-13	0.03890214E+06	0.05234522E+02



Source: SNL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

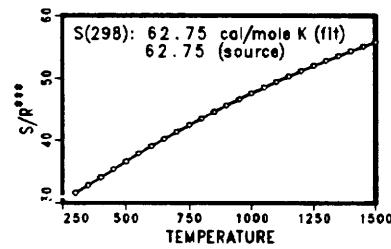
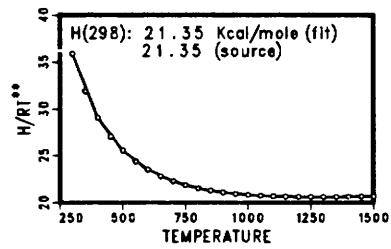
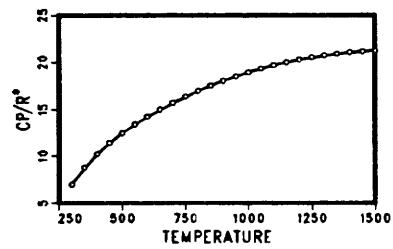
$$\bullet \bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: AL2H6

GAS As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	-0.06800681E+02	0.05080744E+00	0.10397471E-04	-0.11195819E-06	0.08459155E-09	0.10605371E+05	0.05554526E+03
0600-1500K	0.02634884E+02	0.02135952E+00	0.03154151E-05	-0.07684674E-07	0.02335831E-10	0.08871346E+05	0.09827515E+02



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

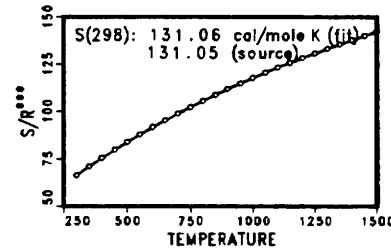
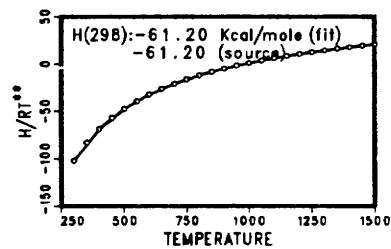
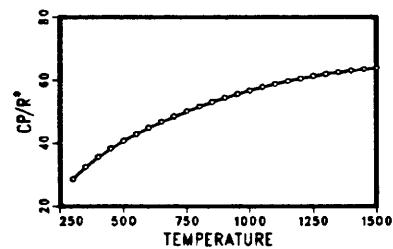
Species: AL2ME6

("ME" = CH<sub>3</sub>,METHYL)

GAS As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	-0.07159750E+01	0.10671087E+00	0.02117604E-03	-0.02193211E-05	0.16441438E-09	-0.03515546E+06	0.03890762E+03
0600-1500K	0.01773147E+03	0.04935747E+00	0.11968535E-05	-0.16398263E-07	0.04890867E-10	-0.03855560E+06	-0.05053298E+03



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

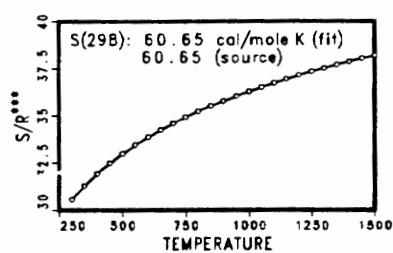
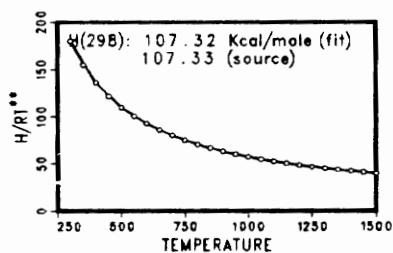
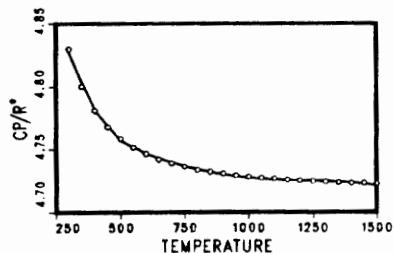
$$\bullet \bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: ALAS

GAS

As of: 6/29/87

Fit  
 Coefficients  $a_1$   $a_2$   $a_3$   $a_4$   $a_5$   $a_6$   $a_7$   
 0300-0600K 0.05047764E+02 -0.06419947E-02 -0.14320714E-05 0.04754390E-07 -0.03297621E-10 0.05254264E+06 0.01985205E+02  
 0600-1500K 0.04790026E+02 -0.01908225E-03 -0.01983390E-05 0.02239358E-08 -0.06904706E-12 0.05259290E+06 0.03259703E+02



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

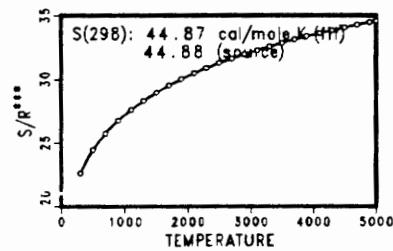
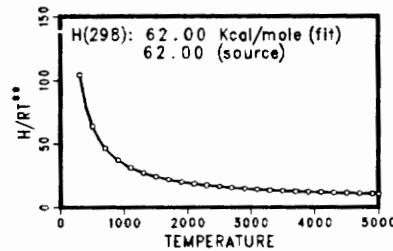
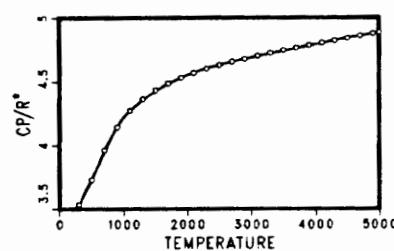
Species: ALH

ALUMINUM MONOHYDRIDE

GAS

As of: 6/29/87

Fit  
 Coefficients  $a_1$   $a_2$   $a_3$   $a_4$   $a_5$   $a_6$   $a_7$   
 0300-1000K 0.03071503E+02 0.02165549E-01 -0.03275638E-04 0.04136983E-07 -0.01877120E-10 0.03021221E+06 0.04548855E+02  
 1000-5000K 0.03392644E+02 0.12153990E-02 -0.04676595E-05 0.08691624E-09 -0.06022668E-13 0.03006845E+06 0.02758899E+02



Source: SNL FIT TO JANAF TABLES

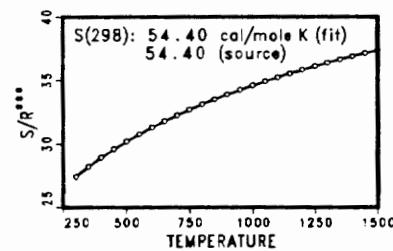
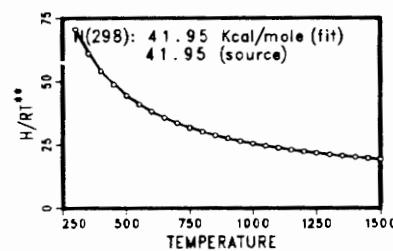
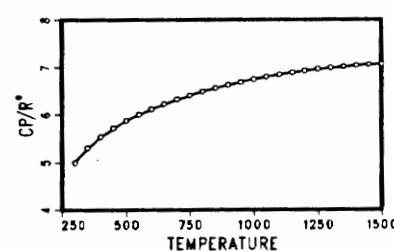
$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: ALH2

GAS

As of: 6/29/87

Fit  
 Coefficients  $a_1$   $a_2$   $a_3$   $a_4$   $a_5$   $a_6$   $a_7$   
 0300-0600K 0.02442136E+02 0.09915913E-01 0.02471082E-05 -0.02119583E-06 0.01710233E-09 0.01997587E+06 0.10652699E+02  
 0600-1500K 0.04486543E+02 0.03128831E-01 -0.01969438E-05 -0.010160304E-08 0.03497468E-11 0.01960959E+06 0.08167897E+01



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

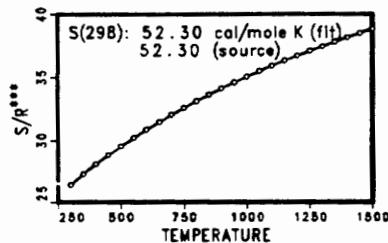
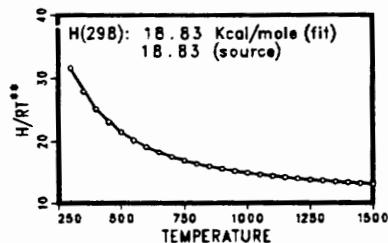
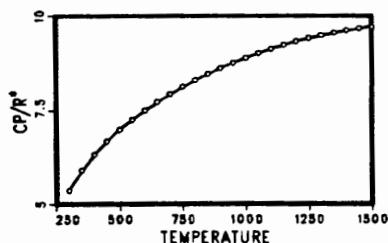
Species: ALH3

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.10083231E+01	0.16403245E-01	0.01976746E-04	-0.03528558E-06	0.02753377E-09	0.08484656E+05	0.15858377E+02
0600-1500K	0.04186837E+02	0.06159249E-01	-0.03877593E-06	-0.02061928E-07	0.06600276E-11	0.07908078E+05	0.05134396E+01



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: ALME

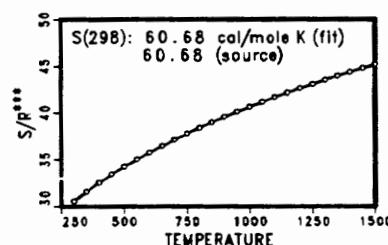
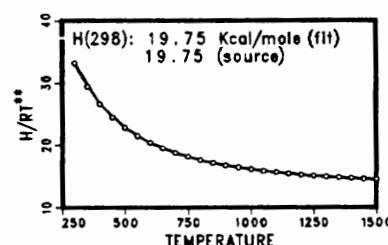
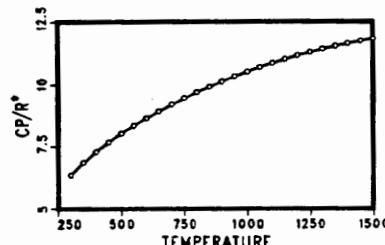
("ME" = CH<sub>3</sub>,METHYL)

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.02664176E+02	0.13249141E-01	0.02525847E-04	-0.02394396E-06	0.01761854E-09	0.08574173E+05	0.11474494E+02
0600-1500K	0.04662737E+02	0.07097939E-01	0.02520013E-05	-0.02114863E-07	0.06097489E-11	0.08203227E+05	0.01769244E+02



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: ALME2

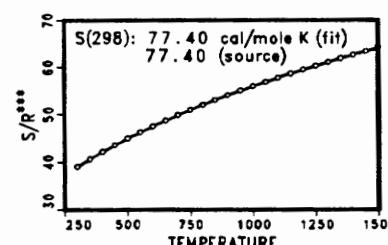
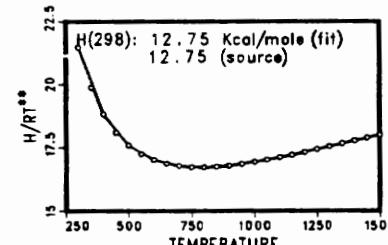
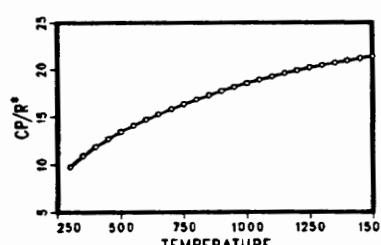
("ME" = CH<sub>3</sub>,METHYL)

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.09494573E+01	0.03206353E+00	0.06134020E-04	-0.06500042E-06	0.04911485E-09	0.04761408E+05	0.02419465E+03
0600-1500K	0.06481282E+02	0.14746049E-01	0.05816529E-05	-0.04621347E-07	0.13960405E-11	0.03745072E+05	-0.02603325E+02



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: ALME3

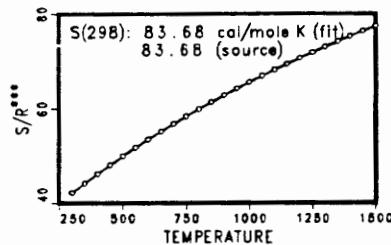
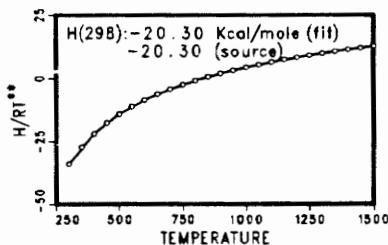
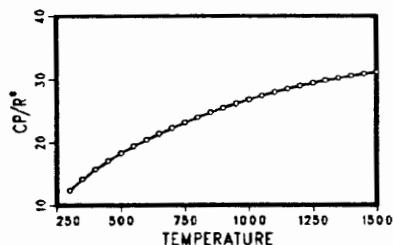
("ME" = CH<sub>3</sub>,METHYL)

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	-0.07027567E+01	0.04682764E+00	0.11499028E-04	-0.09160441E-06	0.06687293E-09	-0.12037989E+05	0.03232771E+03
0600-1500K	0.06654948E+02	0.02455144E+00	0.11765745E-05	-0.07815023E-07	0.02255622E-10	-0.13409524E+05	-0.03454481E+02



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6 T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: AR

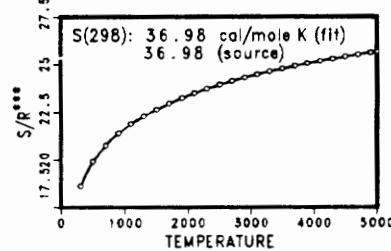
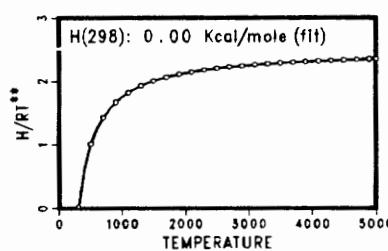
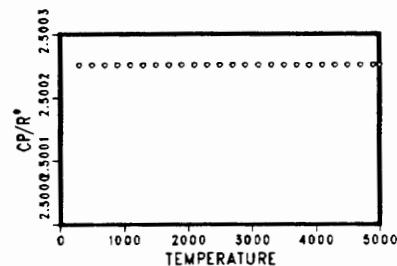
ARGON, MONATOMIC (REF ST)

GAS

As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	-0.07453750E+04	0.04366000E+02
1000-5000K	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	-0.07453750E+04	0.04366000E+02



Source: NASA FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6 T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: AR+

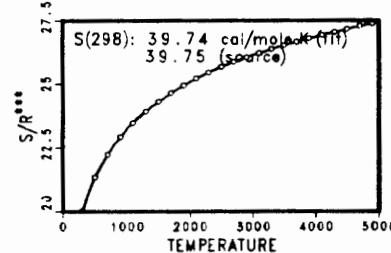
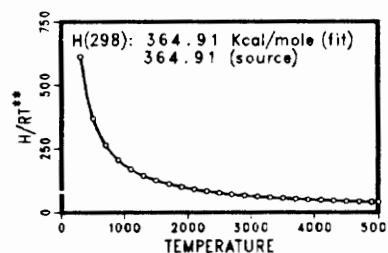
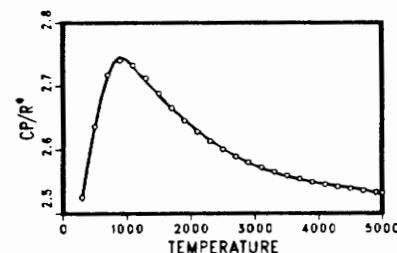
ARGON, UNIPOSITIVE ION

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02301341E+02	0.08035528E-02	-0.01758805E-05	-0.01781093E-08	-0.08937268E-13	0.01829281E+07	0.06659358E+02
1000-5000K	0.02864864E+02	-0.12035732E-03	-0.10651992E-07	0.09074839E-10	-0.09623876E-14	0.01627230E+07	0.03543584E+02



Source: SNL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6 T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

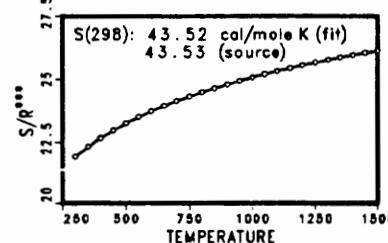
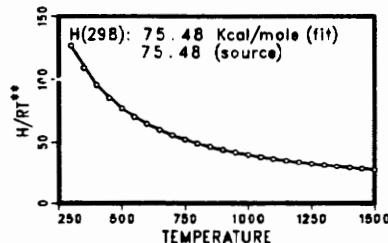
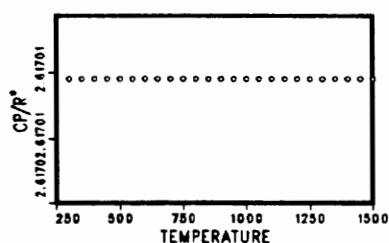
Species: AS

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.02617010E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.03720454E+06	0.06995524E+02
0600-1500K	0.02617010E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.03720454E+06	0.06995524E+02



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

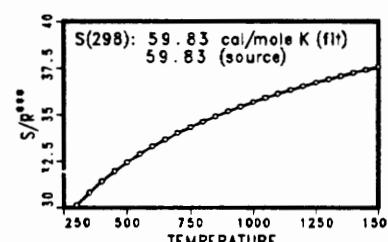
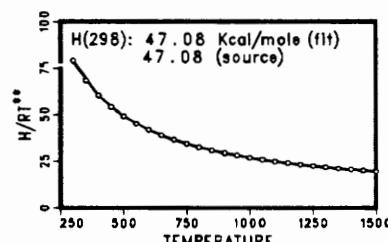
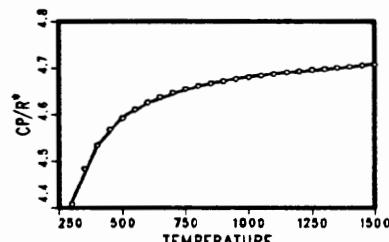
Species: AS2

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.03682891E+02	0.03121811E-01	-0.10740519E-05	-0.05629472E-07	0.0517881E-10	0.02247355E+06	0.08283423E+02
0600-1500K	0.04394201E+02	0.05389968E-02	-0.02379401E-05	-0.06541924E-09	0.05184186E-12	0.02235093E+06	0.04897918E+02



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

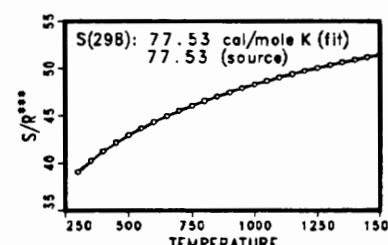
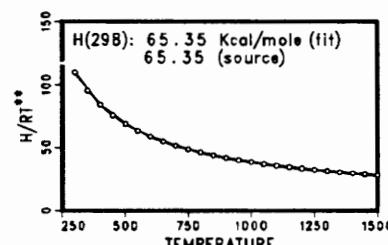
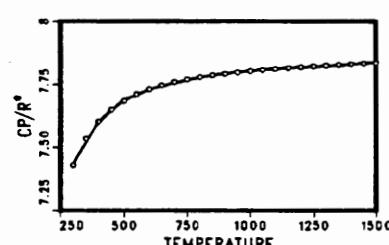
Species: AS3

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.06403142E+02	0.04477098E-01	-0.01866642E-04	-0.07394750E-07	0.07012752E-10	0.03080965E+06	0.13371355E+01
0600-1500K	0.07404036E+02	0.07818425E-02	-0.03918297E-05	-0.05203629E-09	0.06291907E-12	0.03063825E+06	-0.03417323E+02



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

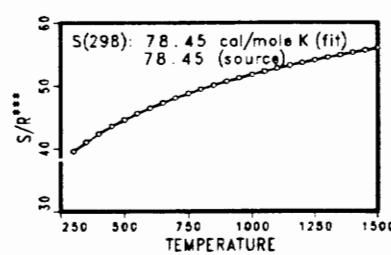
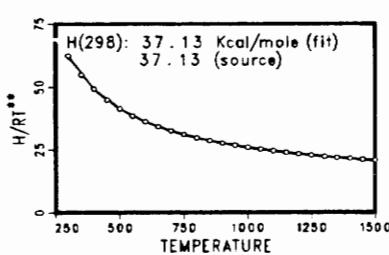
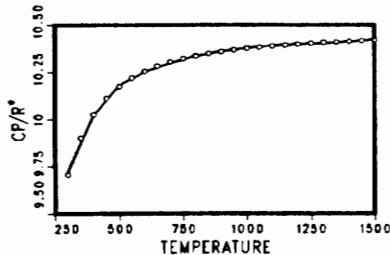
Species: AS4

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.07853760E+02	0.07916509E-01	-0.02329820E-04	-0.15263119E-07	0.13774348E-10	0.16036290E+05	-0.07409755E+02
0600-1500K	0.09695766E+02	0.13062585E-02	-0.05519564E-05	-0.02150873E-08	0.14579349E-12	0.15717321E+05	-0.16188696E+02



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: ASALME

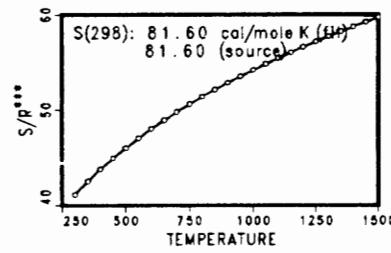
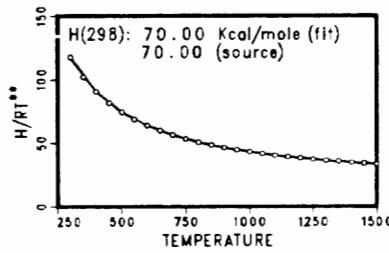
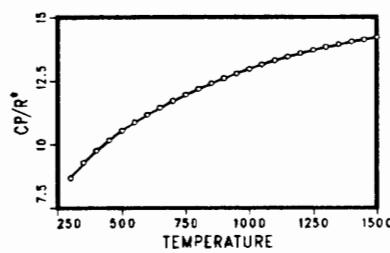
("ME" = CH<sub>3</sub>,METHYL)

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.04053423E+02	0.01726125E+00	0.018333498E-04	-0.03386952E-06	0.02626980E-09	0.03329309E+06	0.12996653E+02
0600-1500K	0.07127107E+02	0.07357863E-01	0.02300796E-06	-0.02226398E-07	0.06927227E-11	0.03273438E+06	-0.01847179E+02



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: ASALME2

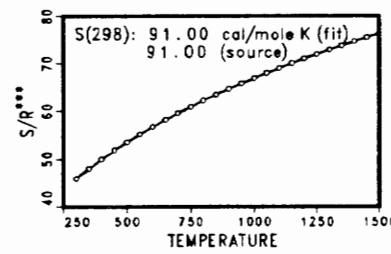
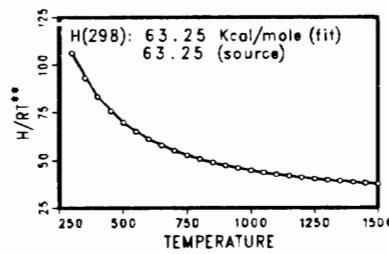
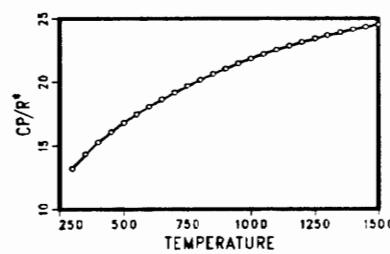
("ME" = CH<sub>3</sub>,METHYL)

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.04808530E+02	0.03067687E+00	0.05048000E-04	-0.05908099E-06	0.04462290E-09	0.02908816E+06	0.09471621E+02
0600-1500K	0.09909938E+02	0.14638499E-01	0.04118730E-05	-0.04444657E-07	0.13295010E-11	0.02815111E+06	-0.15235312E+02



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

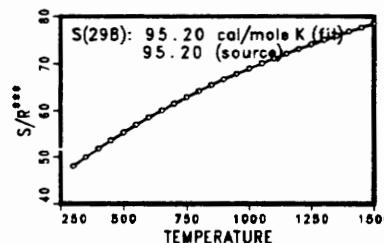
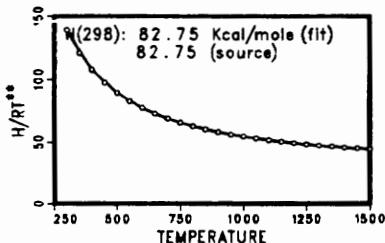
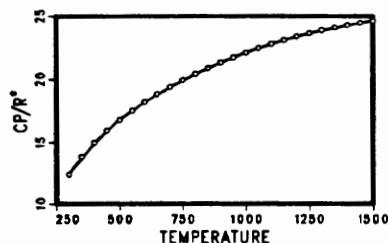
$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: ASGAET ("ET" = C2H5, ETHYL) GAS As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.06364698E+01	0.04382467E+00	0.06144686E-04	-0.09491641E-06	0.07374197E-09	0.03960893E+06	0.03164673E+03
0600-1500K	0.09081073E+02	0.16746316E-01	0.12831301E-06	-0.05590435E-07	0.017B1314E-10	0.03807443E+06	-0.09142782E+02



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

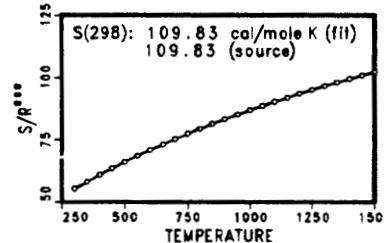
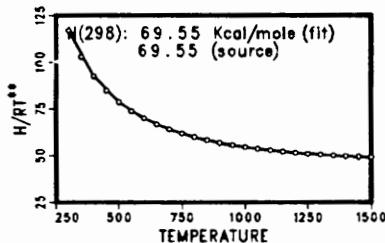
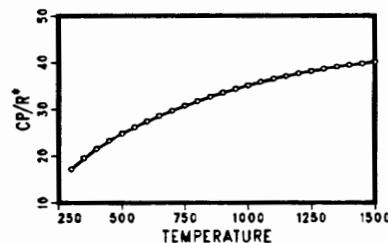
$$\bullet \text{H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: ASGAET2 ("ET" = C2H5, ETHYL) GAS As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	-0.03539248E+01	0.06369772E+00	0.13597417E-04	-0.12861423E-06	0.09572181E-09	0.03236903E+06	0.03865086E+03
0600-1500K	0.10324288E+02	0.03073570E+00	0.10863354E-05	-0.09971948E-07	0.02945979E-10	0.03039490E+06	-0.13164016E+02



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

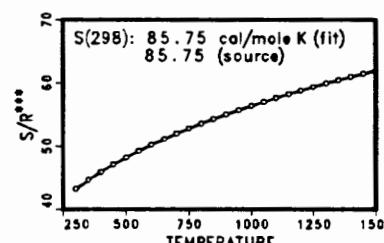
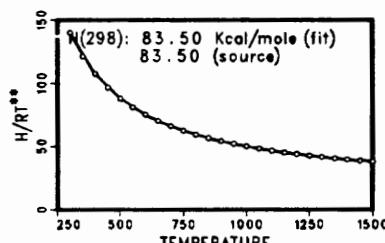
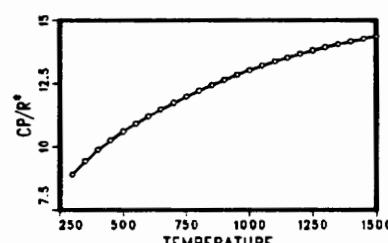
$$\bullet \text{H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: ASGAME ("ME" = CH3, METHYL) GAS As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.04877266E+02	0.14825589E-01	0.16521240E-05	-0.02712058E-06	0.02080195E-09	0.03994071E+06	0.11076703E+02
0600-1500K	0.07322183E+02	0.06995478E-01	0.10693509E-06	-0.01995283E-07	0.06040446E-11	0.03949448E+06	-0.07416680E+01



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

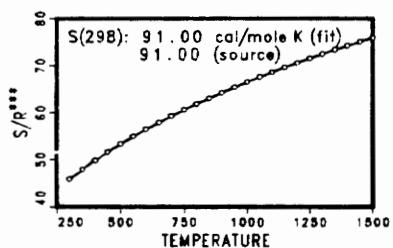
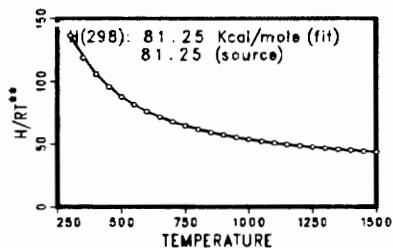
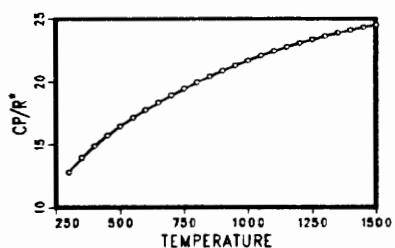
$$\bullet \text{H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: ASGAME2 ("ME" = CH<sub>3</sub>,METHYL) GAS As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.04382076E+02	0.03056344E+00	0.05477057E-04	-0.05834108E-06	0.04373509E-09	0.03827434E+06	0.11911109E+02
0600-1500K	0.09352436E+02	0.15048197E-01	0.05157975E-05	-0.04553518E-07	0.13487630E-11	0.03735855E+06	-0.12181144E+02



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP}/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

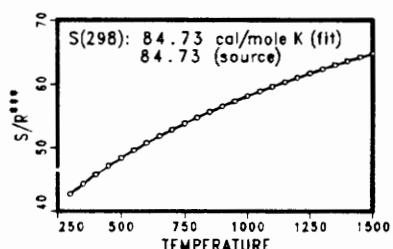
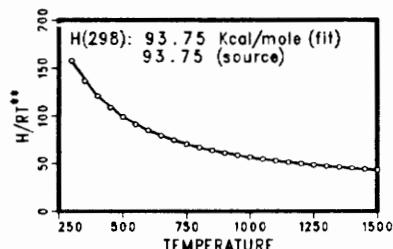
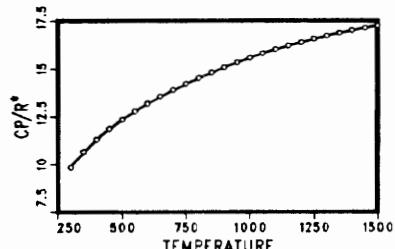
$$\bullet\bullet \text{H}/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet\bullet\bullet \text{S}/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: ASGAMEH ("ME" = CH<sub>3</sub>,METHYL) GAS As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.03585119E+02	0.02336317E+00	0.02873356E-04	-0.04737894E-06	0.03674461E-09	0.04512702E+06	0.15471604E+02
0600-1500K	0.07842794E+02	0.09682097E-01	0.10603061E-06	-0.02991402E-07	0.09382673E-11	0.04435297E+06	-0.05093455E+02



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP}/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

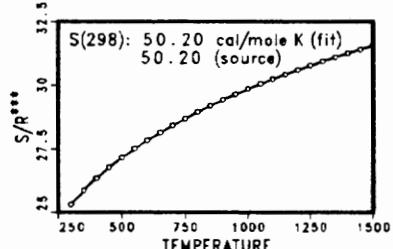
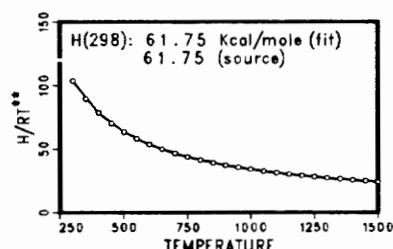
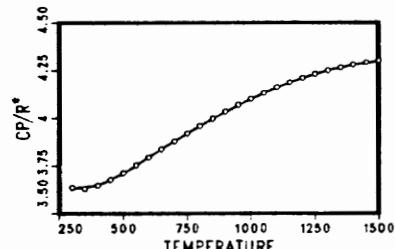
$$\bullet\bullet \text{H}/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet\bullet\bullet \text{S}/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: ASH GAS As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.03865843E+02	-0.11575710E-02	-0.03494371E-05	0.07079686E-07	-0.06014027E-10	0.02996829E+06	0.03549869E+02
0600-1500K	0.03219848E+02	0.10012498E-02	-0.04874997E-08	-0.11076533E-09	-0.09254321E-13	0.03008175E+06	0.06647311E+02



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP}/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet\bullet \text{H}/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet\bullet\bullet \text{S}/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

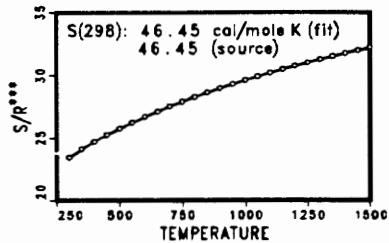
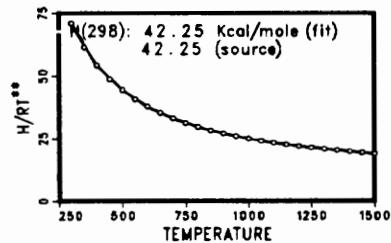
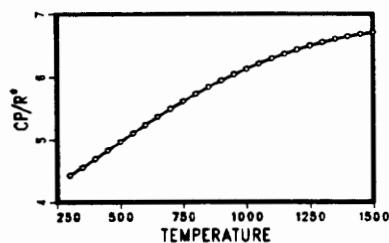
Species: ASH2

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.03778945E+02	0.01759233E-01	0.08070806E-05	0.02358763E-07	-0.03043521E-10	0.02004861E+06	0.12729740E+01
0600-1500K	0.03428307E+02	0.03181140E-01	0.14604843E-06	-0.07937145E-08	0.01694413E-11	0.02010282E+06	0.02904703E+02



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

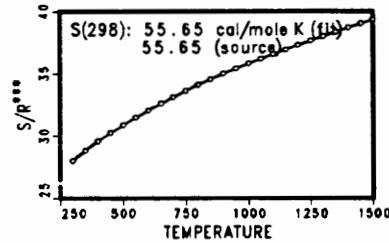
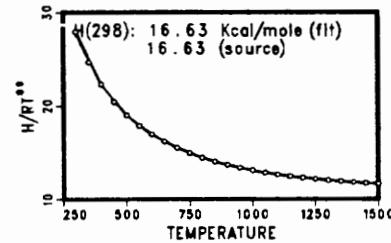
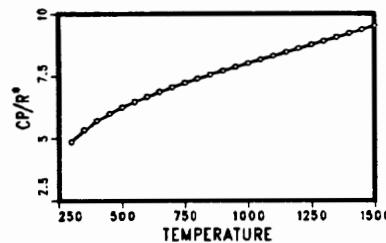
Species: ASH3

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.09446356E+01	0.15084686E-01	0.12016960E-05	-0.03397465E-06	0.02767656E-09	0.07459168E+05	0.01832267E+03
0600-1500K	0.04172022E+02	0.04371322E-01	0.02177574E-05	-0.11832641E-08	0.04536373E-11	0.06882915E+05	0.02803476E+02



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: ASME

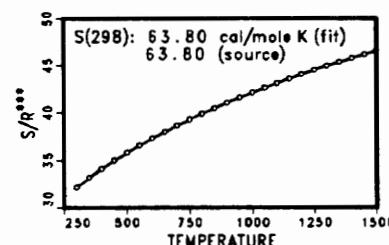
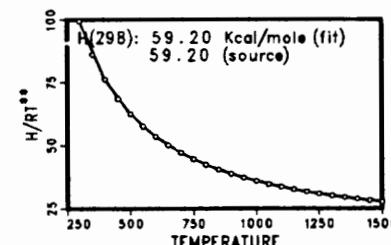
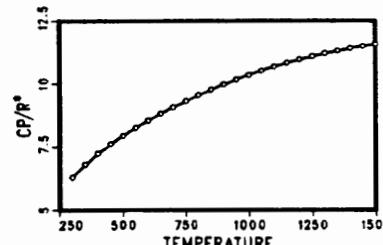
("ME" = CH<sub>3</sub>,METHYL)

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.02625270E+02	0.13252423E-01	0.02441628E-04	-0.02419566E-06	0.01786943E-09	0.02844080E+06	0.13273359E+02
0600-1500K	0.04657260E+02	0.06976297E-01	0.02147556E-05	-0.02101159E-07	0.06082149E-11	0.02806422E+06	0.03409834E+02



Source: SNL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

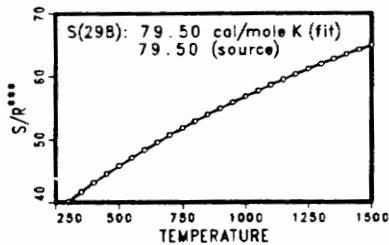
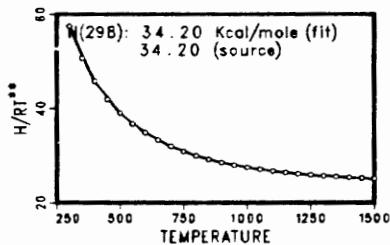
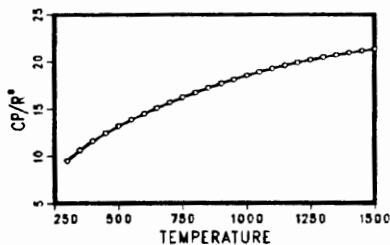
$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: ASME2 ("ME" = CH<sub>3</sub>,METHYL) GAS As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.13903998E+01	0.02923331E+00	0.06598870E-04	-0.05620559E-06	0.04130367E-09	0.15533022E+05	0.02349980E+03
0600-1500K	0.05981395E+02	0.15212837E-01	0.06993355E-05	-0.04721619E-07	0.13699115E-11	0.14679847E+05	0.11927411E+01



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

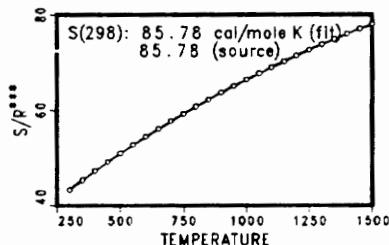
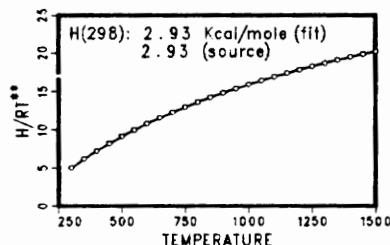
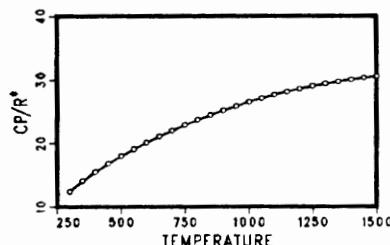
Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} \bullet \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: ASME3 ("ME" = CH<sub>3</sub>,METHYL) GAS As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.02667388E+01	0.04253171E+00	0.11651064E-04	-0.07914706E-06	0.05603126E-09	-0.04685539E+04	0.02904590E+03
0600-1500K	0.06347764E+02	0.02466454E+00	0.11546286E-05	-0.07877435E-07	0.02202225E-10	-0.16173225E+04	-0.06316786E+01



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

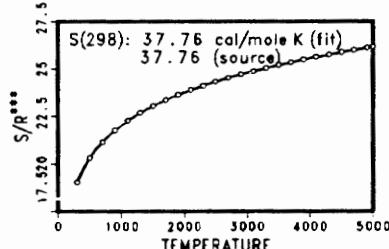
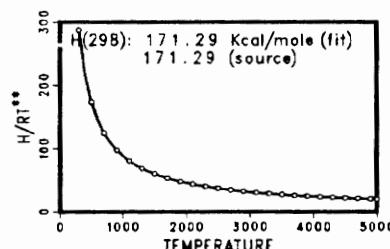
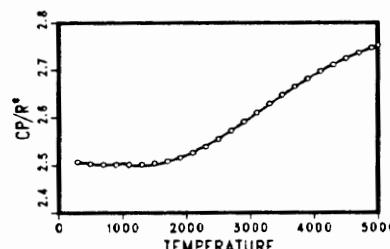
Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} \bullet \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C CARBON, MONATOMIC GAS As of: 12/10/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02498584E+02	0.08085776E-03	-0.02697697E-05	0.03040729E-08	-0.11066518E-12	0.08545878E+06	0.04753459E+02
1000-5000K	0.02602087E+C2	-0.01787081E-02	0.09087041E-06	-0.11499333E-10	0.03310844E-14	0.08542154E+06	0.04195177E+02



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C(S)

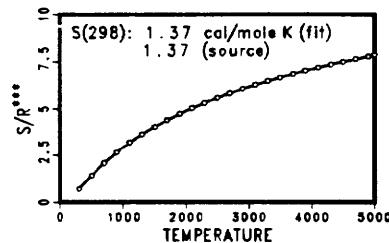
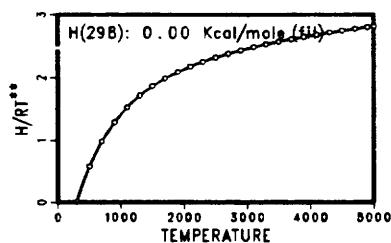
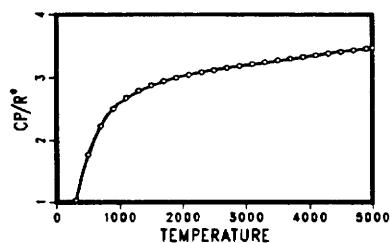
CARBON (REF ST), GRAPHITE

SOLID

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	-0.06705661E+01	0.07181499E-01	-0.05632921E-04	0.02142298E-07	-0.04168562E-11	-0.07339498E+03	0.02601595E+02
1000-5000K	0.14901664E+01	0.16621256E-02	-0.06687204E-05	0.12908796E-09	-0.09205334E-13	-0.07074018E+04	-0.08717785E+02



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 T \\ \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C+

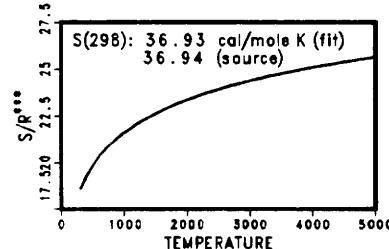
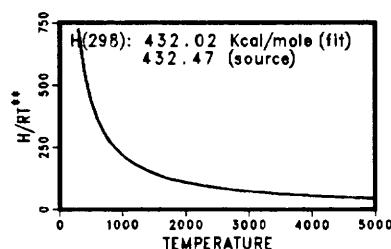
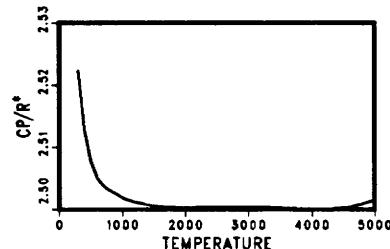
CARBON, UNIPOSITIVE ION

GAS

As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02595384E+02	-0.04068664E-02	0.06892366E-05	-0.05266488E-08	0.15083378E-12	0.02166628E+07	0.03895729E+02
1000-5000K	0.02511827E+02	-0.01735978E-03	0.09504267E-07	-0.02218851E-10	0.01862189E-14	0.02166772E+07	0.04286130E+02



Source: NASA FIT TO NASA LEWIS DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 T \\ \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C-

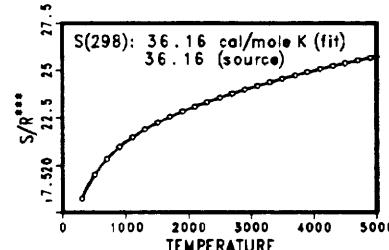
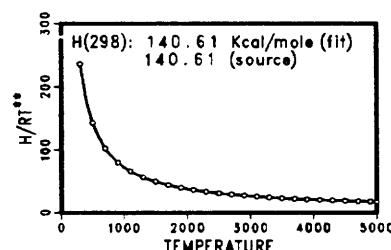
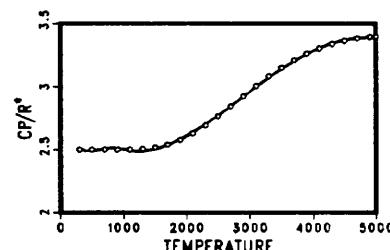
CARBON, UNINEGATIVE ION

GAS

As of: 12/16/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02783902E+02	-0.01774287E-01	0.03696760E-04	-0.03066693E-07	0.08637622E-11	0.0699851E+06	0.02726281E+02
1000-5000K	0.02990221E+02	-0.09184596E-02	0.05055560E-05	-0.07703410E-09	0.03163271E-13	0.06983931E+06	0.12594533E+01



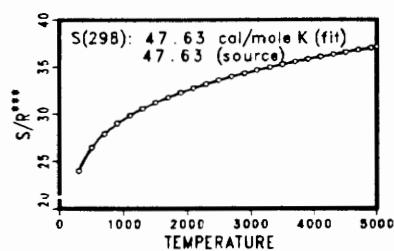
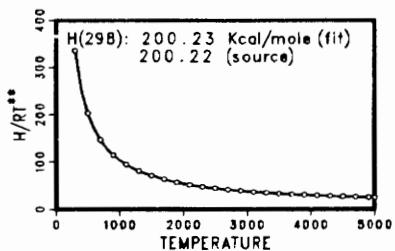
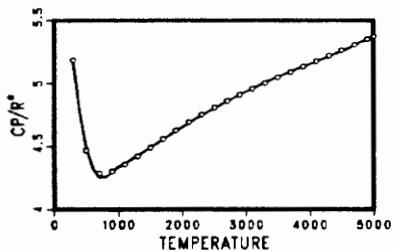
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 T \\ \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C2 CARBON, DIATOMIC GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.06996045E+02	-0.07400601E-01	0.03234703E-04	0.04802535E-07	-0.03295917E-10	0.09897487E+06	-0.13862268E+02
1000-5000K	0.04135978E+02	0.06531618E-03	0.01837099E-05	-0.05295085E-09	0.04712137E-13	0.09967272E+06	0.07472923E+01



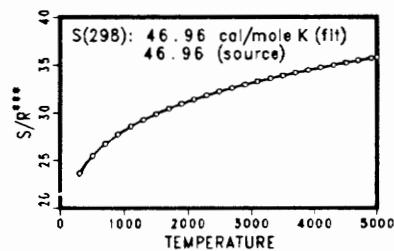
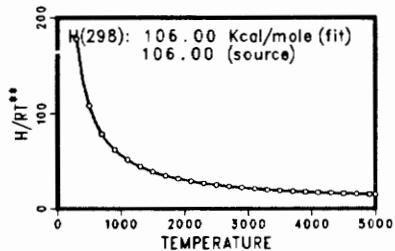
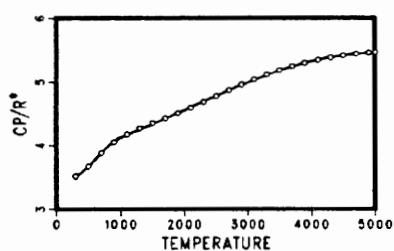
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C2- DIMERIC CARBON, UNINEGATIVE ION GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03468011E+02	-0.02352874E-02	0.12439123E-05	0.04705960E-08	-0.08164274E-11	0.05231215E+06	0.03886699E+02
1000-5000K	0.03796891E+02	0.02530049E-02	0.09709118E-06	-0.16148038E-10	-0.03212893E-15	0.05207981E+06	0.16581468E+01



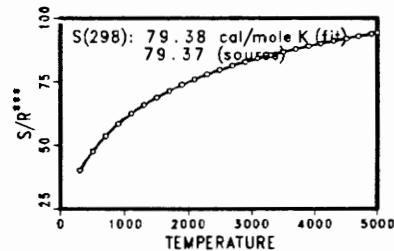
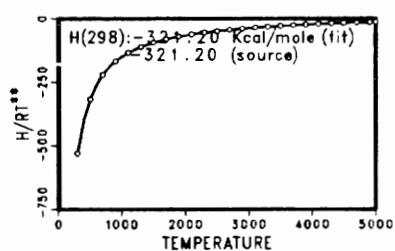
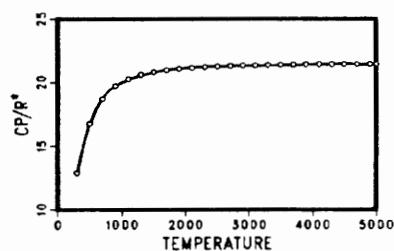
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C2F6 HEXAFLUOROETHANE GAS As of: 8/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03577448E+02	0.03913670E+00	-0.02714862E-03	0.04348459E-08	0.04007135E-10	-0.16421741E+06	0.09098384E+02
1000-5000K	0.16020573E+02	0.06273007E-01	-0.02797778E-04	0.05517547E-08	-0.04004651E-12	-0.16756543E+06	-0.05519459E+03



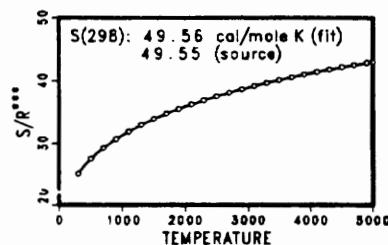
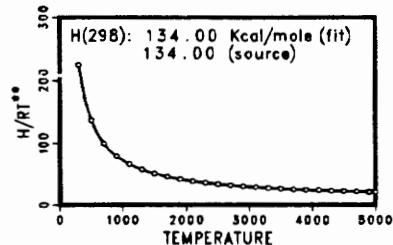
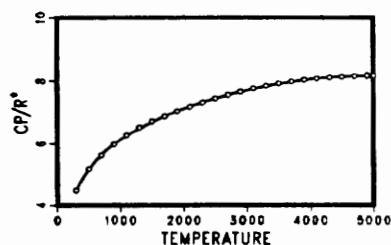
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C2H CCH RADICAL GAS As of: 2/03/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03050667E+02	0.06051674E-01	-0.04956634E-04	0.02804159E-07	-0.08193332E-11	0.06630011E+06	0.05954361E+02
1000-5000K	0.04427688E+02	0.02216268E-01	-0.06048952E-05	0.09882517E-09	-0.07351179E-13	0.06590415E+06	-0.11994418E+01



Source: SNLL FIT TO JANAF TABLES WITH H298=134 PER MILLER

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

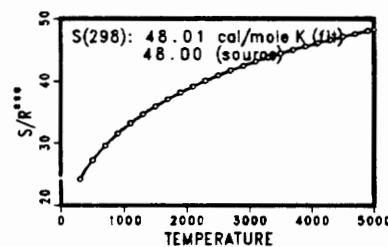
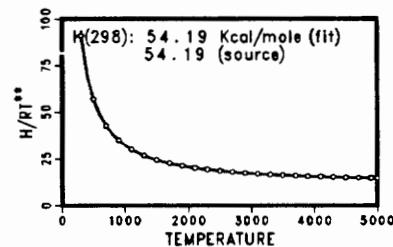
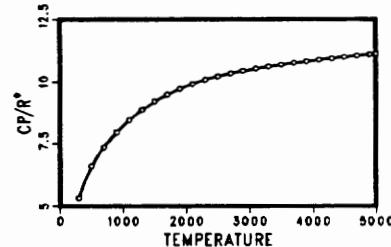
$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C2H2 ACETYLENE GAS As of: 12/13/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02013562E+02	0.15190446E-01	-0.16163189E-04	0.09078992E-07	-0.01912746E-10	0.02612444E+06	0.08805378E+02
1000-5000K	0.04436770E+02	0.05376039E-01	-0.01912816E-04	0.03286379E-08	-0.02156709E-12	0.02566766E+06	-0.02800338E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

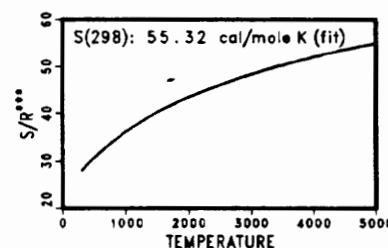
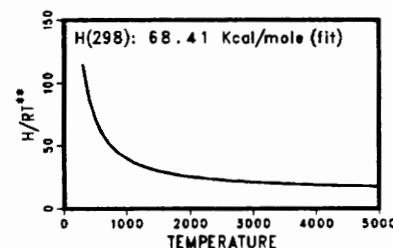
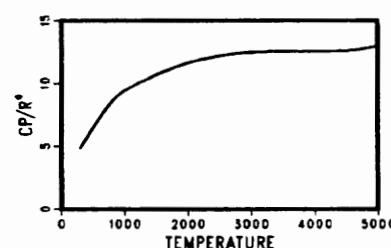
$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C2H3 VINYL-RAD GAS As of: 1/27/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02459276E+02	0.07371476E-01	0.02109872E-04	-0.13216421E-08	-0.11847838E-11	0.03335225E+06	0.11556202E+02
1000-5000K	0.05933468E+02	0.04017745E-01	-0.03966739E-05	-0.14412666E-09	0.02378643E-12	0.03185434E+06	-0.08530313E+02



Source: RECALC. OF BURCAT FIT (TECHNION), H298=68.4 PER MILLER

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

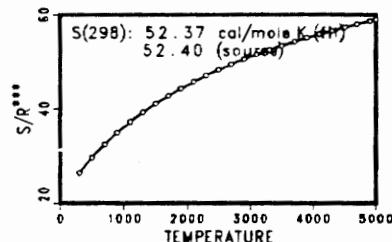
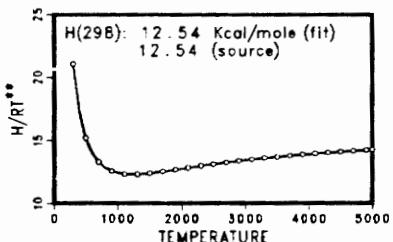
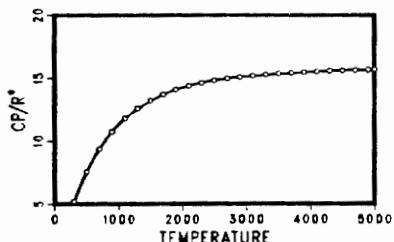
$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C2H4 ETHYLENE GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	-0.08614880E+01	0.02796162E+00	-0.03388677E-03	0.02785152E-06	-0.09737879E-10	0.05573046E+05	0.02421148E+03
1000-5000K	0.03528418E+02	0.11485185E-01	-0.04418385E-04	0.07844600E-08	-0.05266848E-12	0.04428288E+05	0.02230389E+02



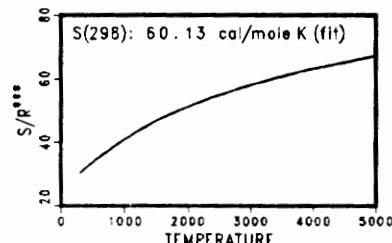
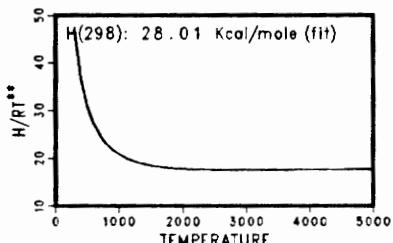
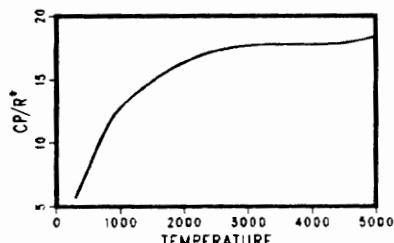
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C2H5 ETHYL RAD GAS As of: 1/23/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02690701E+02	0.08719133E-01	0.04419838E-04	0.09338703E-08	-0.03927773E-10	0.12870404E+05	0.12138195E+02
1000-5000K	0.07190480E+02	0.06484077E-01	-0.06428064E-05	-0.02347879E-08	0.03880877E-12	0.10674549E+05	-0.14780892E+02



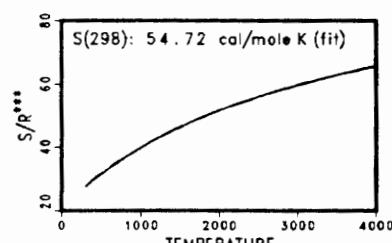
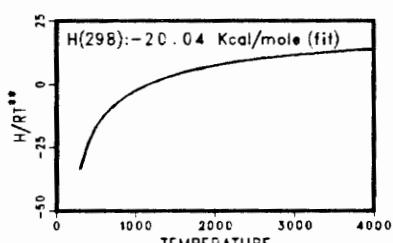
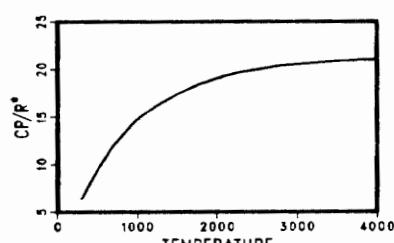
Source: RECALC. OF BURCAT FIT (TSIV TABLES), H298=28 PER MILLER

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C2H6 ETHANE GAS As of: 12/16/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.14625388E+01	0.15494667E-01	0.05780507E-04	-0.12578319E-07	0.04586267E-10	-0.11239176E+05	0.14432295E+02
1000-4000K	0.04825938E+02	0.13840429E-01	-0.04557258E-04	0.06724967E-08	-0.03598161E-12	-0.12717793E+05	-0.05239506E+02



Source: BURCAT (TECHNION REPORTS)

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C2HCL

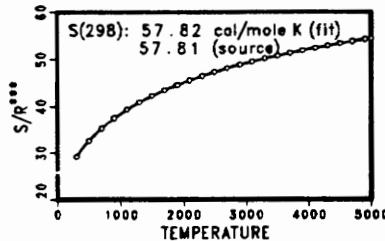
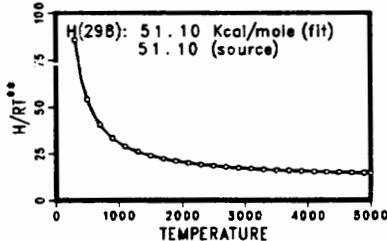
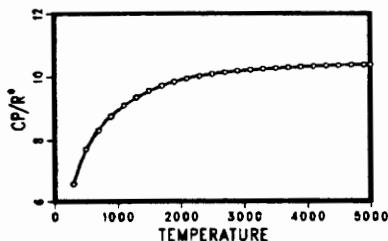
## CHLOROACETYLENE

GAS

As of: 11/29/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03618443E+02	0.13319791E-01	-0.13218222E-04	0.06092023E-07	-0.08879026E-11	0.02415385E+06	0.05050645E+02
1000-5000K	0.06295372E+02	0.03883113E-01	-0.15060494E-05	0.02700003E-08	-0.01830213E-12	0.02357278E+06	-0.08137063E+02



Source: SNLL FIT TO JANNAF DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C2N

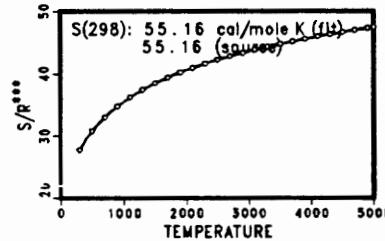
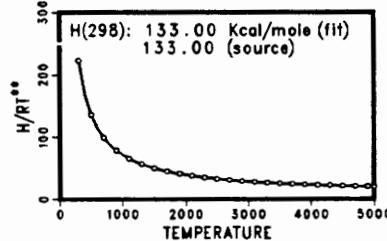
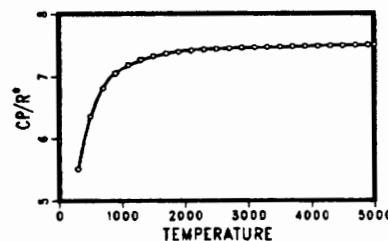
## CNC RADICAL

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03498545E+02	0.08554433E-01	-0.06288697E-04	0.08638478E-08	0.04915996E-11	0.06556611E+06	0.05548374E+02
1000-5000K	0.06151561E+02	0.15116498E-02	-0.06629362E-05	0.12861485E-09	-0.09160830E-13	0.06484318E+06	-0.08177850E+02



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C2N2

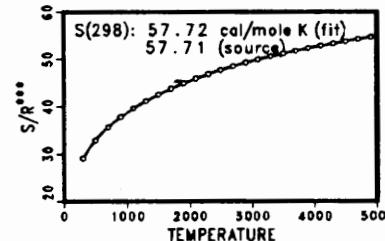
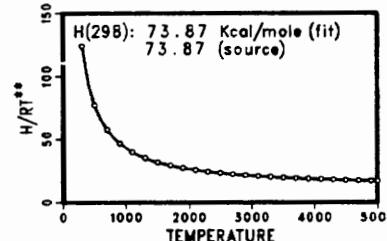
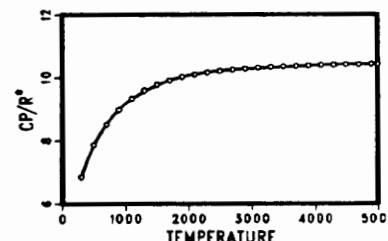
## CYANOGEN

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04265459E+02	0.11922569E-01	-0.13420142E-04	0.09192297E-07	-0.02778941E-10	0.03547887E+06	0.01713212E+02
1000-5000K	0.06548002E+02	0.03984707E-01	-0.16342164E-05	0.03038596E-08	-0.02111069E-12	0.03490716E+06	-0.09735790E+02



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C20

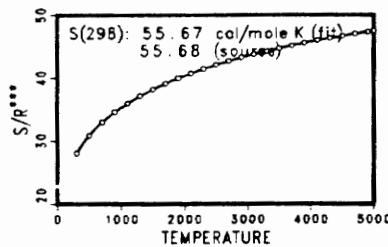
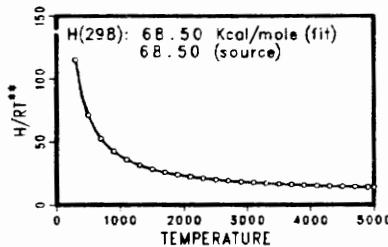
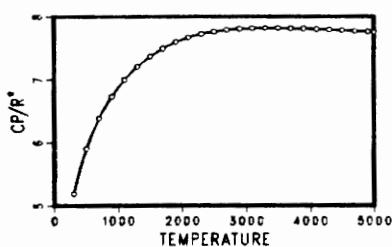
CCO RADICAL

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03368850E+02	0.08241803E-01	-0.08765145E-04	0.05569262E-07	-0.15400086E-11	0.03317081E+06	0.06713314E+02
1000-5000K	0.04849809E+02	0.02947585E-01	-0.10907286E-05	0.01792562E-08	-0.11157585E-13	0.03282055E+06	-0.06453225E+01



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: C3

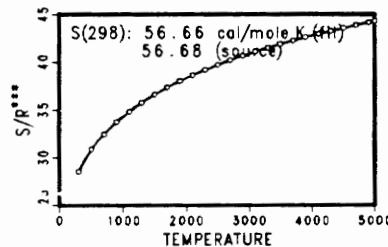
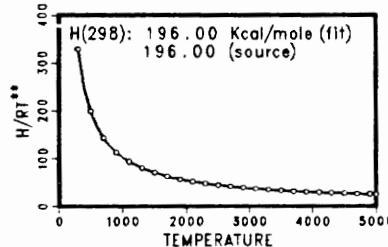
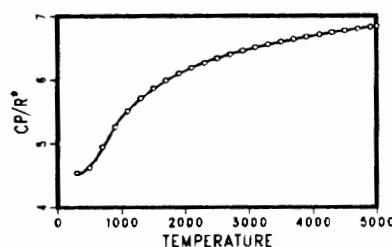
CARBON, TRIATOMIC

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04345527E+02	0.12644661E-02	-0.04652557E-04	0.08695855E-07	-0.04243535E-10	0.09731403E+06	0.03519437E+02
1000-5000K	0.03803709E+02	0.02253566E-01	-0.07704534E-05	0.13162939E-09	-0.08694264E-13	0.09736135E+06	0.06128062E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: C3H2

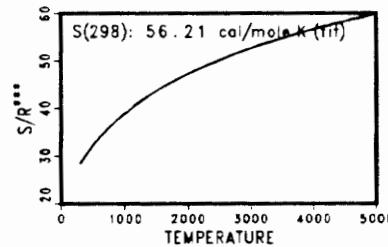
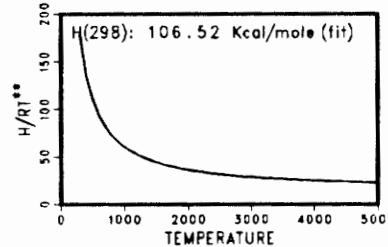
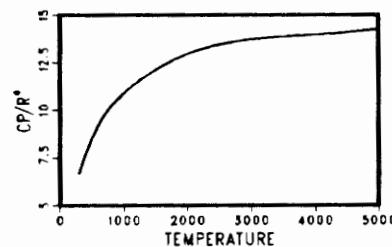
C3H2 RAD

GAS

As of: 12/16/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02691077E+02	0.14803664E-01	-0.03250551E-04	-0.08644363E-07	0.05284877E-10	0.05219072E+06	0.08757391E+02
1000-5000K	0.06530853E+02	0.05870316E-01	-0.01720776E-04	0.02127498E-08	-0.08291910E-13	0.05115213E+06	-0.11227278E+02



Source: BURCAT (LSU CALCULATIONS)

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: C3H4

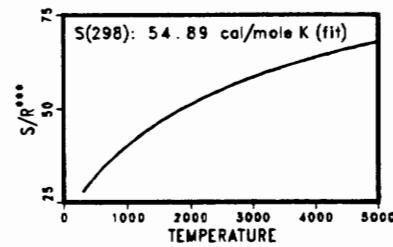
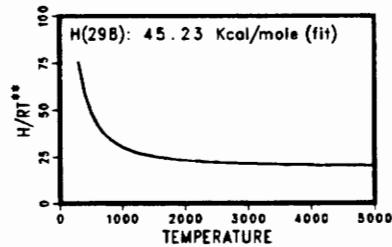
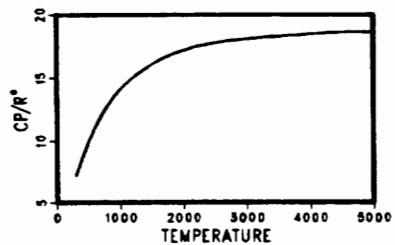
ALLENE

GAS

As of: 4/06/87

Fit

Coefficients	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	a <sub>4</sub>	a <sub>5</sub>	a <sub>6</sub>	a <sub>7</sub>
0300-1000K	-0.02131968E+01	0.03358713E+00	-0.03804870E-03	0.02745838E-06	-0.08690044E-10	0.02162048E+06	0.02029392E+03
1000-5000K	0.05729144E+02	0.12368045E-01	-0.04805626E-04	0.08601364E-08	-0.05812802E-12	0.02012984E+06	-0.09448668E+02



Source: SNLL FIT TO BURCAT VIBRATIONAL FREQUENCIES

Comments: (ERROR IN BURCAT COEFFICIENTS)

$$\begin{aligned} \bullet \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C3H4C

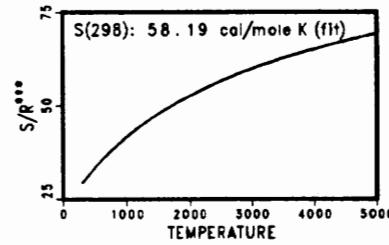
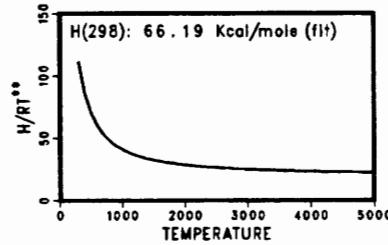
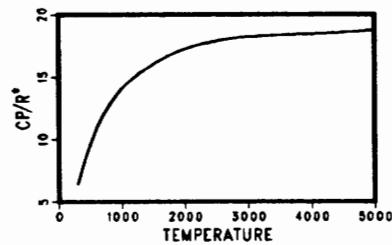
CYCLOPROPENE

GAS

As of: 12/16/86

Fit

Coefficients	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	a <sub>4</sub>	a <sub>5</sub>	a <sub>6</sub>	a <sub>7</sub>
0300-1000K	-0.02462104E+00	0.02319721E+00	-0.01847435E-04	-0.15927594E-07	0.08684615E-10	0.03233413E+06	0.02271659E+03
1000-5000K	0.06699993E+02	0.10357372E-01	-0.03455116E-04	0.05065295E-08	-0.02668227E-12	0.03019905E+06	-0.13391933E+02



Source: BURCAT (TECHNION REPORTS)

$$\begin{aligned} \bullet \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C3H4P

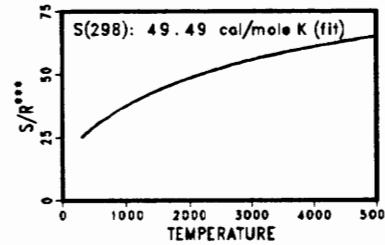
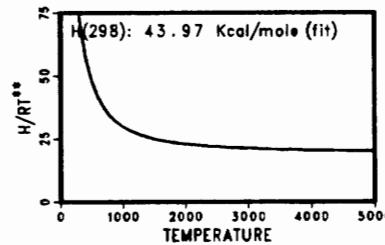
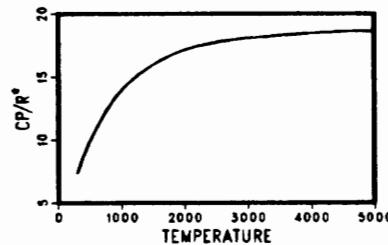
PROPYNE

GAS

As of: 4/06/87

Fit

Coefficients	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	a <sub>4</sub>	a <sub>5</sub>	a <sub>6</sub>	a <sub>7</sub>
0300-1000K	0.06271447E+01	0.03116179E+00	-0.03747663E-03	0.02964117E-06	-0.09987381E-10	0.02083492E+06	0.13468796E+02
1000-5000K	0.05511034E+02	0.12469562E-01	-0.04814164E-04	0.08573770E-08	-0.05771561E-12	0.01961967E+06	-0.10794748E+02



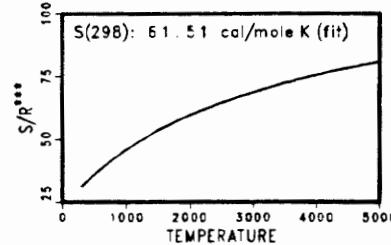
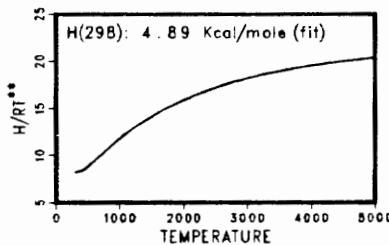
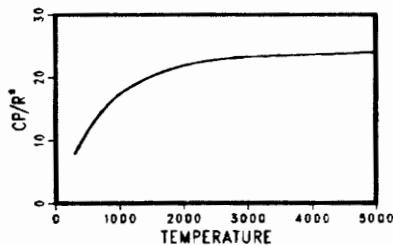
Source: SNLL FIT TO BURCAT VIBRATIONAL FREQUENCIES

Comments: (ERROR IN BURCAT COEFFICIENTS)

$$\begin{aligned} \bullet \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C3H6 PROPYLENE GAS As of: 12/01/86

Fit  
 Coefficients       $a_1$        $a_2$        $a_3$        $a_4$        $a_5$        $a_6$        $a_7$   
 0300-1000K    0.14933071E+01    0.02092517E+00    0.04486794E-04    -0.16689121E-07    0.07158146E-10    0.10748264E+04    0.16145340E+02  
 1000-5000K    0.06732257E+02    0.14908336E-01    -0.04949899E-04    0.07212022E-08    -0.03766204E-12    -0.09235703E+04    -0.13313348E+02

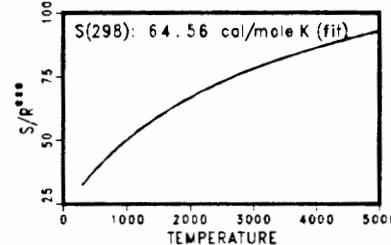
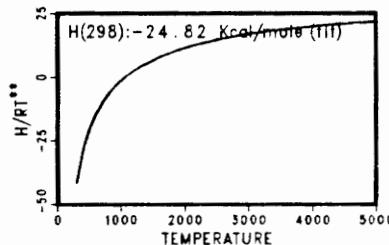
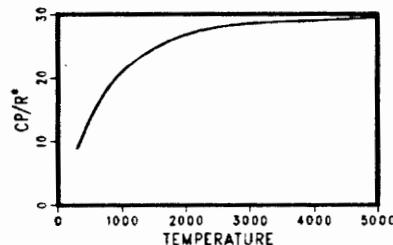


Source: BURCAT (TECHNION REPORTS)

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C3H8 PROPANE GAS As of: 12/01/86

Fit  
 Coefficients       $a_1$        $a_2$        $a_3$        $a_4$        $a_5$        $a_6$        $a_7$   
 0300-1000K    0.08969208E+01    0.02668986E+00    0.05431425E-04    -0.02126000E-06    0.09243330E-10    -0.13954918E+05    0.01935533E+03  
 1000-5000K    0.07525217E+02    0.01889034E+00    -0.06283924E-04    0.09179373E-08    -0.04812410E-12    -0.16464548E+05    -0.01784390E+03

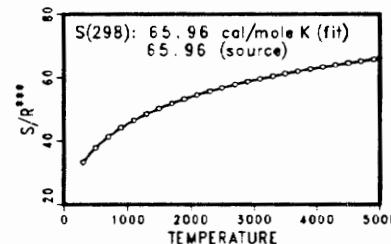
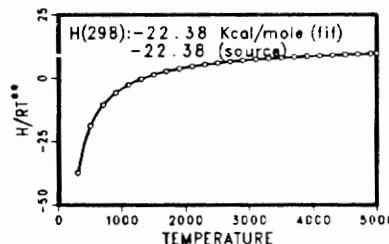
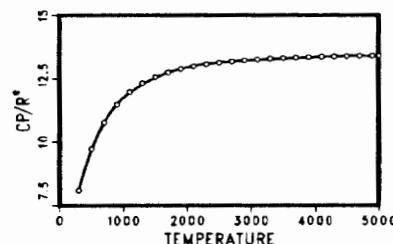


Source: BURCAT (NASA LEWIS TABLES)

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C3O2 CARBON SUBOXIDE GAS As of: 12/12/86

Fit  
 Coefficients       $a_1$        $a_2$        $a_3$        $a_4$        $a_5$        $a_6$        $a_7$   
 0300-1000K    0.04018127E+02    0.01836660E+00    -0.01907148E-03    0.11855871E-07    -0.03418747E-10    -0.13128236E+05    0.05582083E+02  
 1000-5000K    0.08098897E+02    0.05560039E-01    -0.02312264E-04    0.04340709E-08    -0.03036387E-12    -0.14214353E+05    -0.15219745E+02



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C4

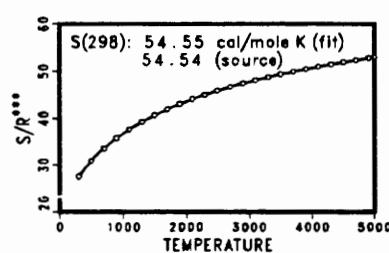
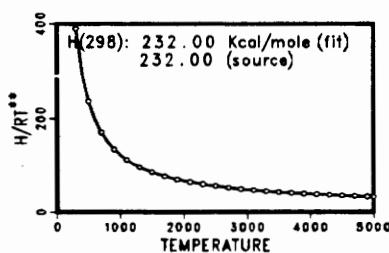
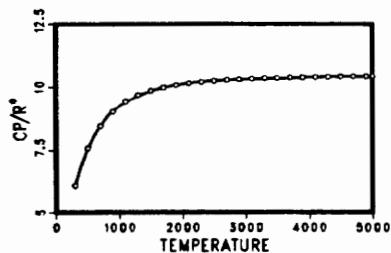
CARBON, TETRATOMIC

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02343028E+02	0.16429811E-01	-0.15279858E-04	0.07343826E-07	-0.15822743E-11	0.11545384E+06	0.09826204E+02
1000-5000K	0.06500180E+02	0.04228632E-01	-0.01790717E-04	0.03404812E-08	-0.02403978E-12	0.11434008E+06	-0.11488894E+02



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C4H

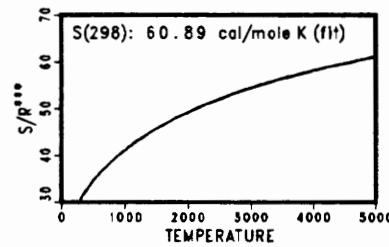
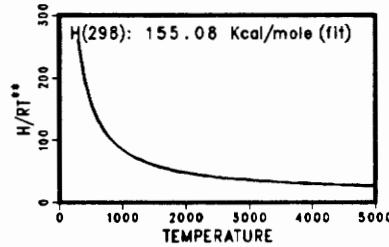
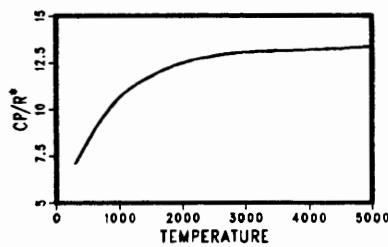
C4H RAD

GAS

As of: 12/16/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.05023247E+02	0.07092375E-01	-0.06073762E-07	-0.02275752E-07	0.08086994E-11	0.07623812E+06	-0.06942594E+00
1000-5000K	0.06242882E+02	0.06193682E-01	-0.02085931E-04	0.03082203E-08	-0.16364826E-13	0.07568019E+06	-0.07210806E+02



Source: BURCAT (TECHNION REPORTS)

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C4H2

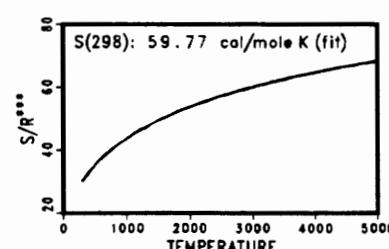
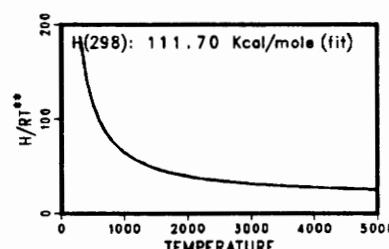
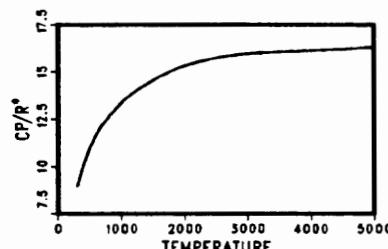
BUTADIYNE

GAS

As of: 12/16/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04005191E+02	0.01981000E+00	-0.09865877E-04	-0.06635158E-07	0.06077413E-10	0.05424065E+06	0.01845736E+02
1000-5000K	0.09031407E+02	0.06047252E-01	-0.01948788E-04	0.02754863E-08	-0.13856080E-13	0.05294735E+06	-0.02385067E+03



Source: BURCAT (LSU CALCULATIONS)

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

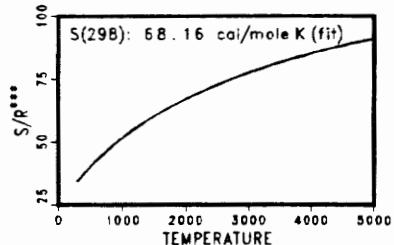
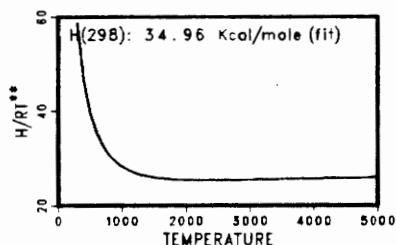
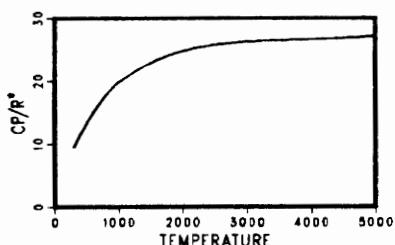
Species: C4H6

2-BUTAYN (DIMETHYLACETYLENE) GAS

As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03197108E+02	0.02025591E+00	0.06510192E-04	-0.16584423E-07	0.06400282E-10	0.15715203E+05	0.09895660E+02
1000-5000K	0.08046583E+02	0.16485251E-01	-0.05522227E-04	0.08123593E-08	-0.04295078E-12	0.13701305E+05	-0.01800457E+03



Source: BURCAT (TECHNION REPORTS)

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

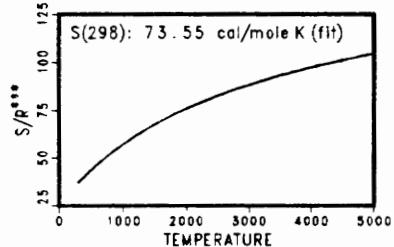
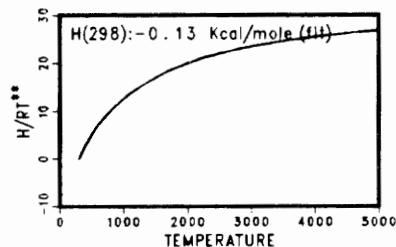
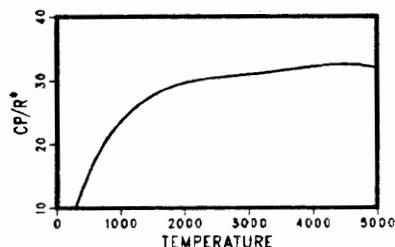
Species: C4H8

1-BUTENE GAS

As of: 12/03/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.11811380E+01	0.03085338E+00	0.05086524E-04	-0.02465488E-06	0.11110192E-10	-0.01790400E+05	0.02106247E+03
1000-5000K	0.02053584E+02	0.03435050E+00	-0.15883196E-04	0.03308966E-07	-0.02536104E-11	-0.02139723E+05	0.15543201E+02



Source: BURCAT (TECHNION REPORTS)

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

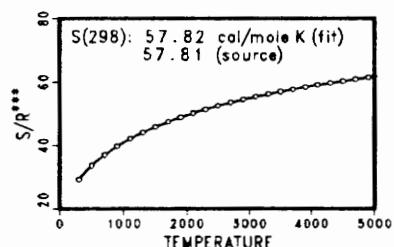
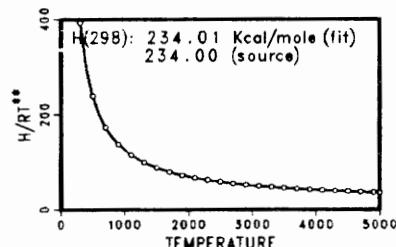
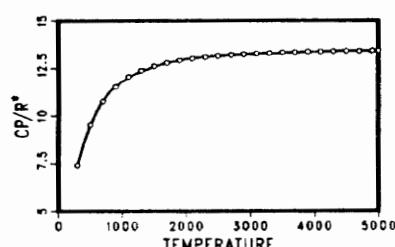
Species: C5

CARBON, PENTATOMIC GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02115273E+02	0.02326331E+00	-0.02109499E-03	0.09072734E-07	-0.15400926E-11	0.11627381E+06	0.10976027E+02
1000-5000K	0.08078081E+02	0.05743464E-01	-0.02436405E-04	0.04638916E-08	-0.03278909E-12	0.11470216E+06	-0.01953023E+03



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C5H

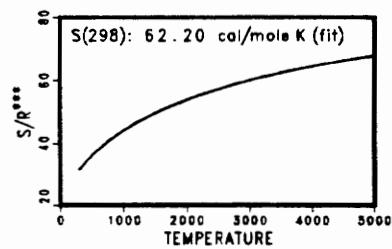
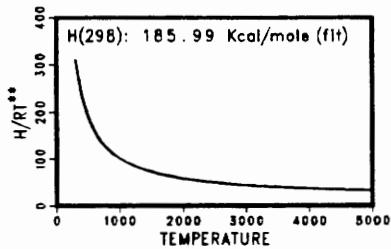
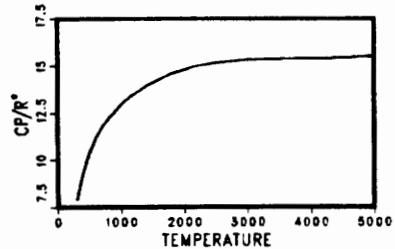
C5H RAD

GAS

As of: 2/03/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.16348248E+01	0.02509538E+00	-0.12066364E-04	-0.10465110E-07	0.08809988E-10	0.09212488E+06	0.15121937E+02
1000-5000K	0.08695749E+02	0.06054301E-01	-0.02016010E-04	0.02892892E-08	-0.14700996E-13	0.09031069E+06	-0.02101594E+03



Source: BURCAT FIT (TECHNION REPORTS)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C5H12

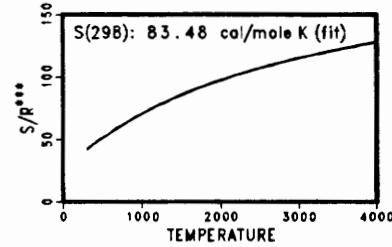
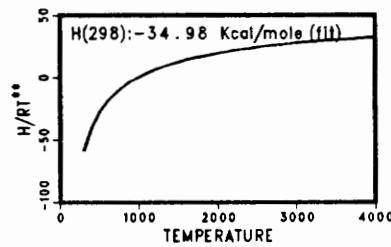
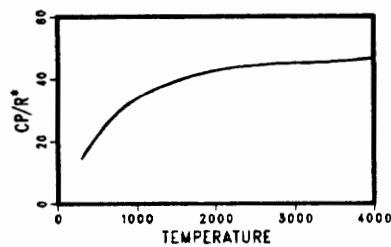
N-PENTANE

GAS

As of: 2/03/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.01877907E+02	0.04121645E+00	0.12532337E-04	-0.03701536E-06	0.15255685E-10	-0.02003815E+06	0.01877256E+03
1000-4000K	0.16677979E+02	0.02114483E+00	-0.03533321E-04	-0.05742202E-08	0.15159483E-12	-0.02553670E+06	-0.06372940E+03



Source: BURCAT FIT (TECHNION REPORTS)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C5H2

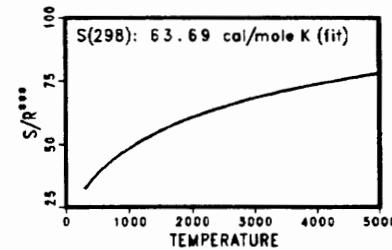
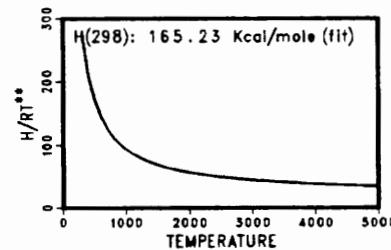
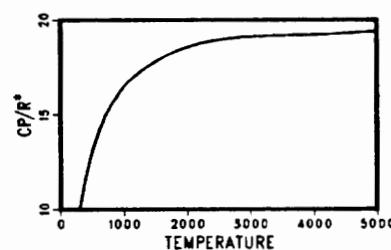
C5H2 RAD

GAS

As of: 2/05/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03062321E+02	0.02709998E+00	-0.10091697E-04	-0.12727451E-07	0.09167219E-10	0.08114969E+06	0.07071078E+02
1000-5000K	0.11329175E+02	0.07424056E-01	-0.02628188E-04	0.04082541E-08	-0.02301332E-12	0.07878706E+06	-0.03617117E+03



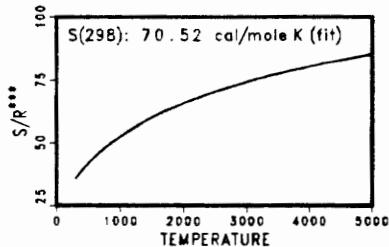
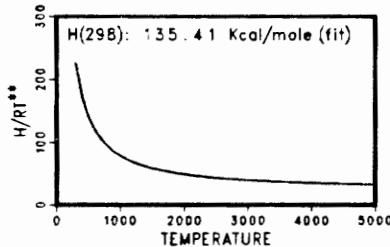
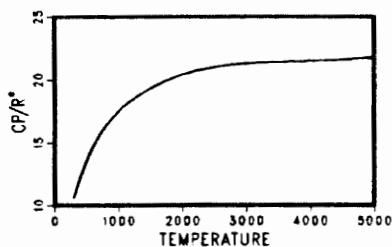
Source: BURCAT FIT (TECHNION REPORTS)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C5H3                    C5H3 RAD                    GAS                    As of: 2/03/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04328720E+02	0.02352480E+00	-0.05856723E-04	-0.12154494E-07	0.07726478E-10	0.06588531E+06	0.04173258E+02
1000-5000K	0.10787622E+02	0.09539619E-01	-0.03206744E-04	0.04733323E-08	-0.02512135E-12	0.06392904E+06	-0.03005444E+03



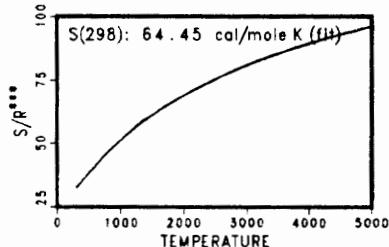
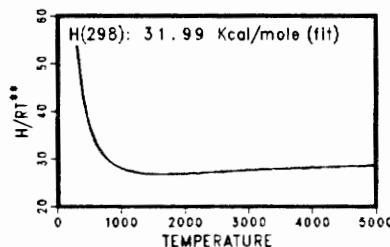
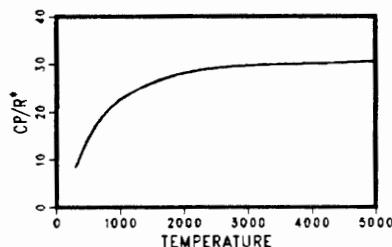
Source: BURCAT (TECHNION REPORTS)

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C5H6                    CYCLOPENTADIENE                    GAS                    As of: 2/03/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	-0.03196739E+02	0.04081361E+00	0.06816505E-05	-0.03137459E-06	0.15772230E-10	0.15290676E+05	0.03869938E+03
1000-5000K	0.09689815E+02	0.01838262E+00	-0.06264884E-04	0.09393377E-08	-0.05087708E-12	0.11021242E+05	-0.03122908E+03



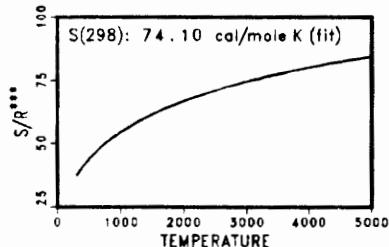
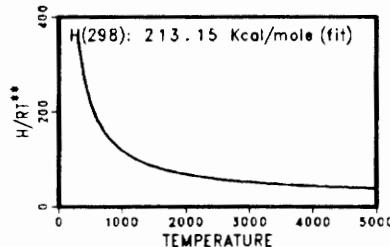
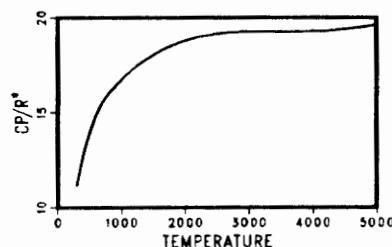
Source: BURCAT FIT (TECHNION REPORTS)

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C6H                    C6H RAD                    GAS                    As of: 12/16/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04769648E+02	0.02457279E+00	-0.07561252E-04	-0.14806908E-07	0.09768053E-10	0.10485231E+06	0.03241530E+02
1000-5000K	0.11587352E+02	0.07295362E-01	-0.02466008E-04	0.03407045E-08	-0.14981855E-13	0.10314481E+06	-0.03172578E+03



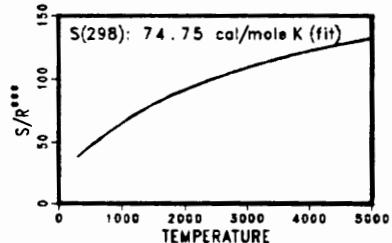
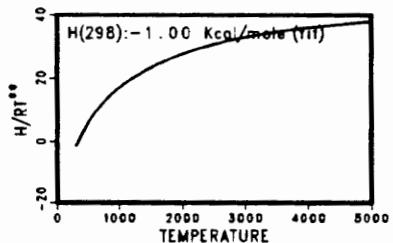
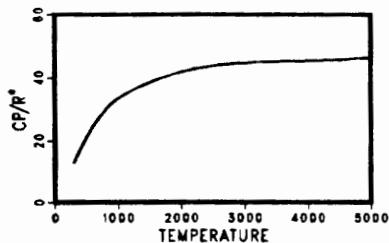
Source: BURCAT (LSU CALCULATIONS)

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C6H10 CYCLOHEXENE GAS As of: 2/03/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	-0.13942280E+01	0.04720693E+00	0.11960419E-04	-0.04162895E-06	0.01740335E-09	-0.02217790E+05	0.03129603E+03
1000-5000K	0.15927771E+02	0.02374412E+00	-0.06908672E-04	0.08109777E-08	-0.02683122E-12	-0.08642656E+05	-0.06525186E+03



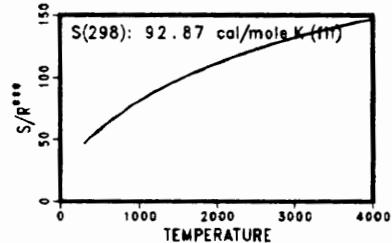
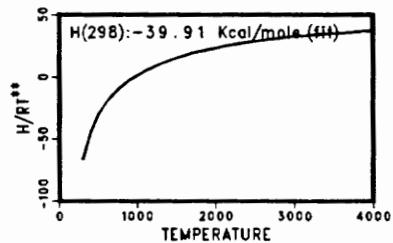
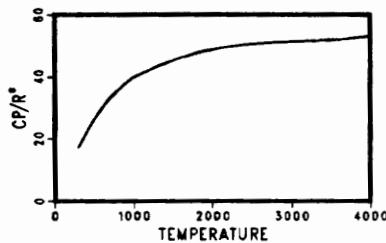
Source: BURCAT FIT (LSU CALCULATIONS)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C6H14 N-HEXANE GAS As of: 2/03/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.01836174E+02	0.05098461E+00	0.12595857E-04	-0.04428362E-06	0.01872237E-09	-0.02292749E+06	0.02088145E+03
1000-4000K	0.02280471E+03	0.02097989E+00	-0.03530674E-04	-0.05466245E-08	0.14789499E-12	-0.03073756E+06	-0.09583162E+03



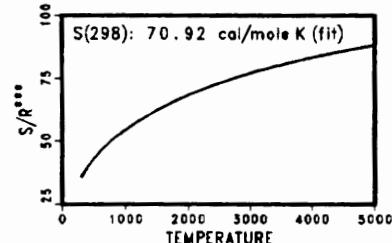
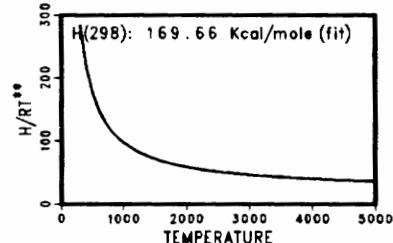
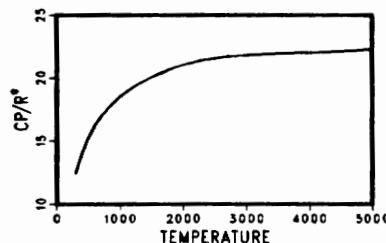
Source: BURCAT FIT (TECHNION REPORTS)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C6H2 HEXATRIYNE GAS As of: 12/16/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.05751085E+02	0.02636719E+00	-0.11667596E-04	-0.10714498E-07	0.08790297E-10	0.08262012E+06	-0.04335532E+02
1000-5000K	0.12756519E+02	0.08034381E-01	-0.02618215E-04	0.03725060E-08	-0.01878850E-12	0.08075469E+06	-0.04041262E+03



Source: BURCAT (LSU CALCULATIONS)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C6H3

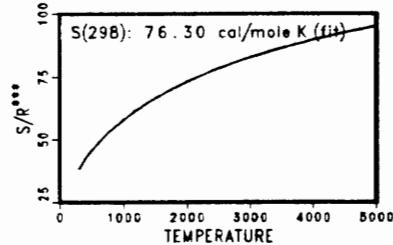
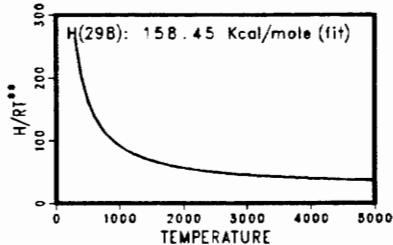
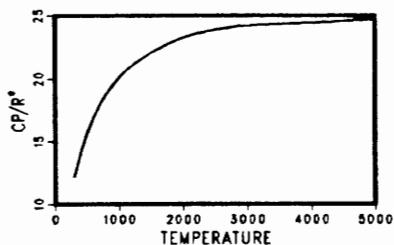
C6H3 RAD

GAS

As of: 2/03/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.05007089E+02	0.02692851E+00	-0.05919865E-04	-0.15272335E-07	0.09408310E-10	0.07713200E+06	0.02225621E+02
1000-5000K	0.12761181E+02	0.10385573E-01	-0.03479192E-04	0.05109733E-08	-0.02690965E-12	0.07477706E+06	-0.03891745E+03



Source: BURCAT FIT (LSU CALCULATIONS)

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C6H4

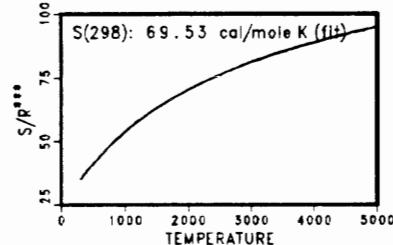
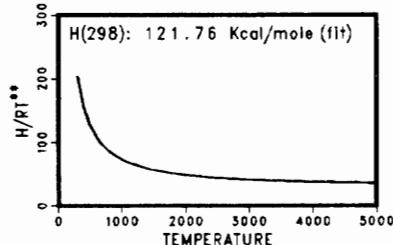
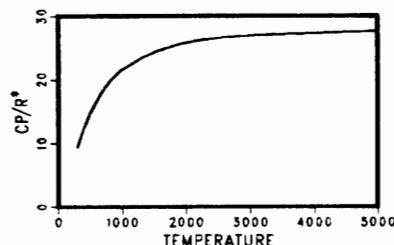
BENZYNE

GAS

As of: 2/03/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	-0.13004846E+01	0.03866476E+00	-0.03643944E-04	-0.02668580E-06	0.14509357E-10	0.06002907E+06	0.03124939E+03
1000-5000K	0.10062741E+02	0.01690304E+00	-0.06473045E-04	0.11240806E-08	-0.07307566E-12	0.05645373E+06	-0.02969310E+03



Source: BURCAT FIT (LSU CALCULATIONS)

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: C6H5

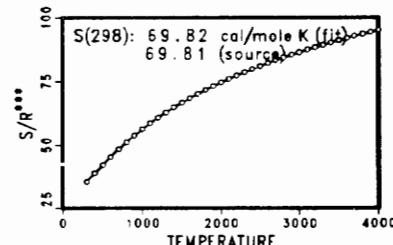
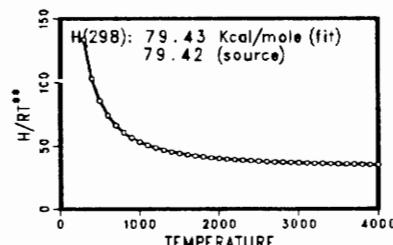
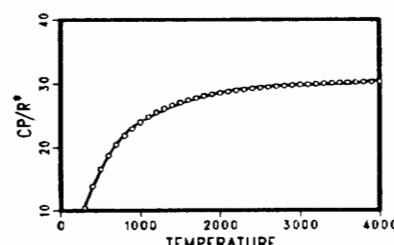
PHENYL

GAS

As of: 8/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.11435567E+00	0.03627324E+00	0.11582856E-05	-0.02196964E-06	0.08463556E-10	0.03836054E+06	0.02380117E+03
1000-4000K	0.15775887E+02	0.09651109E-01	-0.09429416E-05	-0.05469111E-08	0.10265216E-12	0.03302698E+06	-0.06176280E+03



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

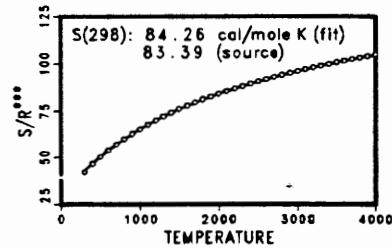
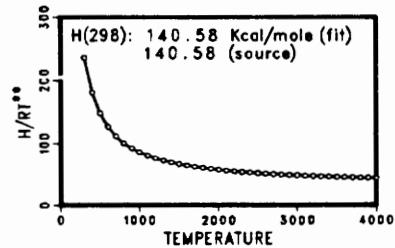
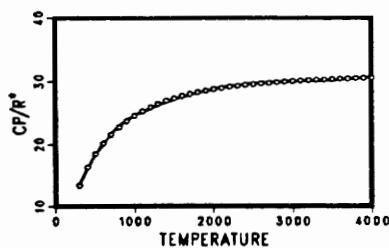
Species: C6H5(L)

HCCCHCHCHCH CCCCCIS HCCH CIS 2A' GAS

As of: 8/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04854268E+02	0.03031659E+00	0.01742892E-05	-0.01811010E-06	0.07392511E-10	0.06798733E+06	0.05854934E+02
1000-4000K	0.01721540E+03	0.08621068E-01	-0.08221340E-05	-0.04752164E-08	0.08844086E-12	0.06385819E+06	-0.06139128E+03



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C6H5O

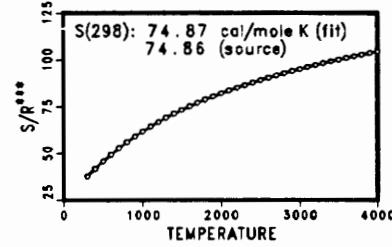
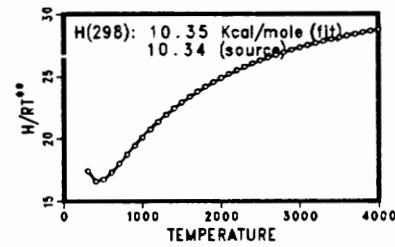
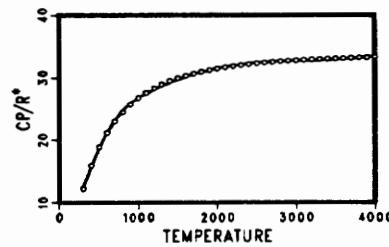
PHENOXY

GAS

As of: 8/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.11074965E+01	0.03956945E+00	0.08497295E-05	-0.02436311E-06	0.09650659E-10	0.03159672E+05	0.01973496E+03
1000-4000K	0.01822638E+03	0.10039851E-01	-0.09915668E-05	-0.05672804E-08	0.10683716E-12	-0.02620846E+05	-0.07361390E+03



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

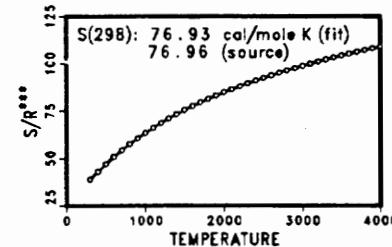
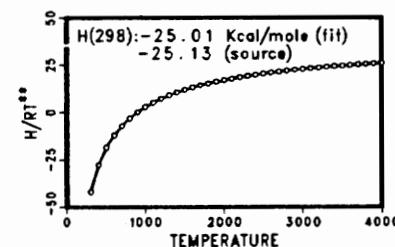
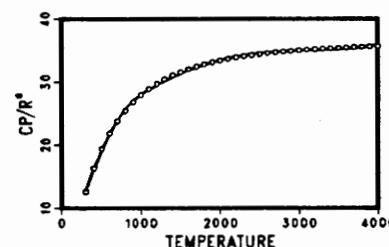
Species: C6H5OH

GAS

As of: 8/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.13914556E+01	0.03931957E+00	0.01777096E-04	-0.02277673E-06	0.08309659E-10	-0.14721809E+05	0.01917813E+03
1000-4000K	0.01821632E+03	0.11424269E-01	-0.10966843E-05	-0.06427442E-08	0.11988930E-12	-0.02053664E+06	-0.07304233E+03



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: C6H6

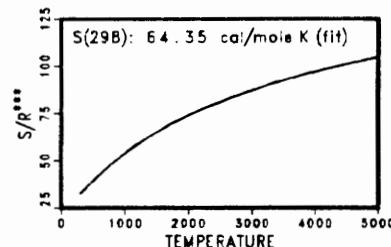
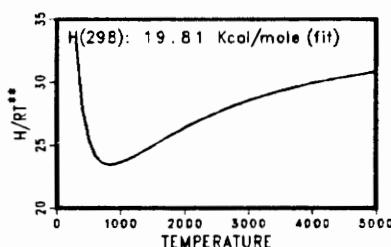
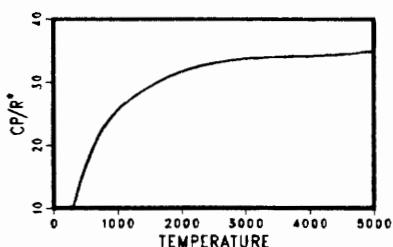
BENZENE

GAS

As of: 2/03/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	-0.03138012E+02	0.04723103E+00	-0.02962207E-04	-0.03262819E-06	0.01718691E-09	0.08890031E+05	0.03657573E+03
1000-5000K	0.12910740E+02	0.01723296E+00	-0.05024210E-04	0.05893497E-08	-0.01947521E-12	0.03664511E+05	-0.05002699E+03



Source: BURCAT FIT (LSU CALCULATIONS)

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C6H7

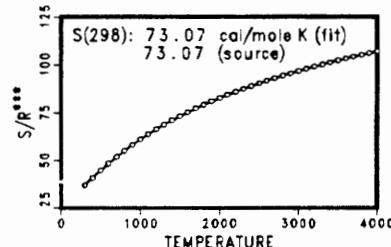
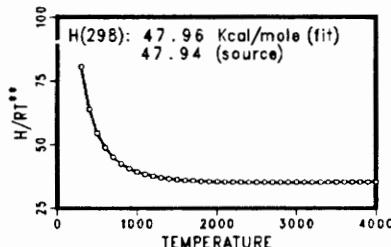
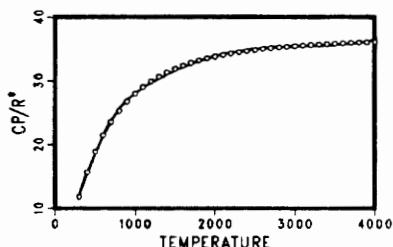
BENZYL 2B1

GAS

As of: 8/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04639166E+01	0.03975928E+00	0.02529095E-04	-0.02223792E-06	0.07557053E-10	0.02225169E+06	0.02235387E+03
1000-4000K	0.01755221E+03	0.12270795E-01	-0.11857424E-05	-0.06959661E-08	0.13013259E-12	0.16245813E+05	-0.07166588E+03



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C8H

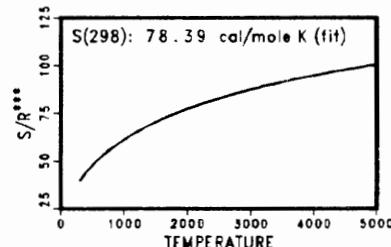
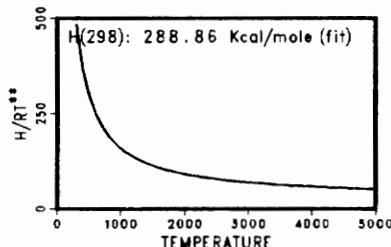
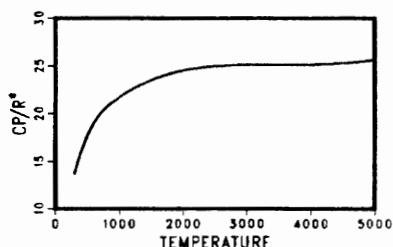
C8H RAD

GAS

As of: 12/16/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04489507E+02	0.03521521E+00	-0.10193898E-04	-0.02197024E-06	0.14214164E-10	0.14259919E+06	0.03996225E+02
1000-5000K	0.14749907E+02	0.09931501E-01	-0.03374841E-04	0.04687592E-08	-0.02073536E-12	0.13994481E+06	-0.04892689E+03



Source: BURCAT (LSU CALCULATIONS)

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: C8H2

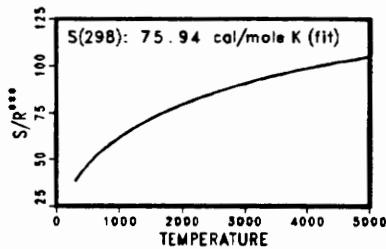
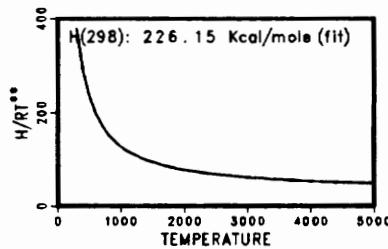
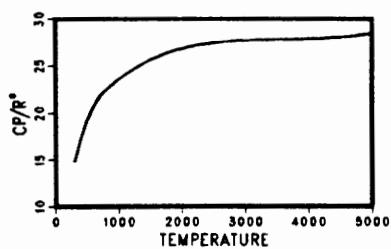
OCTATETRAYNE

GAS

As of: 12/16/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04630427E+02	0.03937080E+00	-0.11480348E-04	-0.02562213E-06	0.16707913E-10	0.11082850E+06	0.08077425E+01
1000-5000K	0.15680213E+02	0.11154614E-01	-0.03724372E-04	0.05197891E-08	-0.02375550E-12	0.10811225E+06	-0.05571437E+03



Source: BURCAT (LSU CALCULATIONS)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: CCL

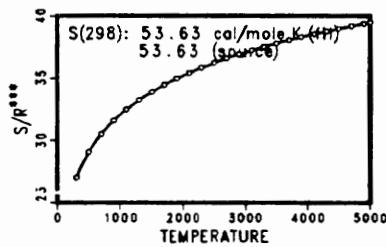
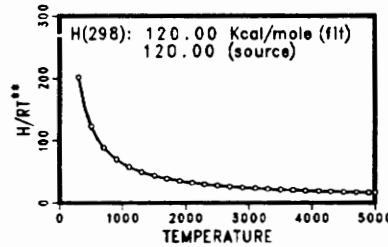
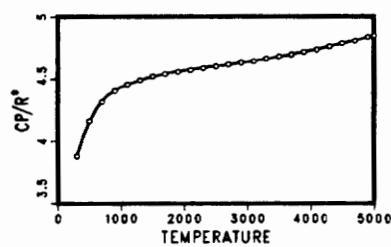
CARBON MONOCHLORIDE

GAS

As of: 11/29/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03188782E+02	0.02965197E-01	-0.02305370E-04	0.04866913E-08	0.09990141E-12	0.05932937E+06	0.08037628E+02
1000-5000K	0.04072804E+02	0.05508787E-02	-0.02319334E-05	0.04669038E-09	-0.03236856E-13	0.05909198E+06	0.03481073E+02



Source: SNLL FIT TO JANNAF DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: CCL2

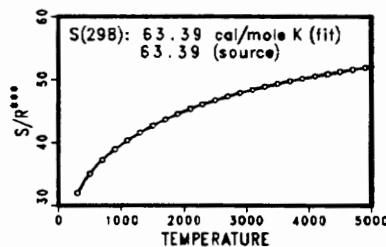
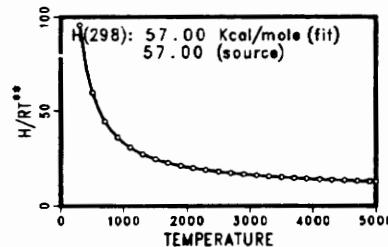
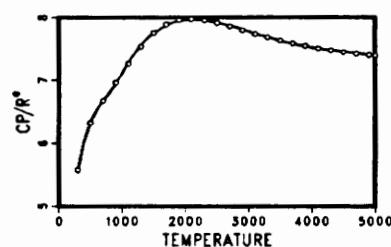
CARBON DICHLORIDE

GAS

As of: 11/29/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02651916E+02	0.15169552E-01	-0.02230162E-03	0.15041039E-07	-0.03452951E-10	0.02739027E+06	0.13136703E+02
1000-5000K	0.03501741E+02	0.05749397E-01	-0.02589721E-04	0.04783950E-08	-0.03188271E-12	0.02763633E+06	0.10829469E+02



Source: SNLL FIT TO JANNAF DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: CCL3

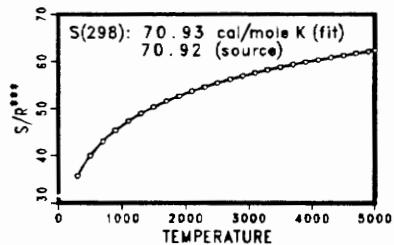
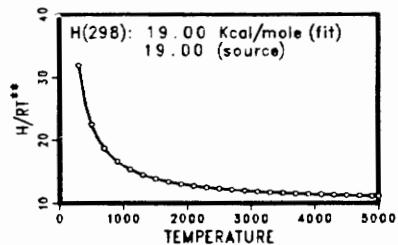
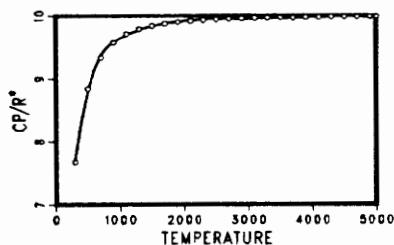
TRICHLOROMETHYL

GAS

As of: 11/29/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04866162E+02	0.11903691E-01	-0.07849049E-04	-0.14484371E-08	0.02169760E-10	0.07655364E+05	0.04781636E+02
1000-5000K	0.08639372E+02	0.15880909E-02	-0.07176410E-05	0.14271238E-09	-0.10407368E-13	0.06701065E+05	-0.14518221E+02



Source: SNLL FIT TO JANNAF DATA

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CCL4

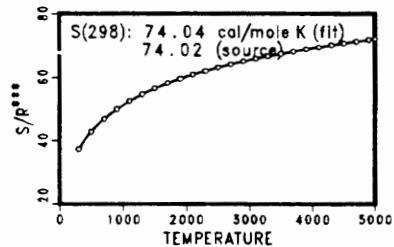
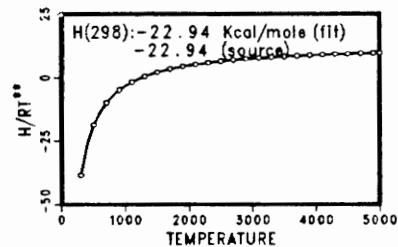
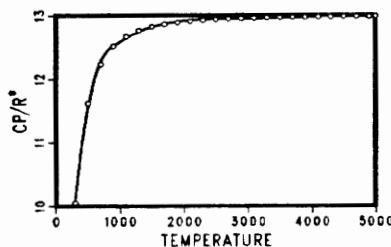
CARBON TETRACHLORIDE

GAS

As of: 11/29/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.06286815E+02	0.15997799E-01	-0.10203526E-04	-0.03043311E-07	0.03546287E-10	-0.14032573E+05	-0.02850812E+02
1000-5000K	0.11369968E+02	0.01933276E-01	-0.08832003E-05	0.01770067E-08	-0.12982896E-13	-0.15283466E+05	-0.02874324E+03



Source: SNLL FIT TO JANNAF DATA

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH

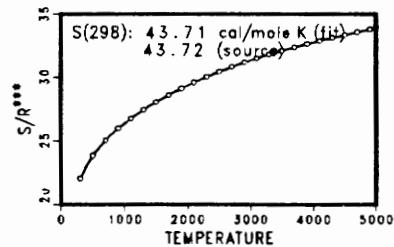
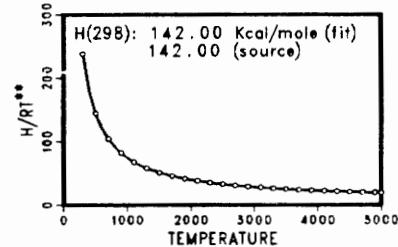
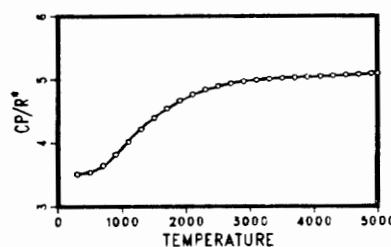
METHYLLIDYNE

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03200202E+02	0.02072875E-01	-0.05134431E-04	0.05733890E-07	-0.01955533E-10	0.07045259E+06	0.03331587E+02
1000-5000K	0.02196223E+02	0.02340381E-01	-0.07058201E-05	0.09007582E-09	-0.03855040E-13	0.07086723E+06	0.09178373E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

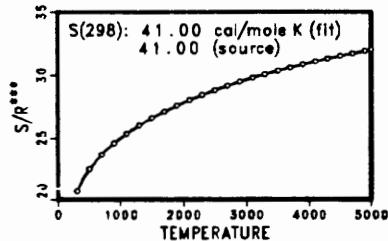
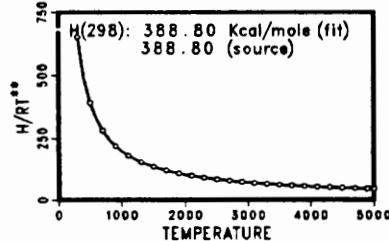
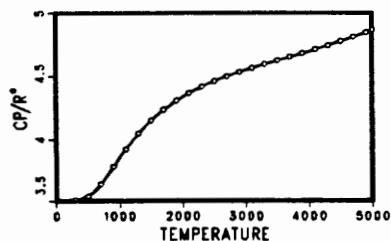
Species: CH+

METHYLDYNE, UNIPOSITIVE ION GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03327207E+02	0.13470505E-02	-0.03895861E-04	0.05129390E-07	-0.02054575E-10	0.01946452E+07	0.14084738E+01
1000-5000K	0.02753358E+02	0.15528998E-02	-0.05368453E-05	0.08921772E-09	-0.05416801E-13	0.01948467E+07	0.04654892E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet\bullet\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH2

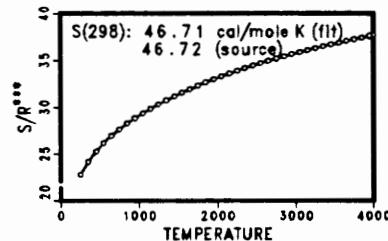
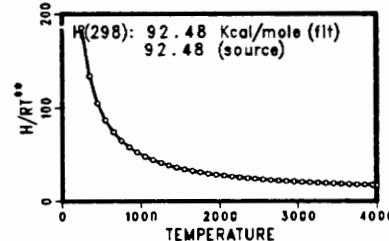
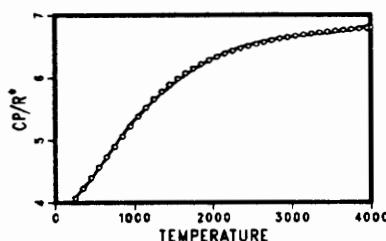
METHYLENE, TRIPLET

GAS

As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0250-1000K	0.03762237E+02	0.11598191E-02	0.02489585E-05	0.08800836E-08	-0.07332435E-11	0.04536790E+06	0.01712577E+02
1000-4000K	0.03636407E+02	0.01933056E-01	-0.01687016E-05	-0.10098994E-09	0.01808255E-12	0.04534134E+06	0.02156560E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet\bullet\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH2(S)

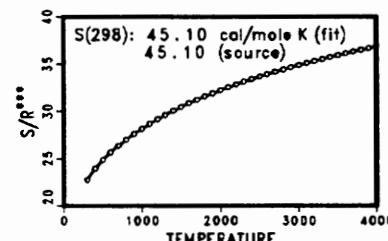
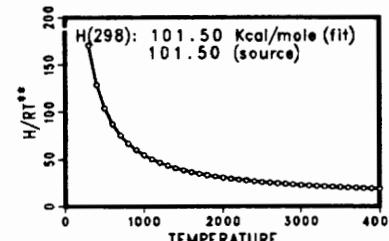
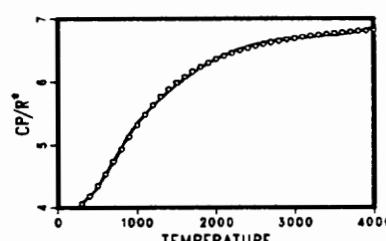
METHYLENE, SINGLET

GAS

As of: 3/12/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03971265E+02	-0.01699088E-02	0.10253689E-05	0.02492550E-07	-0.01981266E-10	0.04989367E+06	0.05753207E+00
1000-4000K	0.03552888E+02	0.02066788E-01	-0.01914116E-05	-0.11046733E-09	0.02021349E-12	0.04984975E+06	0.01686570E+02



Source: FIT TO BAC-MP4 DATA WITH H298=101.5 PER MILLER

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet\bullet\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

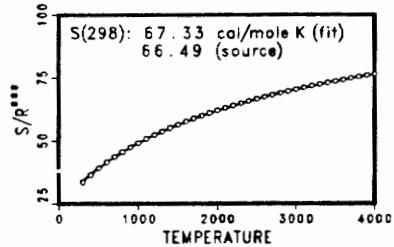
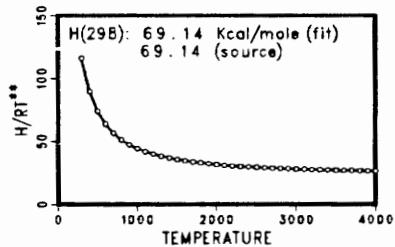
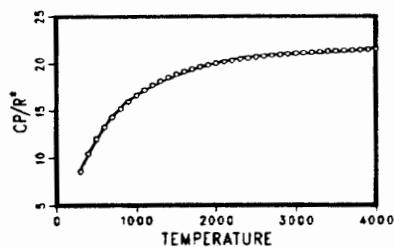
Species: CH<sub>2</sub>CHCCH

BUT-1-YN-3-ENE PLANAR CS GAS

As of: 8/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03233893E+02	0.01865634E+00	0.12703205E-05	-0.09410096E-07	0.02956110E-10	0.03301097E+06	0.09922676E+02
1000-4000K	0.10697773E+02	0.06982014E-01	-0.06567747E-05	-0.03884517E-08	0.07200946E-12	0.03034803E+06	-0.03128430E+03



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: CH<sub>2</sub>CHCCH<sub>2</sub>

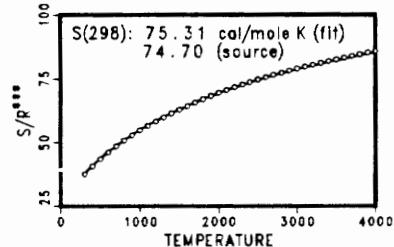
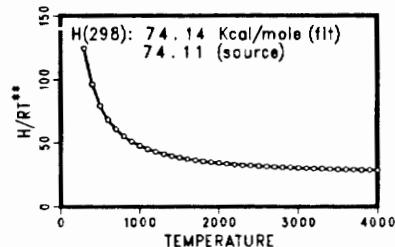
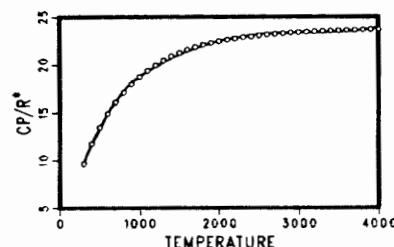
CS

GAS

As of: 8/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03879443E+02	0.01997663E+00	0.01872777E-04	-0.09306953E-07	0.02386116E-10	0.03526859E+06	0.09842152E+02
1000-4000K	0.11997762E+02	0.07990580E-01	-0.08098172E-05	-0.04568733E-08	0.08636911E-12	0.03228493E+06	-0.03528494E+03



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: CH<sub>2</sub>CHCH<sub>2</sub>

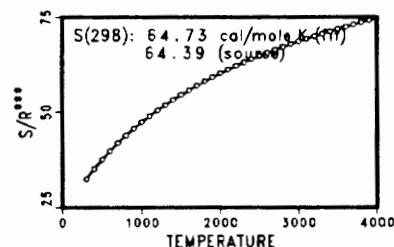
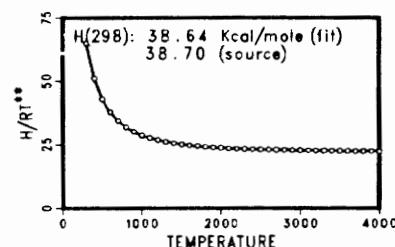
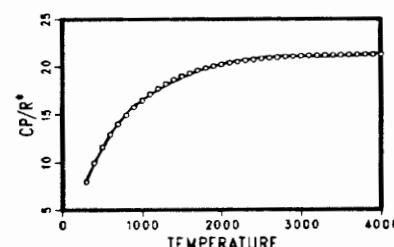
PROP-1-ENYL C2V 2A2

GAS

As of: 8/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02276486E+02	0.01985564E+00	0.11238421E-05	-0.10145757E-07	0.03441342E-10	0.01789496E+06	0.13725151E+02
1000-4000K	0.09651539E+02	0.08075596E-01	-0.07965424E-05	-0.04650696E-08	0.08603281E-12	0.15300955E+05	-0.02686773E+03



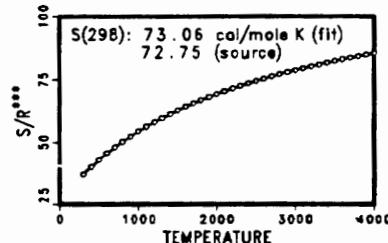
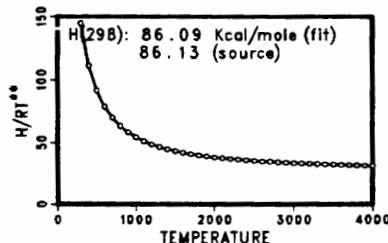
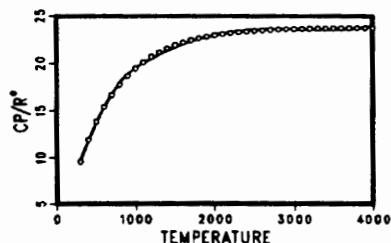
Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: CH<sub>2</sub>CHCHCH      2A' CCCC TRANS HCCH CIS      GAS      As of: 8/24/89

Fit

Coefficients	$\alpha_1$	$\alpha_2$	$\alpha_3$	$\alpha_4$	$\alpha_5$	$\alpha_6$	$\alpha_7$
0300-1000K	0.02995240E+02	0.02288456E+00	0.01975471E-04	-0.11482454E-07	0.03197823E-10	0.04142218E+06	0.12894539E+02
1000-4000K	0.12865971E+02	0.07943369E-01	-0.08626466E-05	-0.04655635E-08	0.08951131E-12	0.03783552E+06	-0.04182502E+03



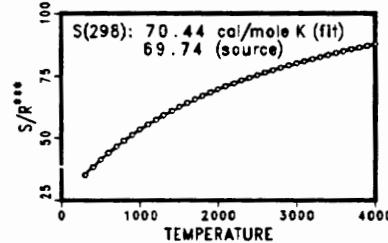
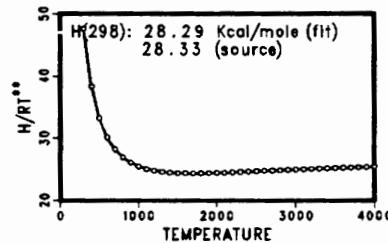
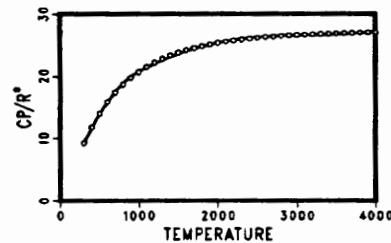
Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= \alpha_1 + \alpha_2 T + \alpha_3 T^2 + \alpha_4 T^3 + \alpha_5 T^4 \\ ** \text{H/RT} &= \alpha_1 + \alpha_2 T / 2 + \alpha_3 T^2 / 3 + \alpha_4 T^3 / 4 + \alpha_5 T^4 / 5 + \alpha_6 / T \\ *** \text{S/R} &= \alpha_1 \ln(T) + \alpha_2 T + \alpha_3 T^2 / 2 + \alpha_4 T^3 / 3 + \alpha_5 T^4 / 4 + \alpha_7 \end{aligned}$$

Species: CH<sub>2</sub>CHCHCH<sub>2</sub>      TRANS-1,3-BUTADIENE      GAS      As of: 12/01/89

Fit

Coefficients	$\alpha_1$	$\alpha_2$	$\alpha_3$	$\alpha_4$	$\alpha_5$	$\alpha_6$	$\alpha_7$
0300-1000K	0.01931624E+02	0.02479030E+00	0.03018071E-04	-0.11546856E-07	0.02586623E-10	0.12554682E+05	0.01701999E+03
1000-4000K	0.12544366E+02	0.09596525E-01	-0.09187012E-05	-0.05429640E-08	0.10053636E-12	0.08597330E+05	-0.04217450E+03



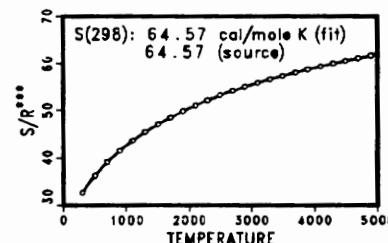
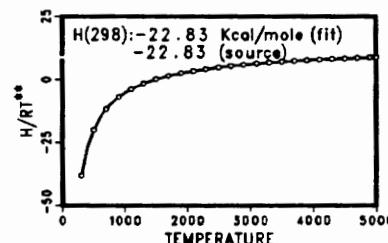
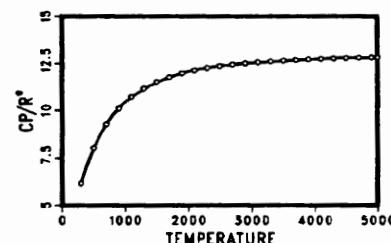
Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= \alpha_1 + \alpha_2 T + \alpha_3 T^2 + \alpha_4 T^3 + \alpha_5 T^4 \\ ** \text{H/RT} &= \alpha_1 + \alpha_2 T / 2 + \alpha_3 T^2 / 3 + \alpha_4 T^3 / 4 + \alpha_5 T^4 / 5 + \alpha_6 / T \\ *** \text{S/R} &= \alpha_1 \ln(T) + \alpha_2 T + \alpha_3 T^2 / 2 + \alpha_4 T^3 / 3 + \alpha_5 T^4 / 4 + \alpha_7 \end{aligned}$$

Species: CH<sub>2</sub>CL<sub>2</sub>      DICHLOROMETHANE      GAS      As of: 11/29/89

Fit

Coefficients	$\alpha_1$	$\alpha_2$	$\alpha_3$	$\alpha_4$	$\alpha_5$	$\alpha_6$	$\alpha_7$
0300-1000K	0.14232844E+01	0.02116658E+00	-0.02178088E-03	0.13458726E-07	-0.03811649E-10	-0.12686636E+05	0.01893445E+03
1000-5000K	0.05917327E+02	0.06762395E-01	-0.02676163E-04	0.04856687E-08	-0.03316973E-12	-0.13859256E+05	-0.03877739E+02



Source: SNLL FIT TO JANNAF DATA

$$\begin{aligned} * \text{CP/R} &= \alpha_1 + \alpha_2 T + \alpha_3 T^2 + \alpha_4 T^3 + \alpha_5 T^4 \\ ** \text{H/RT} &= \alpha_1 + \alpha_2 T / 2 + \alpha_3 T^2 / 3 + \alpha_4 T^3 / 4 + \alpha_5 T^4 / 5 + \alpha_6 / T \\ *** \text{S/R} &= \alpha_1 \ln(T) + \alpha_2 T + \alpha_3 T^2 / 2 + \alpha_4 T^3 / 3 + \alpha_5 T^4 / 4 + \alpha_7 \end{aligned}$$

Species: CH<sub>2</sub>CO

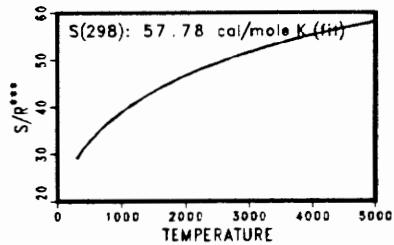
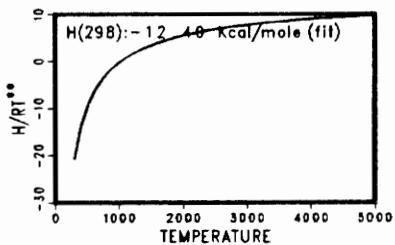
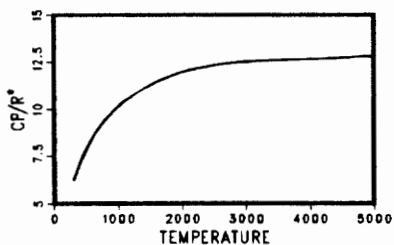
KETENE

GAS

As of: 12/16/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02974970E+02	0.12118712E-01	-0.02345045E-04	-0.06466685E-07	0.03905649E-10	-0.07632636E+05	0.08673553E+02
1000-5000K	0.06038817E+02	0.05804840E-01	-0.01920953E-04	0.02794484E-08	-0.14588676E-13	-0.08563402E+05	-0.07657581E+02



Source: BURCAT (C2H2O) (TECHNION REPORTS)

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: CH<sub>2</sub>F<sub>2</sub>

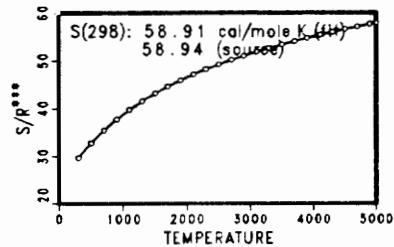
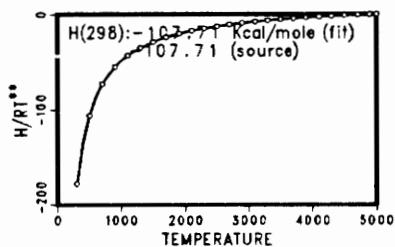
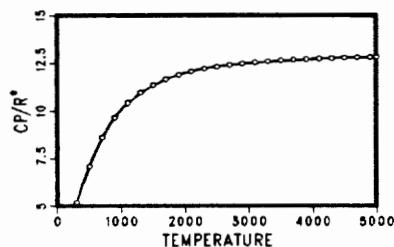
DIFLUOROMETHANE

GAS

As of: 8/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03669433E+01	0.02168917E+00	-0.02441912E-03	0.01942310E-06	-0.06978343E-10	-0.05510102E+06	0.02202214E+03
1000-5000K	0.04730052E+02	0.07997300E-01	-0.03186045E-04	0.05801159E-08	-0.03967925E-12	-0.05637288E+06	-0.04954843E+01



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

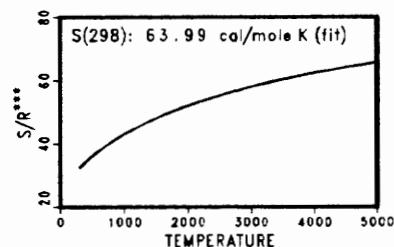
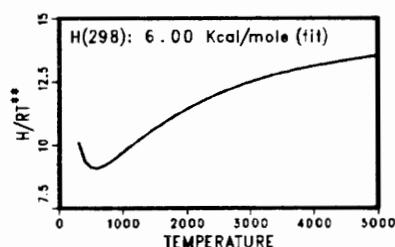
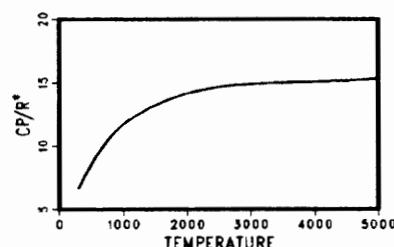
Species: CH<sub>2</sub>HCOCH<sub>2</sub>HCO RAD

GAS

As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03409062E+02	0.10738574E-01	0.01891492E-04	-0.07158583E-07	0.02867385E-10	0.15214766E+04	0.09558290E+02
1000-5000K	0.05975670E+02	0.08130591E-01	-0.02743624E-04	0.04070304E-08	-0.02176017E-12	0.04903218E+04	-0.05045251E+02



Source: BURCAT, C2H30A (CH2CHO) (TECHNION REPORTS)

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: CH<sub>2</sub>O

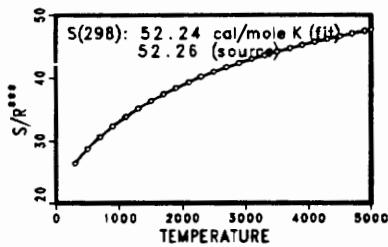
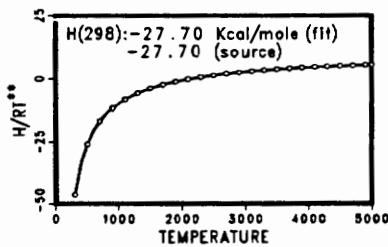
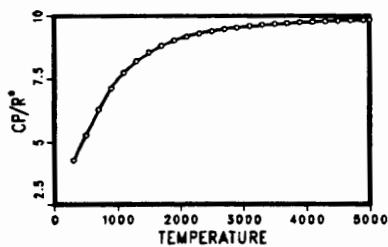
## FORMALDEHYDE

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.16527311E+01	0.12631439E-01	-0.01888168E-03	0.02050031E-06	-0.08413237E-10	-0.14865404E+05	0.13784820E+02
1000-5000K	0.02995606E+02	0.06681321E-01	-0.02628954E-04	0.04737153E-08	-0.03212517E-12	-0.15320369E+05	0.06912572E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: CH<sub>2</sub>OH

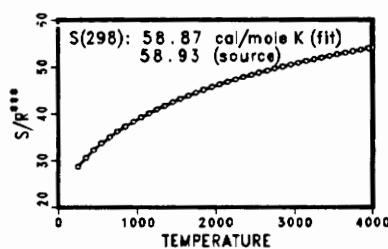
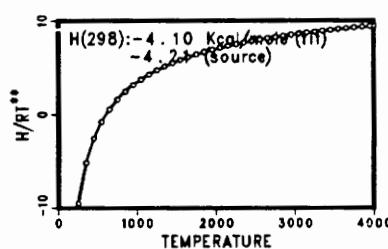
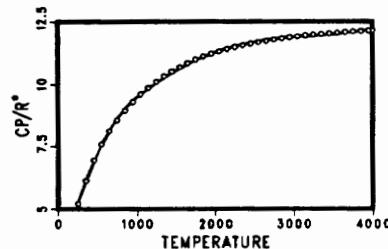
## HYDROXYMETHYLENE RAD

GAS

As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0250-1000K	0.02862628E+02	0.10015273E-01	-0.05285435E-05	-0.05138539E-07	0.02246041E-10	-0.03349678E+05	0.10397938E+02
1000-4000K	0.06327520E+02	0.03608270E-01	-0.03201547E-05	-0.01938750E-08	0.03509704E-12	-0.04474509E+05	-0.08329365E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: CH<sub>3</sub>

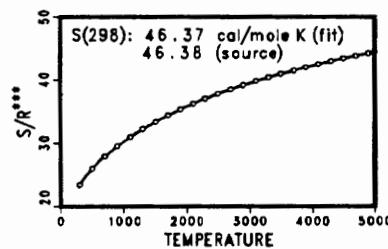
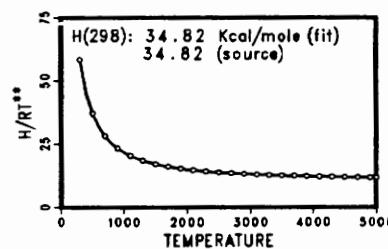
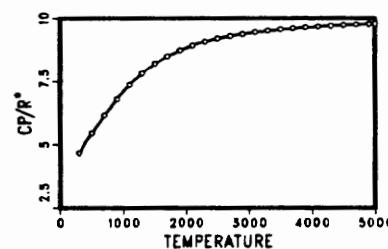
## METHYL

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02430442E+02	0.11124099E-01	-0.01680220E-03	0.16218288E-07	-0.05864952E-10	0.16423781E+05	0.06789794E+02
1000-5000K	0.02844051E+02	0.06137974E-01	-0.02230345E-04	0.03785161E-08	-0.02452159E-12	0.16437809E+05	0.05452697E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

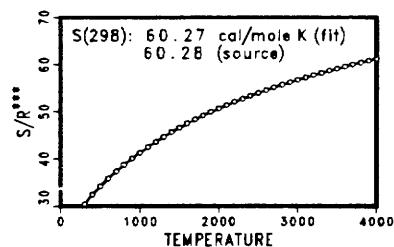
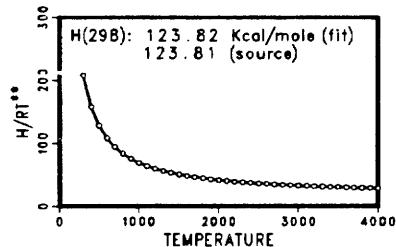
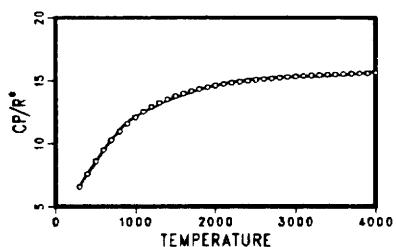
$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: CH<sub>3</sub>CC                          1-PROPYNYL C3V 2A1                          GAS                          As of: 8/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03798751E+02	0.08749062E-01	0.02523014E-04	-0.15293730E-08	-0.14105619E-11	0.06077425E+06	0.05989223E+02
1000-4000K	0.07640221E+02	0.05233556E-01	-0.05053635E-05	-0.02919772E-08	0.05445700E-12	0.05909763E+06	-0.16295735E+02



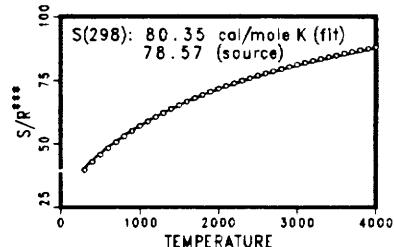
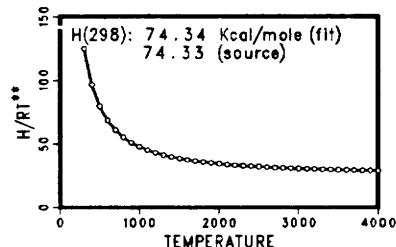
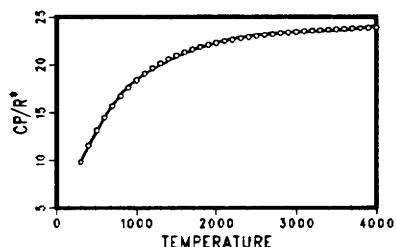
Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP}/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H}/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S}/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: CH<sub>3</sub>CCCH<sub>2</sub>                          HCCC CIS                          GAS                          As of: 8/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.05068450E+02	0.15717475E-01	0.02968975E-04	-0.04990586E-07	-0.02984224E-11	0.03518855E+06	0.06791893E+02
1000-4000K	0.11565059E+02	0.08030297E-01	-0.07649450E-05	-0.04476533E-08	0.08313260E-12	0.03256813E+06	-0.03014066E+03



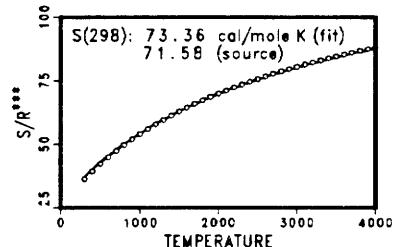
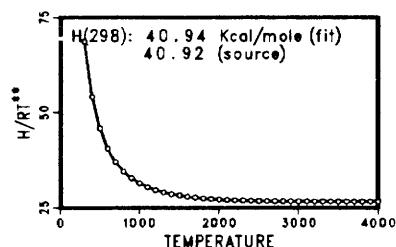
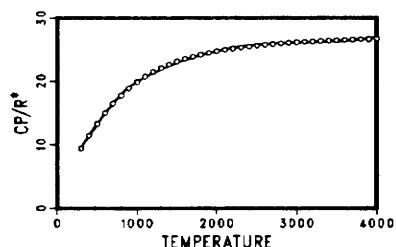
Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP}/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H}/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S}/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: CH<sub>3</sub>CCCH<sub>3</sub>                          2-BUTYNE                          GAS                          As of: 12/01/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04077105E+02	0.01703158E+00	0.04707490E-04	-0.03767239E-07	-0.02066962E-10	0.01859756E+06	0.08444801E+02
1000-4000K	0.11336582E+02	0.10057637E-01	-0.09511323E-05	-0.05660496E-08	0.10494509E-12	0.15476594E+05	-0.03350866E+03



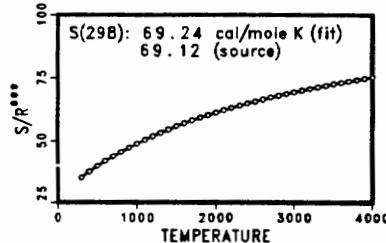
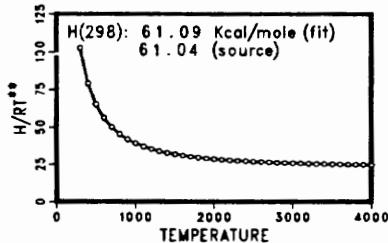
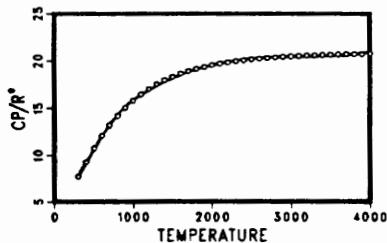
Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP}/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H}/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S}/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: CH<sub>3</sub>CCH<sub>2</sub>      1-METHYL-ETHENYL CS 2A'      GAS      As of: 8/24/89

Fit

	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03385811E+02	0.14045337E-01	0.03204127E-04	-0.03824120E-07	-0.09053742E-11	0.02909066E+06	0.11266487E+02
1000-4000K	0.09101018E+02	0.07964167E-01	-0.07884945E-05	-0.04562036E-08	0.08529212E-12	0.02670680E+06	-0.02150559E+03



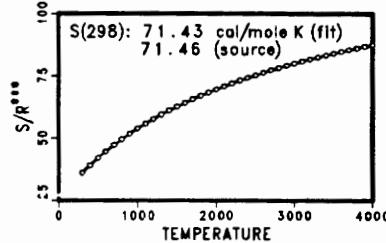
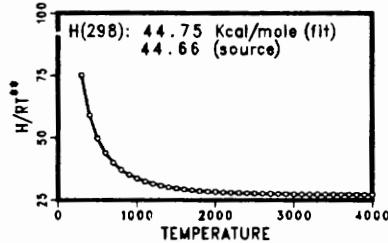
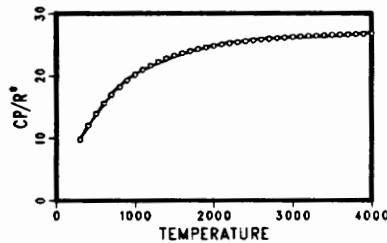
Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: CH<sub>3</sub>CH<sub>2</sub>CCH      1-BUTYNE      GAS      As of: 12/01/89

Fit

	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03726043E+02	0.02053492E+00	0.03021439E-04	-0.08131812E-07	0.10952799E-11	0.02048821E+06	0.08538826E+02
1000-4000K	0.12006946E+02	0.09576069E-01	-0.08995018E-05	-0.05369808E-08	0.09934174E-12	0.01729419E+06	-0.03802692E+03



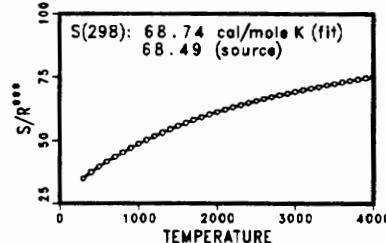
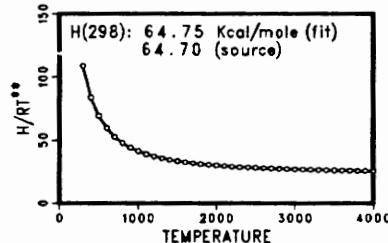
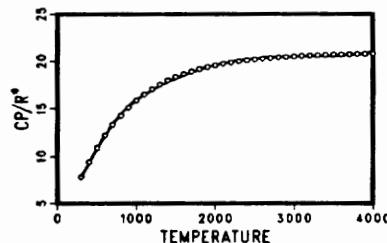
Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: CH<sub>3</sub>CHCH      PROP-1-ENYL HC=CHCIS 2A'      GAS      As of: 8/24/89

Fit

	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03161863E+02	0.15180997E-01	0.02722659E-04	-0.05177112E-07	0.05435286E-12	0.03095547E+06	0.11979733E+02
1000-4000K	0.09209764E+02	0.07871412E-01	-0.07724522E-05	-0.04497357E-08	0.08377272E-12	0.02853967E+06	-0.02232369E+03



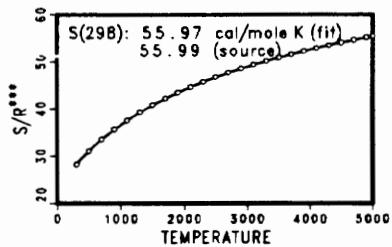
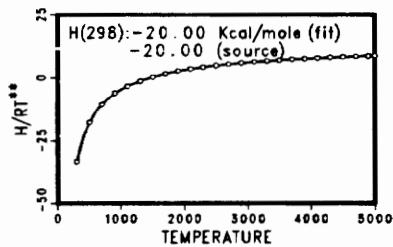
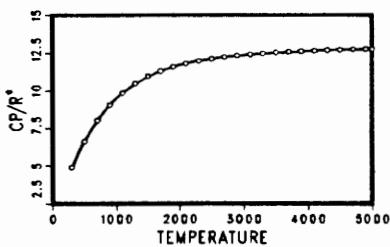
Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: CH3CL      METHYL CHLORIDE      GAS      As of: 11/29/89

Fit

	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04621901E+01	0.02068247E+00	-0.02553133E-03	0.02160310E-06	-0.07706816E-10	-0.10936672E+05	0.02032976E+03
1000-5000K	0.03633875E+02	0.08664625E-01	-0.03343871E-04	0.05950130E-08	-0.04001401E-12	-0.11776588E+05	0.04430651E+02



Source: SNLL FIT TO JANAF DATA

Comments: ALSO CALLED CHLOROMETHANE

$$\begin{aligned} * \text{CP}/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H}/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S}/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: CH3CO

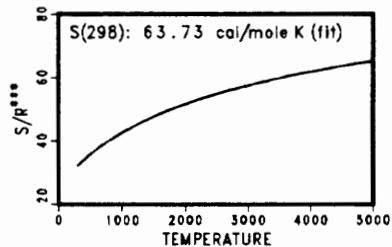
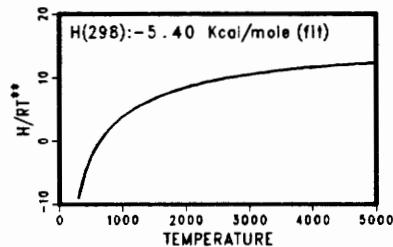
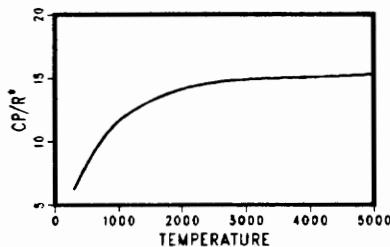
CH3CO RAD

GAS

As of: 12/01/86

Fit

	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03125278E+02	0.09778220E-01	0.04521448E-04	-0.09009462E-07	0.03193717E-10	-0.04108507E+05	0.11228854E+02
1000-5000K	0.05612279E+02	0.08449886E-01	-0.02854147E-04	0.04238376E-08	-0.02268403E-12	-0.05187863E+05	-0.03274949E+02



Source: BURCAT C2H30B (CH3CO) (TECHNION REPORTS)

$$\begin{aligned} * \text{CP}/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H}/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S}/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: CH3F

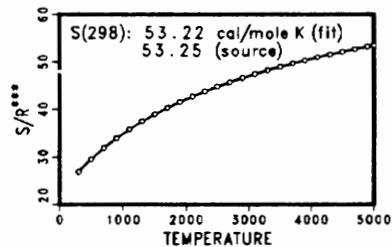
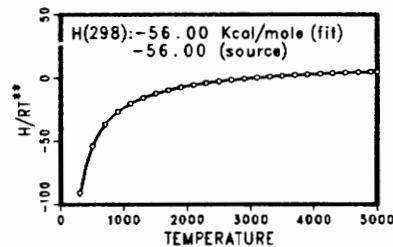
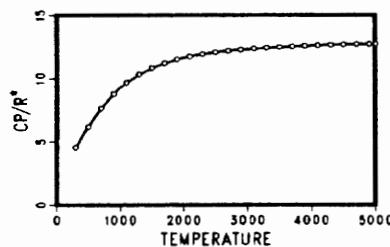
FLUOROMETHANE

GAS

As of: 8/24/89

Fit

	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02600910E+01	0.02000787E+00	-0.02662584E-03	0.02561176E-06	-0.09935237E-10	-0.02896232E+06	0.02031799E+03
1000-5000K	0.03014978E+02	0.09314397E-01	-0.03611697E-04	0.06443728E-08	-0.04339594E-12	-0.02977838E+06	0.06323815E+02



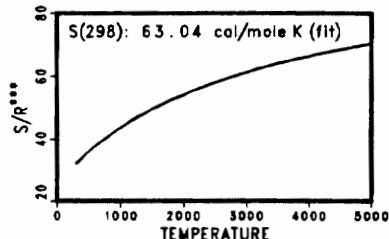
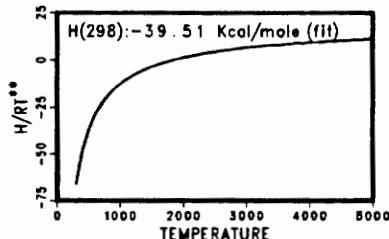
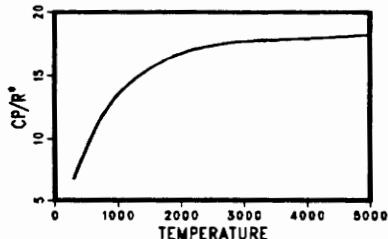
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP}/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H}/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S}/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: CH<sub>3</sub>HCO ACETALDEHYDE GAS As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02505695E+02	0.13369907E-01	0.04671953E-04	-0.11281401E-07	0.04263566E-10	-0.02124588E+06	0.13350887E+02
1000-5000K	0.05868650E+02	0.10794241E-01	-0.03645530E-04	0.05412912E-08	-0.02896844E-12	-0.02264568E+06	-0.06012946E+02



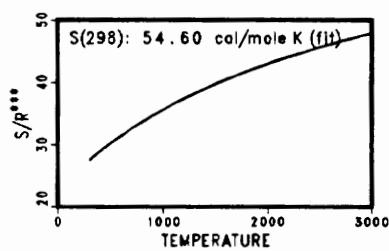
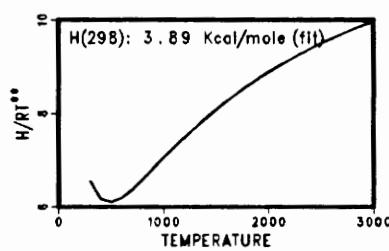
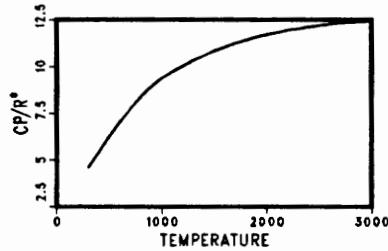
Source: BURCAT (C2H40A) (TECHNION REPORTS)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: CH<sub>3</sub>O METHYLOXIDE (METHOXY RAD) GAS As of: 12/16/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02106204E+02	0.07216595E-01	0.05338472E-04	-0.07377636E-07	0.02075610E-10	0.09786011E+04	0.13152177E+02
1000-3000K	0.03770799E+02	0.07871497E-01	-0.02656384E-04	0.03944431E-08	-0.02112616E-12	0.12783252E+03	0.02929575E+02



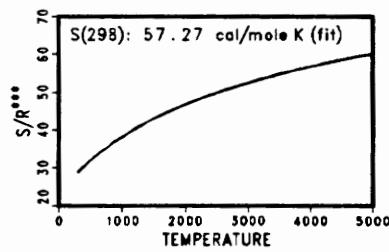
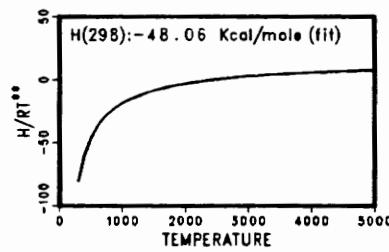
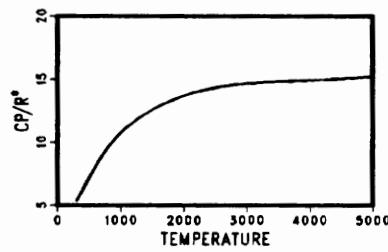
Source: BURCAT (LSU CALCULATIONS)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: CH<sub>3</sub>OH METHANOL GAS As of: 12/16/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02660115E+02	0.07341508E-01	0.07170050E-04	-0.08793194E-07	0.02390570E-10	-0.02535348E+06	0.11232631E+02
1000-5000K	0.04029061E+02	0.09376593E-01	-0.03050254E-04	0.04358793E-08	-0.02224723E-12	-0.02615791E+06	0.02378195E+02



Source: BURCAT (CH40) (TECHNION REPORTS)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: CH<sub>3</sub>SiCl<sub>3</sub>

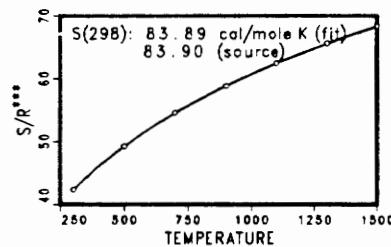
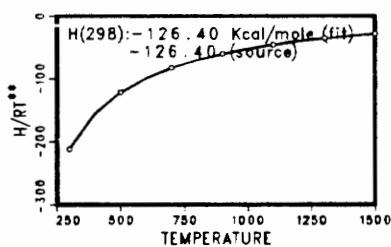
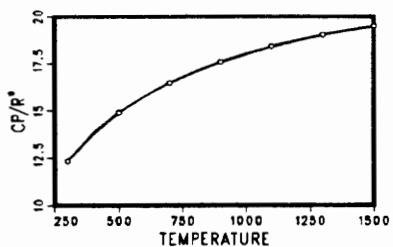
## TRICHLOROMETHYLSILANE

GAS

As of: 11/29/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04637712E+02	0.03733016E+00	-0.04798528E-03	0.03353132E-06	-0.09484405E-10	-0.06629348E+06	0.06524867E+02
1000-1500K	0.11803988E+02	0.07642902E-01	-0.09493348E-06	-0.01852654E-07	0.05302190E-11	-0.06773651E+06	-0.02794492E+03



Source: SNLL FIT TO JANNAF DATA

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CH<sub>4</sub>

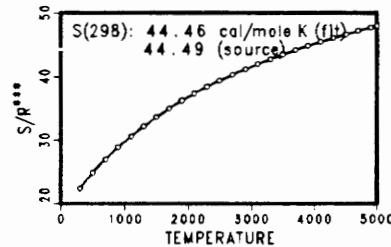
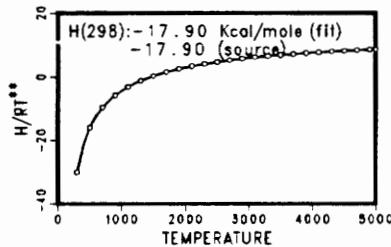
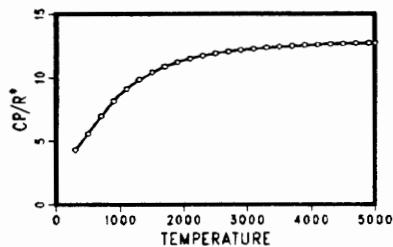
## METHANE

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.07787415E+01	0.01747668E+00	-0.02783409E-03	0.03049708E-06	-0.12239307E-10	-0.09825229E+05	0.13722195E+02
1000-5000K	0.01683478E+02	0.10237236E-01	-0.03875128E-04	0.06785585E-08	-0.04503423E-12	-0.10080787E+05	0.09623395E+02



Source: SNLL FIT TO JANNAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CHCl

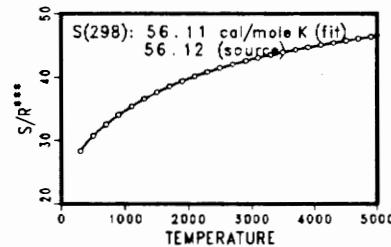
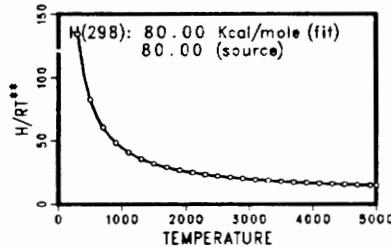
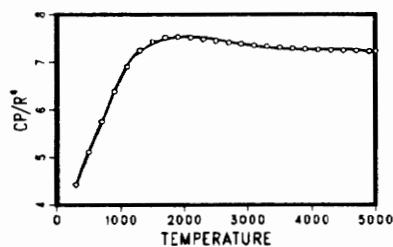
## MONOCHLOROMETHYLENE

GAS

As of: 11/29/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1200K	0.02781262E+02	0.07805384E-01	-0.10637111E-04	0.10654407E-07	-0.03916796E-10	0.03916144E+06	0.10455153E+02
1200-5000K	0.03216518E+02	0.05976969E-01	-0.02918238E-04	0.05912801E-08	-0.04297945E-12	0.03879839E+06	0.07793842E+02



Source: SNLL FIT TO JANNAF DATA

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CHCL<sub>3</sub>

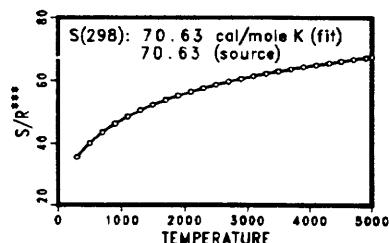
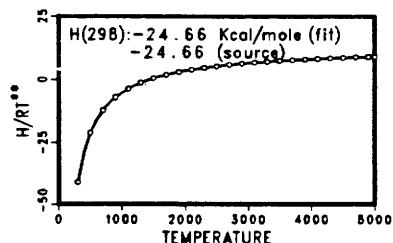
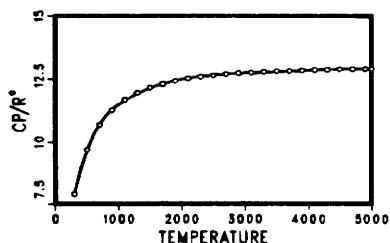
CHLOROFORM

GAS

As of: 11/29/89

Fit

Coefficients	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	a <sub>4</sub>	a <sub>5</sub>	a <sub>6</sub>	a <sub>7</sub>
0300-1000K	0.03437633E+02	0.01941496E+00	-0.16494730E-04	0.05196545E-07	-0.06939614E-12	-0.14161262E+05	0.10863299E+02
1000-5000K	0.08523544E+02	0.04480142E-01	-0.01837282E-04	0.03424891E-08	-0.02387283E-12	-0.15461167E+05	-0.15056193E+02



Source: SNLL FIT TO JANNAF DATA

Comments: ALSO CALLED TRICHLOROMETHANE

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CHF

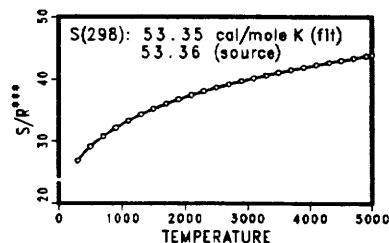
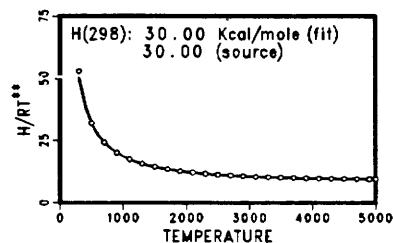
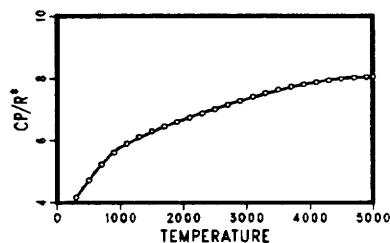
MONOFLUOROMETHYLENE

GAS

As of: 8/24/89

Fit

Coefficients	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	a <sub>4</sub>	a <sub>5</sub>	a <sub>6</sub>	a <sub>7</sub>
0300-1000K	0.03029060E+02	0.04850873E-01	-0.04971678E-04	0.05277968E-07	-0.02403154E-10	0.14014348E+05	0.08324101E+02
1000-5000K	0.04242812E+02	0.02066316E-01	-0.06527951E-05	0.13887000E-09	-0.12133360E-13	0.13559817E+05	0.01680196E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CHF<sub>3</sub>

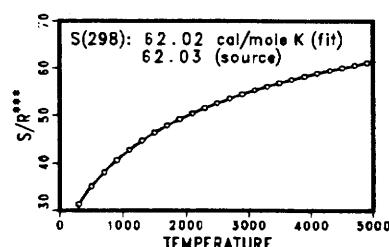
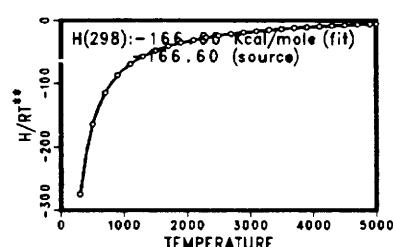
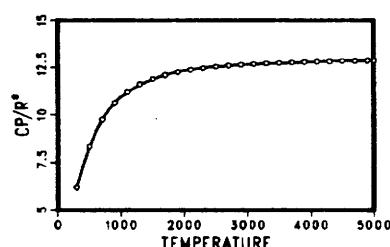
TRIFLUOROMETHANE

GAS

As of: 8/24/89

Fit

Coefficients	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	a <sub>4</sub>	a <sub>5</sub>	a <sub>6</sub>	a <sub>7</sub>
0300-1000K	0.08725142E+01	0.02308431E+00	-0.02123718E-03	0.11144284E-07	-0.02909229E-10	-0.08496391E+06	0.02021498E+03
1000-5000K	0.06834333E+02	0.06248730E-01	-0.02575750E-04	0.04809112E-08	-0.03352074E-12	-0.08663771E+06	-0.10627405E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

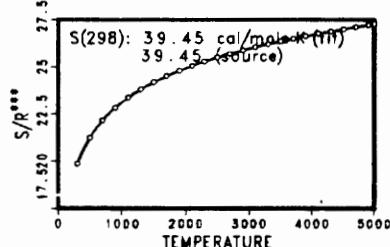
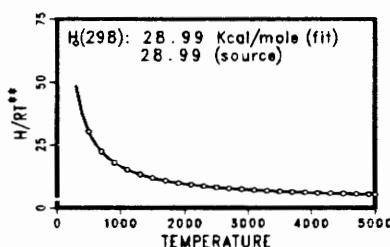
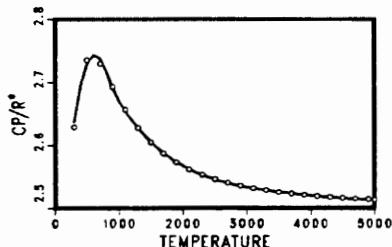
$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: CL CHLORINE, MONATOMIC GAS As of: 4/21/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02381576E+02	0.08891079E-02	0.04070475E-05	-0.02168943E-07	0.11608274E-11	0.13839987E+05	0.06021817E+02
1000-5000K	0.02920236E+02	-0.03597985E-02	0.12942943E-06	-0.02162776E-09	0.13765171E-14	0.13713381E+05	0.03262690E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

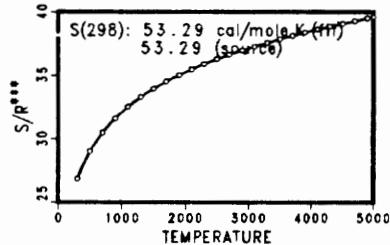
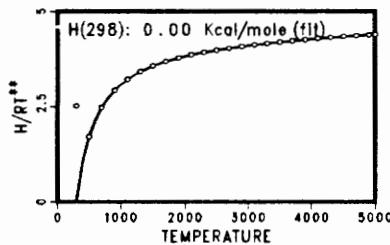
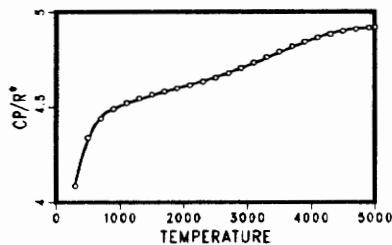
$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: CL2 CHLORINE, DIATOMIC GAS As of: 4/21/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03439587E+02	0.02870774E-01	-0.02385870E-04	0.02892918E-08	0.02915057E-11	-0.11317875E+04	0.06471359E+02
1000-5000K	0.04274586E+02	0.03717336E-02	-0.01893489E-05	0.05337465E-09	-0.05057602E-13	-0.13311486E+04	0.02256946E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

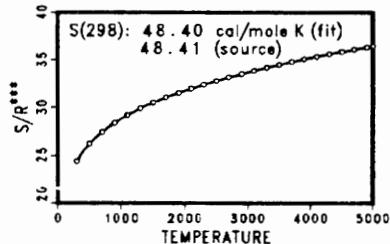
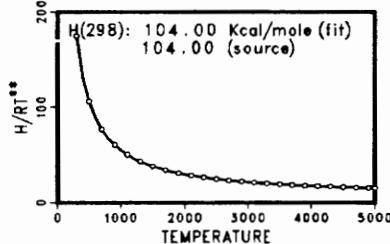
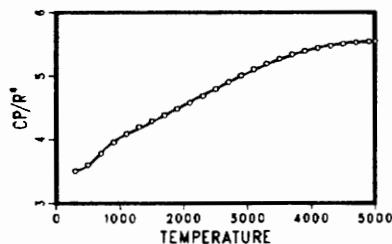
$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: CN CYANO GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03663204E+02	-0.11565290E-02	0.02163409E-04	0.01854208E-08	-0.08214695E-11	0.05128118E+06	0.03739015E+02
1000-5000K	0.03720119E+02	0.15183506E-03	0.01987381E-05	-0.03798371E-09	0.13282296E-14	0.05111626E+06	0.02888597E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

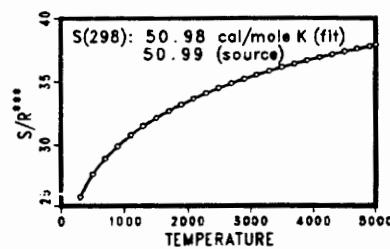
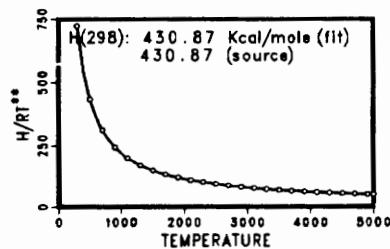
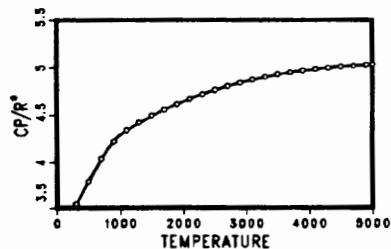
$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: CN+ CYANO, UNIPOSITIVE ION GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03118657E+02	0.15532581E-02	-0.09487764E-05	0.14795005E-08	-0.09096763E-11	0.02158512E+07	0.07456254E+02
1000-5000K	0.03701463E+02	0.07482931E-02	-0.01790173E-05	0.02366368E-09	-0.14370368E-14	0.02155966E+07	0.04108678E+02



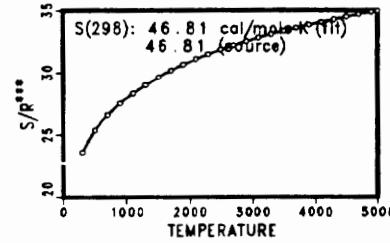
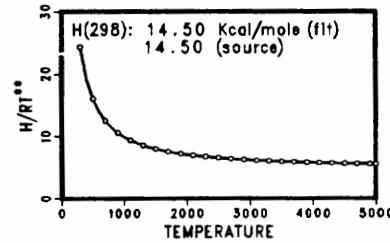
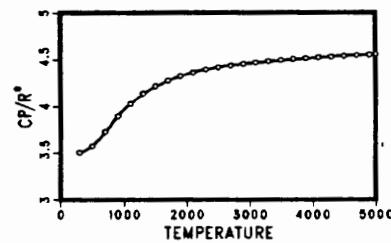
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: CN- CYANO, UNINEGATIVE ION GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03278995E+02	0.14641916E-02	-0.03925899E-04	0.05629874E-07	-0.02473496E-10	0.06279509E+05	0.04568972E+02
1000-5000K	0.02981276E+02	0.14647728E-02	-0.05672737E-05	0.10176226E-09	-0.06870930E-13	0.06346098E+05	0.06171693E+02



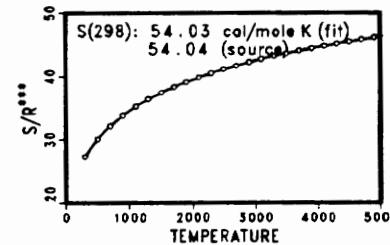
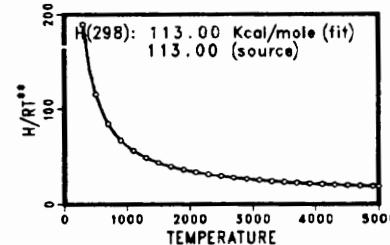
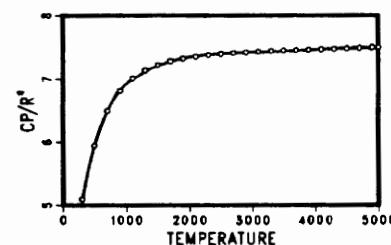
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: CN2 NCN RADICAL GAS As of: 12/16/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03039963E+02	0.08812105E-01	-0.07605508E-04	0.03554357E-07	-0.08746100E-11	0.05563268E+06	0.07555298E+02
1000-5000K	0.05567064E+02	0.02100501E-01	-0.09010517E-05	0.01718571E-08	-0.12062552E-13	0.05489968E+06	-0.05630054E+02



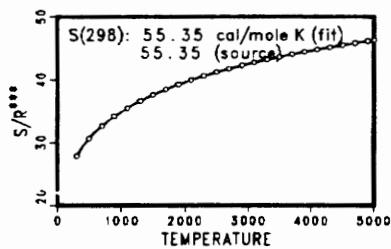
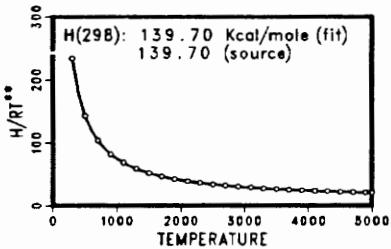
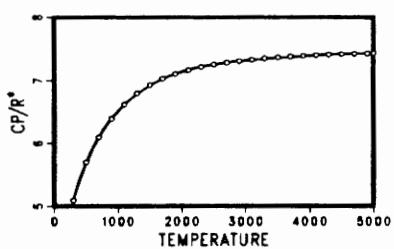
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: CNN CNN RADICAL GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03524436E+02	0.07271923E-01	-0.08272698E-04	0.05628704E-07	-0.16415759E-11	0.06899647E+06	0.05932444E+02
1000-5000K	0.04785930E+02	0.02559553E-01	-0.10031326E-05	0.01807148E-08	-0.12273827E-13	0.06870411E+06	-0.02953957E+01



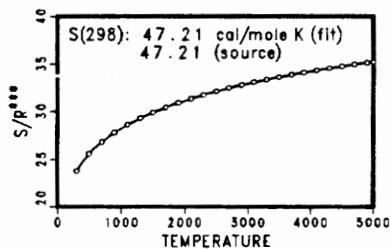
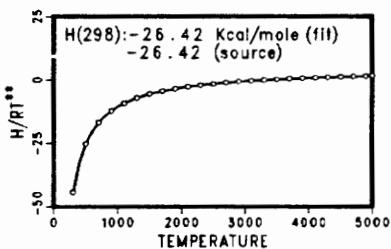
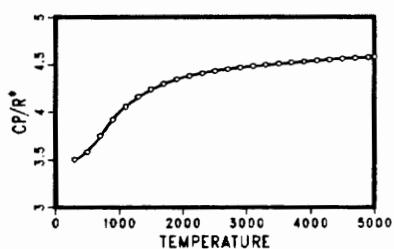
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: CO CARBON MONOXIDE GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03262451E+02	0.15119409E-02	-0.03881755E-04	0.05581944E-07	-0.02474951E-10	-0.14310539E+05	0.04848897E+02
1000-5000K	0.03025078E+02	0.14426885E-02	-0.05630827E-05	0.10185813E-09	-0.06910951E-13	-0.14268350E+05	0.06108217E+02



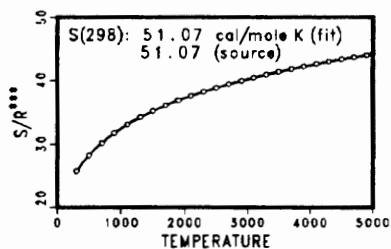
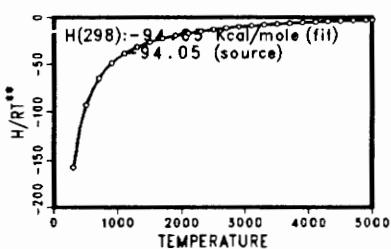
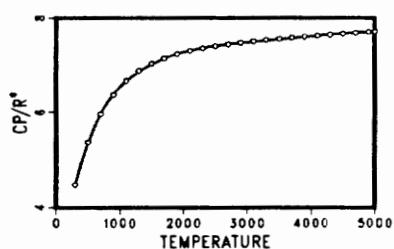
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: CO2 CARBON DIOXIDE GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02275724E+02	0.09922072E-01	-0.10409113E-04	0.06866686E-07	-0.02117280E-10	-0.04837314E+06	0.10188488E+02
1000-5000K	0.04453623E+02	0.03140168E-01	-0.12784105E-05	0.02393996E-08	-0.16690333E-13	-0.04896696E+06	-0.09553959E+01



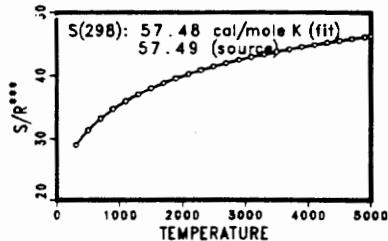
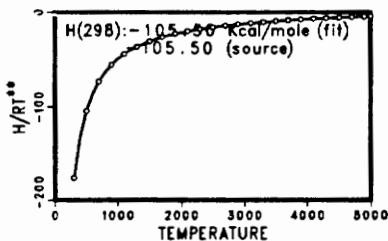
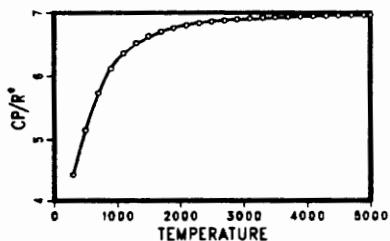
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: CO<sub>2</sub>- CARBON DIOXIDE, UNINEGATIVE ION GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02637077E+02	0.07803230E-01	-0.08196187E-04	0.06537897E-07	-0.02520220E-10	-0.05416772E+06	0.11889549E+02
1000-5000K	0.04610574E+02	0.02532962E-01	-0.10701653E-05	0.02026770E-08	-0.14249581E-13	-0.05479881E+06	0.14496295E+01



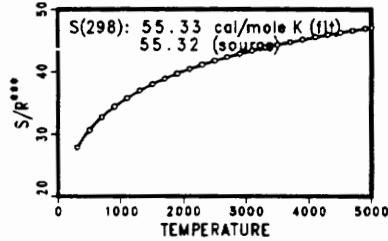
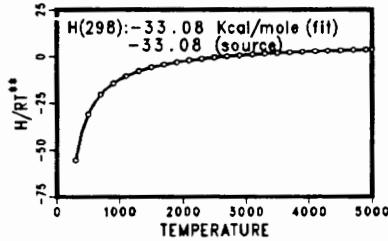
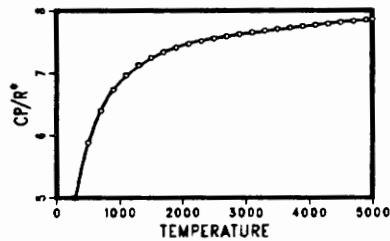
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: COS CARBON OXYSULFIDE GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02858530E+02	0.09515458E-01	-0.08884915E-04	0.04220994E-07	-0.08557340E-11	-0.01785144E+06	0.09081989E+02
1000-5000K	0.05191924E+02	0.02506123E-01	-0.10243963E-05	0.01943914E-08	-0.13707999E-13	-0.01846210E+06	-0.02825755E+02



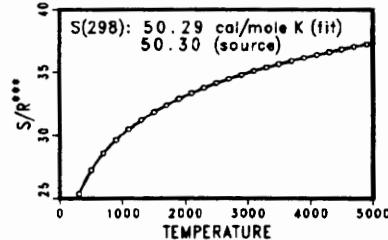
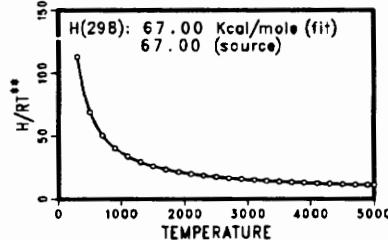
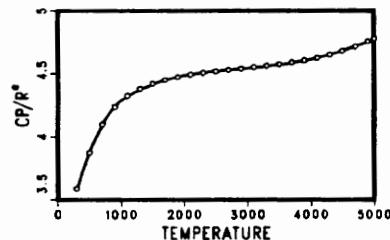
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: CS CARBON MONOSULFIDE GAS As of: 12/16/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02938623E+02	0.02724351E-01	-0.02397706E-04	0.01689500E-07	-0.06665050E-11	0.03273992E+06	0.07848720E+02
1000-5000K	0.03737430E+02	0.08180451E-02	-0.03178918E-05	0.05356801E-09	-0.02886194E-13	0.03247725E+06	0.03576556E+02



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: CS2

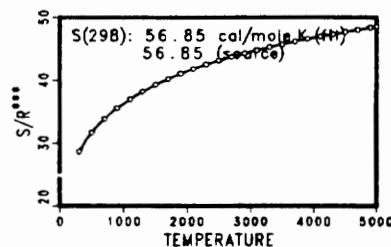
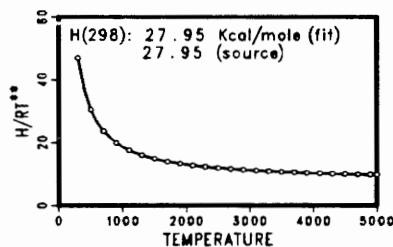
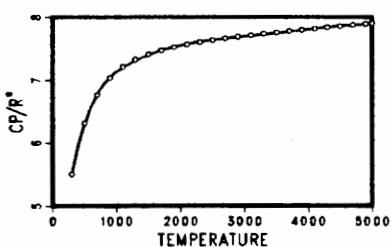
## CARBON DISULFIDE

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03566139E+02	0.08374927E-01	-0.06835704E-04	0.02091214E-07	-0.06737193E-12	0.12688482E+05	0.06085967E+02
1000-5000K	0.05930515E+02	0.01813645E-01	-0.07492172E-05	0.14458920E-09	-0.10326380E-13	0.12051166E+05	-0.06093909E+02



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: E

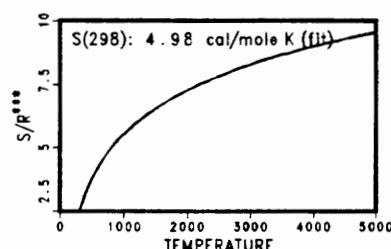
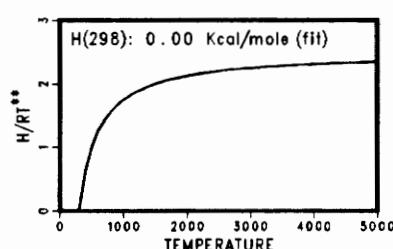
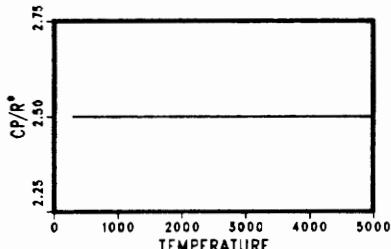
## ELECTRON

GAS

As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	-0.07453750E+04	-0.11734026E+02
1000-5000K	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	-0.07453749E+04	-0.11734026E+02



Source: NASA FIT TO NASA-LEWIS DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: F

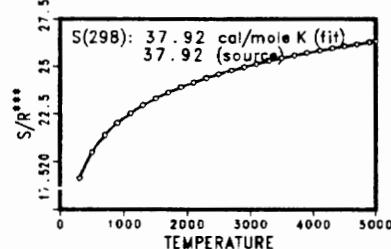
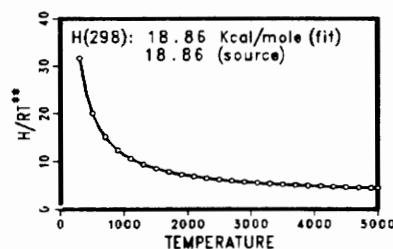
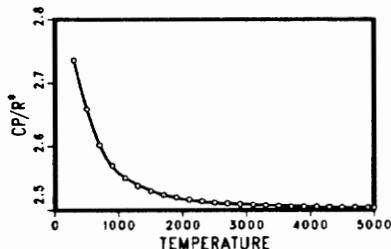
## FLUORINE, MONATOMIC

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02913904E+02	-0.07336339E-02	0.05571015E-05	-0.02666871E-08	0.08643255E-12	0.08651201E+05	0.02677115E+02
1000-5000K	0.02687459E+02	-0.02010358E-02	0.08597957E-06	-0.16449738E-10	0.11661605E-14	0.08722883E+05	0.03882212E+02



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: F2

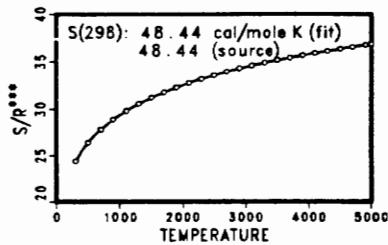
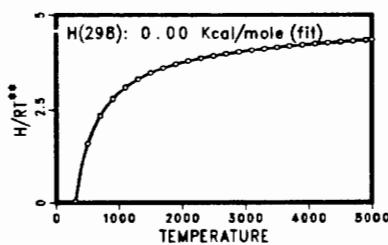
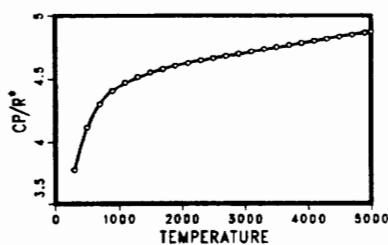
FLUORINE, DIATOMIC (REF ST)

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02940287E+02	0.03491491E-01	-0.02458207E-04	0.01837073E-08	0.02850916E-11	-0.10104296E+04	0.06694194E+02
1000-5000K	0.04018308E+02	0.06221479E-02	-0.02420845E-05	0.04742076E-09	-0.03418141E-13	-0.13007128E+04	0.11263273E+01



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

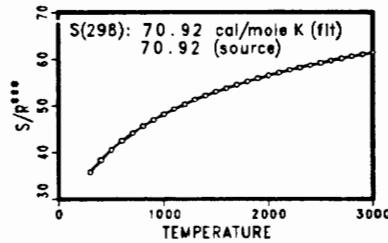
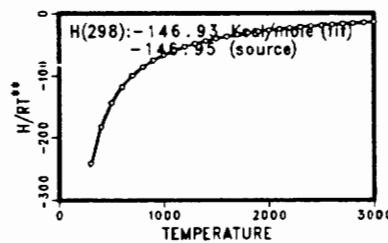
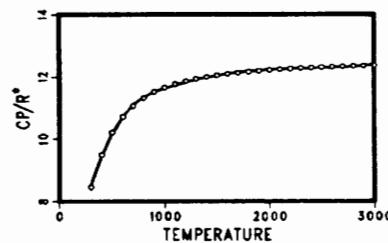
Species: F2SINH

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04951547E+02	0.13296361E-01	-0.02098648E-04	-0.10072757E-07	0.05552285E-10	-0.07597540E+06	0.03690891E+02
1000-3000K	0.10048301E+02	0.01983144E-01	-0.02703168E-05	-0.01767852E-08	0.04444367E-12	-0.07739741E+06	-0.02303888E+03



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: F3SIN

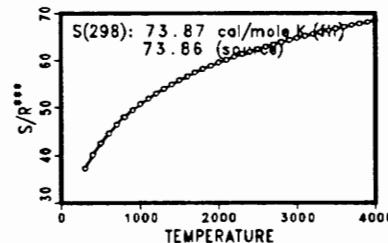
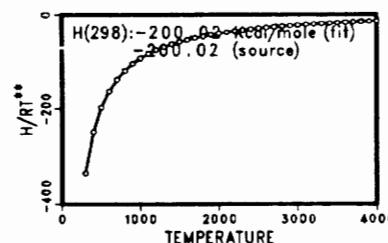
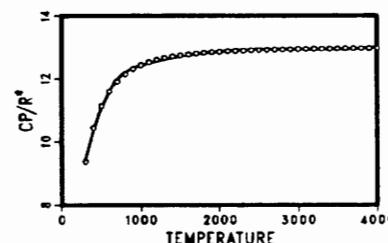
TRIFLUOROSILYL NITRENE

GAS

As of: 2/27/90

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.06028419E+02	0.12786807E-01	-0.01878856E-04	-0.09695426E-07	0.05184847E-10	-0.10299499E+06	-0.08217830E+01
1000-4000K	0.11512423E+02	0.1150295E-02	-0.16054655E-06	-0.05271933E-09	0.11608998E-13	-0.10459191E+06	-0.02981224E+03



Source: SNL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: FNNF

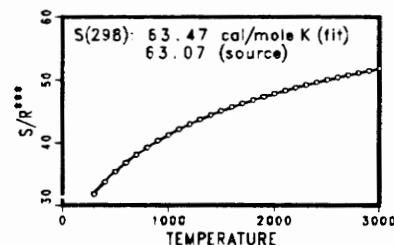
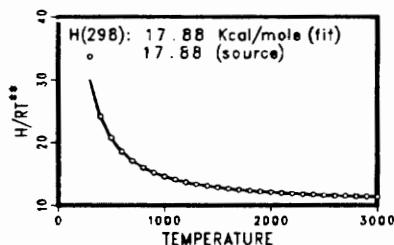
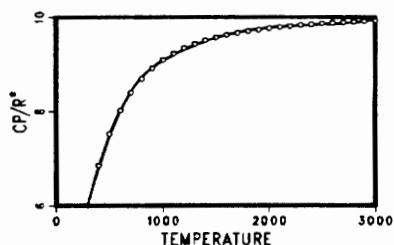
CIS-DIFLUORODIAZINE

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03127143E+02	0.10571342E-01	-0.09746113E-05	-0.07208357E-07	0.03567978E-10	0.07615830E+05	0.11074648E+02
1000-3000K	0.07255211E+02	0.02274409E-01	-0.02793346E-05	-0.02203843E-08	0.05359234E-12	0.06360352E+05	-0.10942477E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: FN03

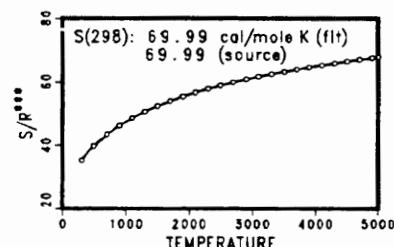
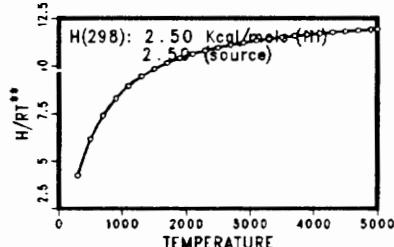
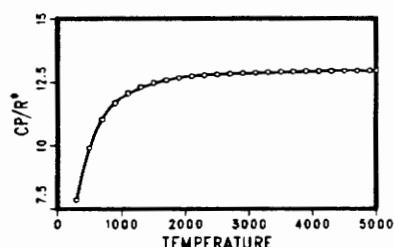
FLUORINE NITRATE

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02985786E+02	0.02094642E+00	-0.16527329E-04	0.04318770E-07	0.16607836E-12	-0.04237215E+04	0.12667929E+02
1000-5000K	0.09176275E+02	0.04219072E-01	-0.01835575E-04	0.03553717E-08	-0.02541078E-12	-0.02118638E+05	-0.01934397E+03



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: FO

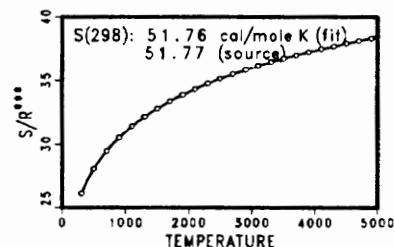
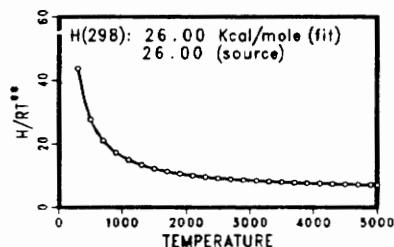
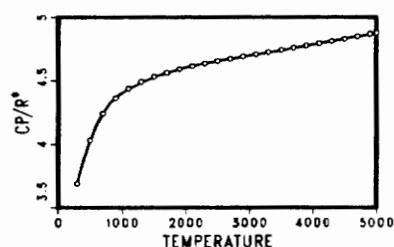
FLUORINE MONOXIDE

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02879578E+02	0.03399121E-01	-0.02572854E-04	0.07422381E-08	-0.04328053E-12	0.12096633E+05	0.08738887E+02
1000-5000K	0.03913735E+02	0.07210714E-02	-0.02796614E-05	0.05337821E-09	-0.03720183E-13	0.11801406E+05	0.03346367E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

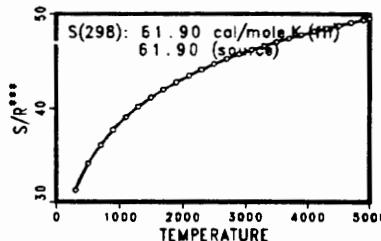
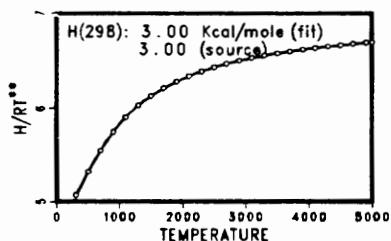
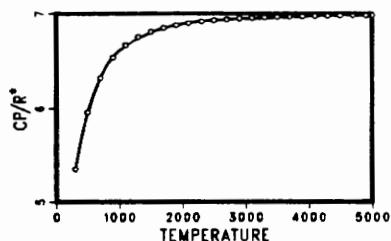
$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: F02 DIOXYGEN FLUORIDE GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03872542E+02	0.06409974E-01	-0.05517784E-04	0.02232770E-07	-0.03876157E-11	0.11570760E+03	0.07406949E+02
1000-5000K	0.05678971E+02	0.14424551E-02	-0.06229546E-05	0.11996118E-09	-0.08543416E-13	-0.03861836E+04	-0.01941811E+02



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

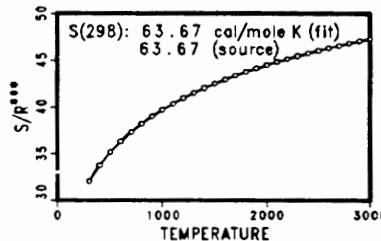
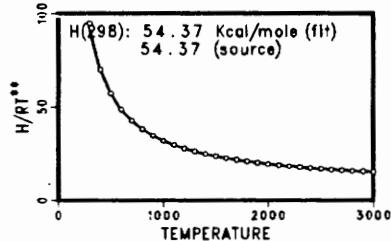
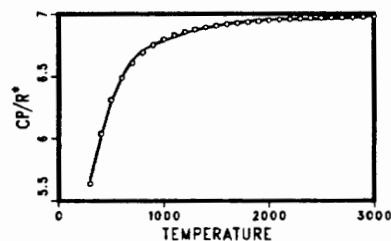
Species: FSIN

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04269969E+02	0.05298358E-01	-0.11038015E-05	-0.03962805E-07	0.02282982E-10	0.02587238E+06	0.06215038E+02
1000-3000K	0.06269572E+02	0.06747867E-02	-0.12419759E-06	-0.04970158E-09	0.14244521E-13	0.02533350E+06	-0.04201141E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

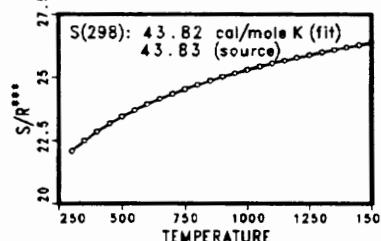
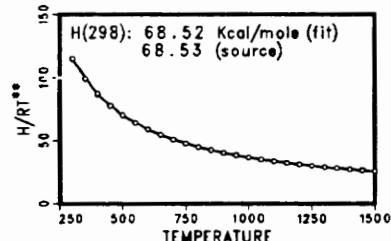
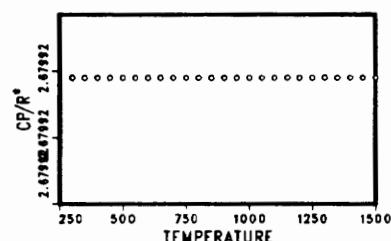
Species: GA

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-600K	0.02679919E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.03368803E+06	0.06788109E+02
600-1500K	0.02679919E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.03368804E+06	0.06788109E+02



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

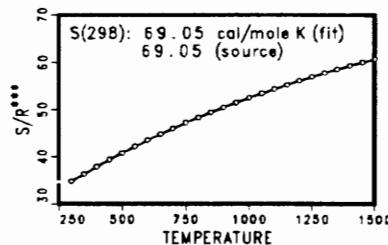
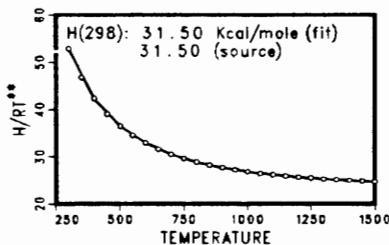
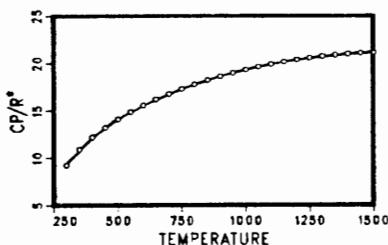
Species: GA2H6

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	-0.03914560E+02	0.04965434E+00	0.07401903E-04	-0.11241373E-06	0.08726339E-09	0.14930795E+05	0.04274882E+03
0600-1500K	0.06016247E+02	0.01788370E+00	-0.12042288E-06	-0.06487881E-07	0.02075367E-10	0.13125479E+05	-0.05228029E+02



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

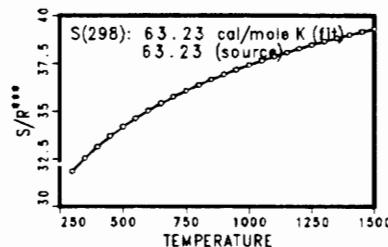
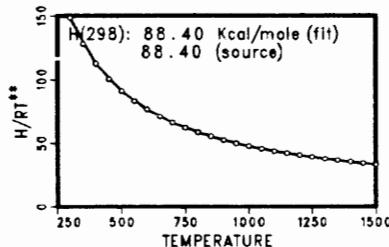
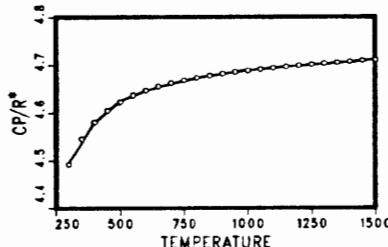
Species: GAAS

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.03967473E+02	0.02318966E-01	-0.11454521E-05	-0.03411430E-07	0.03365821E-10	0.04321919E+06	0.08599628E+02
0600-1500K	0.04471149E+02	0.04238449E-02	-0.02279404E-05	-0.04441172E-10	0.02618952E-12	0.04313359E+06	0.06212470E+02



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

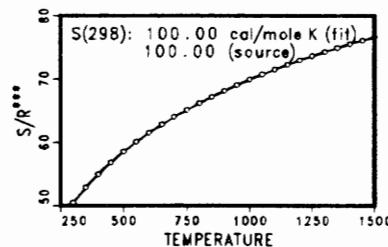
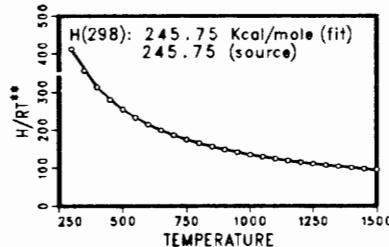
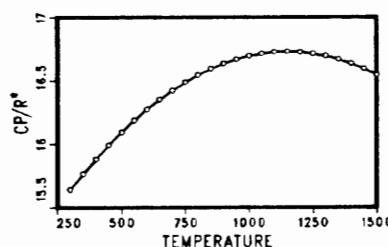
Species: GAAS(3,C)

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.14701892E+02	0.03827728E-01	-0.02945747E-04	0.02465370E-07	-0.15205979E-11	0.11914958E+06	-0.03445955E+03
0600-1500K	0.14852467E+02	0.02959435E-01	-0.07124246E-05	-0.05316048E-08	0.12673211E-12	0.11912617E+06	-0.03514144E+03



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

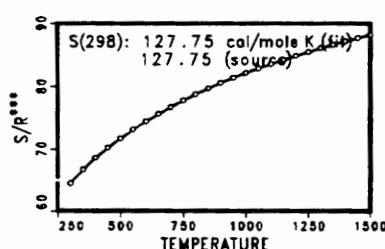
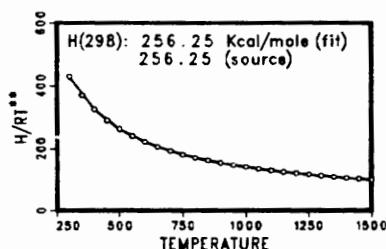
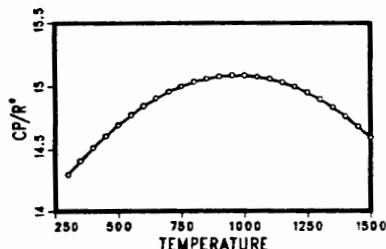
Species: GAAS(3,L)

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.13412763E+02	0.03617689E-01	-0.02726208E-04	0.01877183E-07	-0.12591780E-11	0.12482649E+06	-0.13091947E+02
0600-1500K	0.13568498E+02	0.02802435E-01	-0.07969918E-05	-0.06437098E-08	0.15602546E-12	0.12480055E+06	-0.13810628E+02



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet\bullet \text{H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet\bullet\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

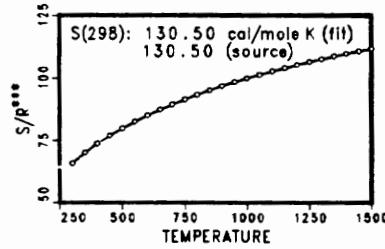
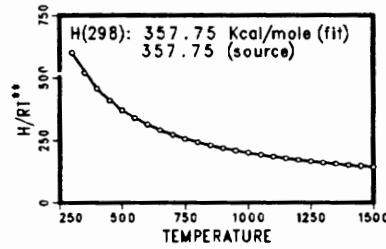
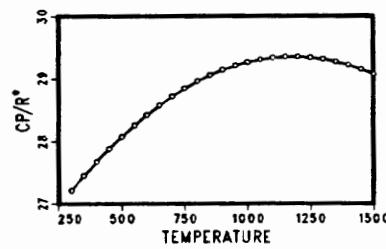
Species: GAAS(5,C)

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.02546511E+03	0.07014337E-01	-0.04881356E-04	0.03825484E-07	-0.02450420E-10	0.01721819E+07	-0.08130267E+03
0600-1500K	0.02573672E+03	0.05523956E-01	-0.12034680E-05	-0.10437431E-08	0.02528930E-11	0.01721381E+07	-0.08254488E+03



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet\bullet \text{H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet\bullet\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

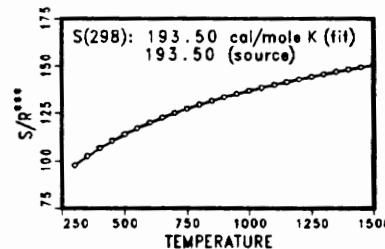
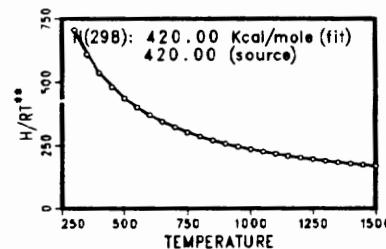
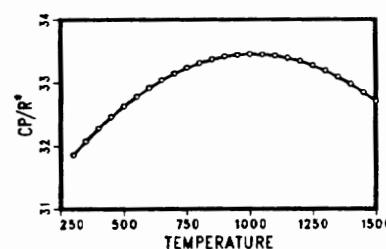
Species: GAAS(5,L)

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.03015255E+03	0.07234394E-01	-0.06497993E-04	0.05559584E-07	-0.03339653E-10	0.02021150E+07	-0.07630866E+03
0600-1500K	0.03045793E+03	0.05403151E-01	-0.16494765E-05	-0.09968843E-08	0.02413154E-11	0.02020691E+07	-0.07768010E+03



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet\bullet \text{H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet\bullet\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: GAET

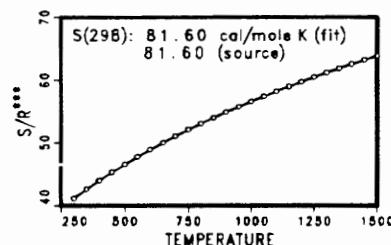
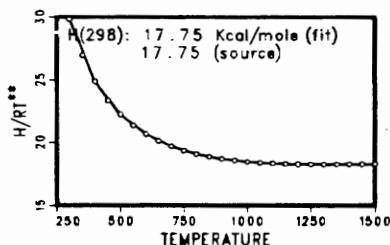
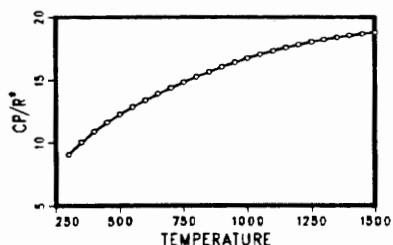
("ET" = C<sub>2</sub>H<sub>5</sub>, ETHYL)

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.01846399E+02	0.02592050E+00	0.05522393E-04	-0.04977960E-06	0.03654361E-09	0.07264445E+05	0.02294638E+03
0600-1500K	0.05932970E+02	0.13424544E-01	0.04110518E-05	-0.04286069E-07	0.12387095E-11	0.06504863E+05	0.03090838E+02



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: GAET2

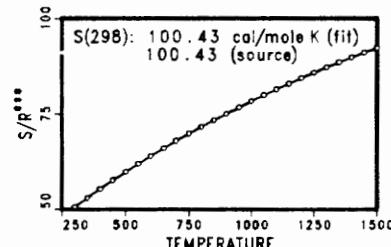
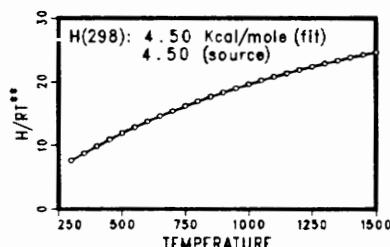
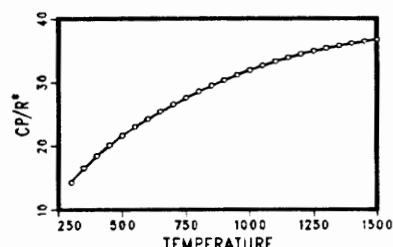
("ET" = C<sub>2</sub>H<sub>5</sub>, ETHYL)

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	-0.02162930E+02	0.05892512E+00	0.14471449E-04	-0.11686023E-06	0.08526654E-09	0.03561840E+04	0.04552626E+03
0600-1500K	0.07213832E+02	0.03055227E+00	0.12494508E-05	-0.09990274E-07	0.02881965E-10	-0.13921194E+04	-0.07795098E+00



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: GAET3

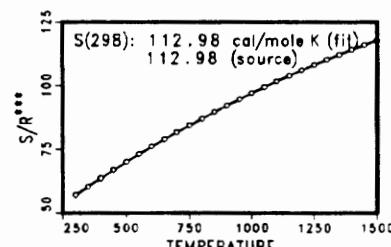
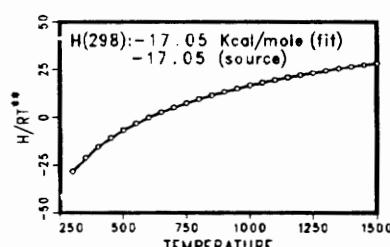
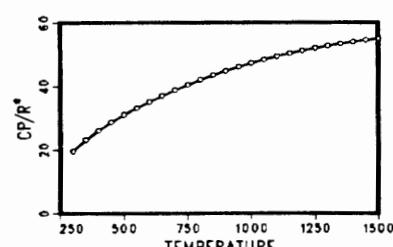
("ET" = C<sub>2</sub>H<sub>5</sub>, ETHYL)

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	-0.06544288E+02	0.09332246E+00	0.02364121E-03	-0.01874104E-05	0.13677210E-09	-0.10676594E+05	0.06666796E+03
0600-1500K	0.08436453E+02	0.04804950E+00	0.02119157E-04	-0.15816849E-07	0.04571778E-10	-0.13469963E+05	-0.06196490E+02



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

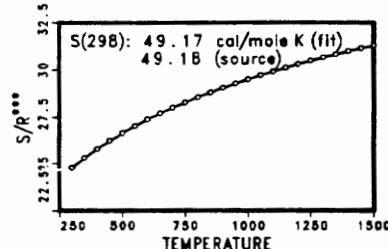
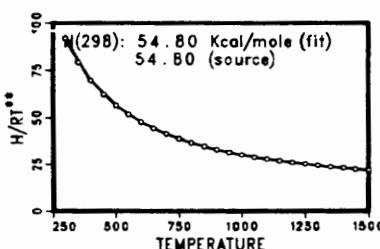
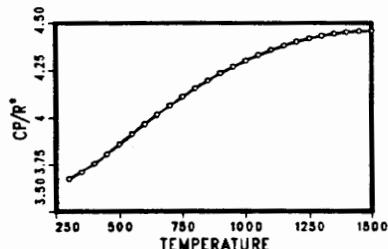
Species: GAH

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.03524579E+02	0.03386213E-02	-0.02064013E-05	0.03220998E-07	-0.02936132E-10	0.02651074E+06	0.04554066E+02
0600-1500K	0.03232142E+02	0.13432469E-02	-0.04325498E-06	-0.02791841E-08	0.04973590E-12	0.02656059E+06	0.05947896E+02



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet\bullet\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

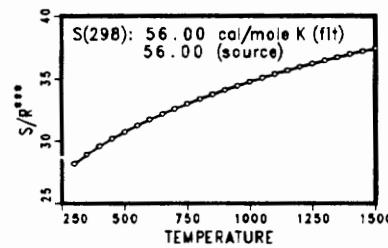
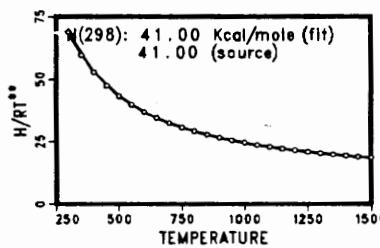
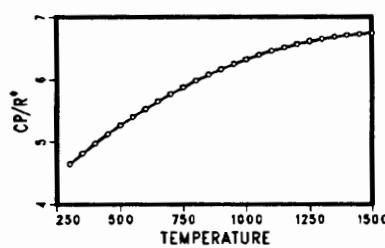
Species: GAH2

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.03559710E+02	0.03676741E-01	0.06484499E-05	-0.03109349E-07	0.15854136E-11	0.01940976E+06	0.06803081E+02
0600-1500K	0.03762384E+02	0.03210792E-01	0.02180096E-06	-0.08908394E-08	0.02219062E-11	0.01936646E+06	0.05783398E+02



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet\bullet\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

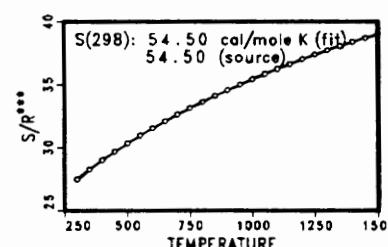
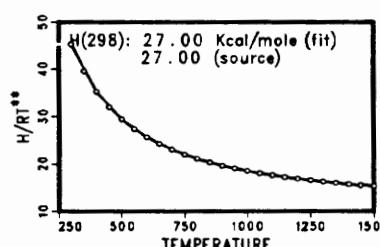
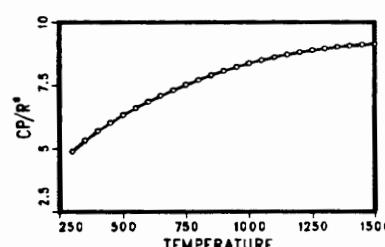
Species: GAH3

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.01726153E+02	0.11247386E-01	0.02447526E-04	-0.02026314E-06	0.14470000E-10	0.12586196E+05	0.14284450E+02
0600-1500K	0.03345475E+02	0.06399313E-01	0.11229964E-06	-0.02065899E-07	0.05780202E-11	0.12281851E+05	0.06394841E+02



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

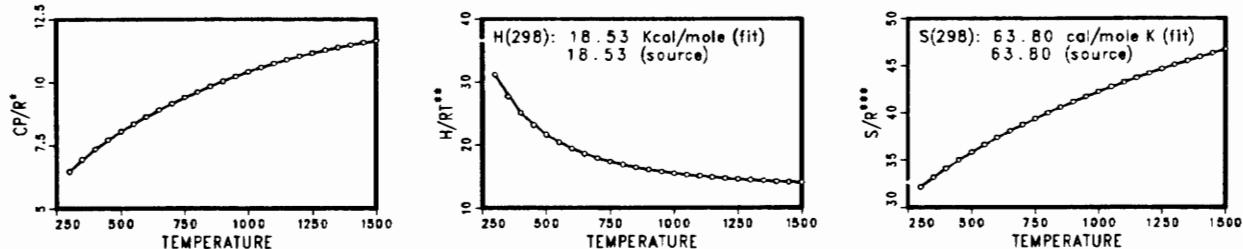
$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet\bullet\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: GAME ("ME" = CH<sub>3</sub>,METHYL) GAS As of: 6/29/87

Fit  
 Coefficients       $\alpha_1$        $\alpha_2$        $\alpha_3$        $\alpha_4$        $\alpha_5$        $\alpha_6$        $\alpha_7$   
 0300-0600K    0.03054536E+02    0.12186402E-01    0.02332213E-04    -0.02121866E-06    0.15442261E-10    0.07885868E+05    0.111287B1E+02  
 0600-1500K    0.04809857E+02    0.06824206E-01    0.02258235E-05    -0.02018341E-07    0.05736453E-11    0.07558677E+05    0.02595904E+02

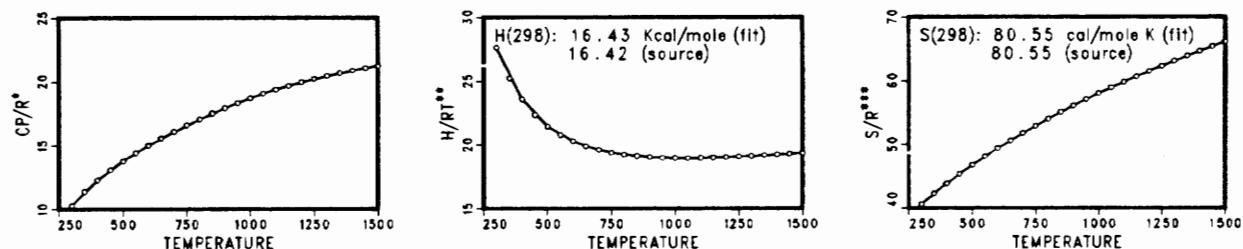


Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * \text{CP/R} &= \alpha_1 + \alpha_2 T + \alpha_3 T^2 + \alpha_4 T^3 + \alpha_5 T^4 \\ ** \text{H/RT} &= \alpha_1 + \alpha_2 T / 2 + \alpha_3 T^2 / 3 + \alpha_4 T^3 / 4 + \alpha_5 T^4 / 5 + \alpha_6 / T \\ *** \text{S/R} &= \alpha_1 \ln(T) + \alpha_2 T + \alpha_3 T^2 / 2 + \alpha_4 T^3 / 3 + \alpha_5 T^4 / 4 + \alpha_7 \end{aligned}$$

Species: GAME2 ("ME" = CH<sub>3</sub>,METHYL) GAS As of: 6/29/87

Fit  
 Coefficients       $\alpha_1$        $\alpha_2$        $\alpha_3$        $\alpha_4$        $\alpha_5$        $\alpha_6$        $\alpha_7$   
 0300-0600K    0.02257655E+02    0.02916445E+00    0.05669861E-04    -0.05709755E-06    0.04268905E-09    0.06341297E+05    0.01915435E+03  
 0600-1500K    0.07068372E+02    0.14216021E-01    0.05120694E-05    -0.04421986E-07    0.13096413E-11    0.05453790E+05    -0.04173960E+02

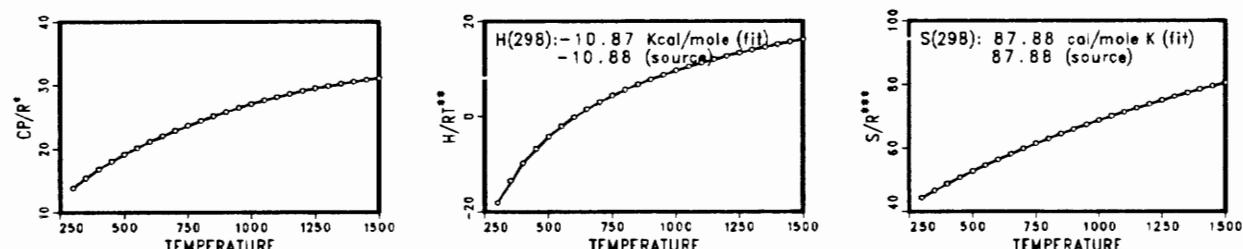


Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * \text{CP/R} &= \alpha_1 + \alpha_2 T + \alpha_3 T^2 + \alpha_4 T^3 + \alpha_5 T^4 \\ ** \text{H/RT} &= \alpha_1 + \alpha_2 T / 2 + \alpha_3 T^2 / 3 + \alpha_4 T^3 / 4 + \alpha_5 T^4 / 5 + \alpha_6 / T \\ *** \text{S/R} &= \alpha_1 \ln(T) + \alpha_2 T + \alpha_3 T^2 / 2 + \alpha_4 T^3 / 3 + \alpha_5 T^4 / 4 + \alpha_7 \end{aligned}$$

Species: GAME3 ("ME" = CH<sub>3</sub>,METHYL) GAS As of: 6/29/87

Fit  
 Coefficients       $\alpha_1$        $\alpha_2$        $\alpha_3$        $\alpha_4$        $\alpha_5$        $\alpha_6$        $\alpha_7$   
 0300-0600K    0.02120238E+02    0.04161029E+00    0.09959505E-04    -0.07846792E-06    0.05693396E-09    -0.07911968E+05    0.01988516E+03  
 0600-1500K    0.08410636E+02    0.02262803E+00    0.10430190E-05    -0.07049610E-07    0.02015307E-10    -0.09087271E+05    -0.10722496E+02



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * \text{CP/R} &= \alpha_1 + \alpha_2 T + \alpha_3 T^2 + \alpha_4 T^3 + \alpha_5 T^4 \\ ** \text{H/RT} &= \alpha_1 + \alpha_2 T / 2 + \alpha_3 T^2 / 3 + \alpha_4 T^3 / 4 + \alpha_5 T^4 / 5 + \alpha_6 / T \\ *** \text{S/R} &= \alpha_1 \ln(T) + \alpha_2 T + \alpha_3 T^2 / 2 + \alpha_4 T^3 / 3 + \alpha_5 T^4 / 4 + \alpha_7 \end{aligned}$$

Species: H

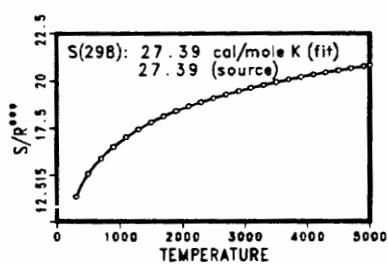
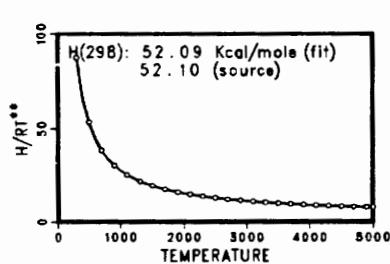
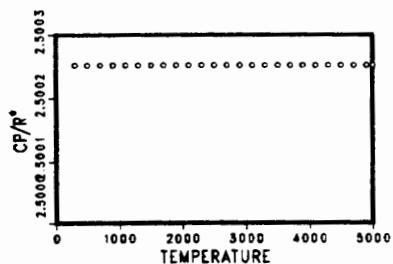
HYDROGEN, MONATOMIC

GAS

As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.0250000E+02	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.02547162E+06	-0.04601176E+01
1000-5000K	0.0250000E+02	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.02547162E+06	-0.04601176E+01



Source: NASA FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H+

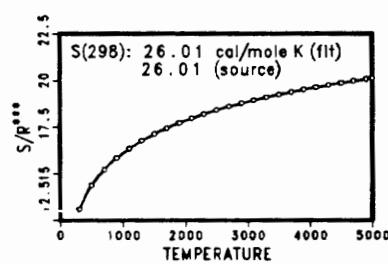
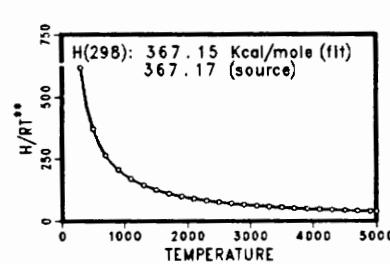
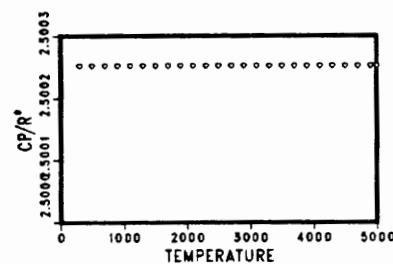
PROTON

GAS

As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.0250000E+02	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.01840334E+07	-0.11538621E+01
1000-5000K	0.0250000E+02	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.01840334E+07	-0.11538620E+01



Source: NASA FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H-

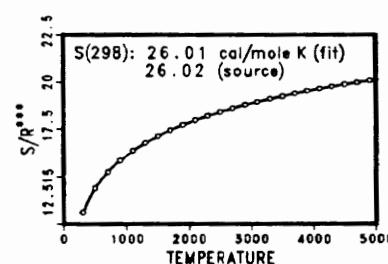
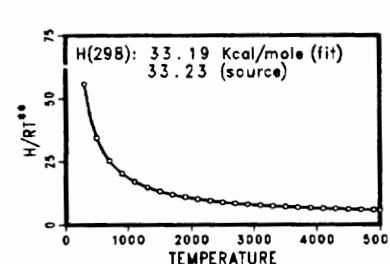
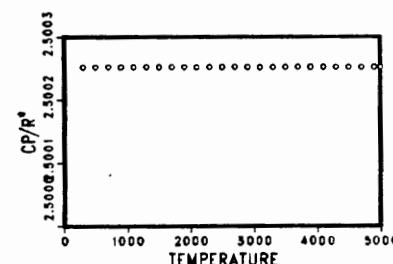
HYDROGEN, UNINEGATIVE ION

GAS

As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.0250000E+02	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.15961045E+05	-0.11524486E+01
1000-5000K	0.0250000E+02	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.15961045E+05	-0.11524488E+01



Source: NASA FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

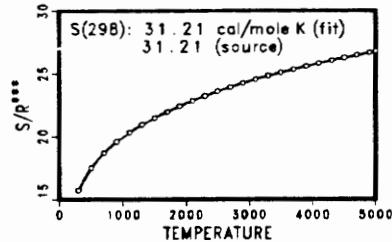
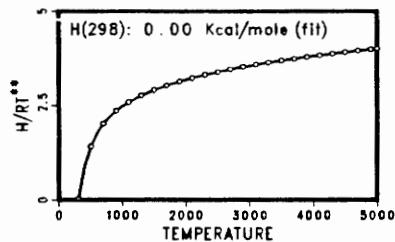
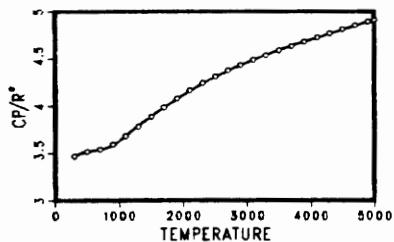
Species: H2

HYDROGEN, DIATOMIC (REF ST) GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03298124E+02	0.08249441E-02	-0.08143015E-05	-0.09475434E-09	0.04134872E-11	-0.10125209E+04	-0.03294094E+02
1000-5000K	0.02991423E+02	0.07000644E-02	-0.05633828E-06	-0.09231578E-10	0.15827519E-14	-0.08350340E+04	-0.13551101E+01



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet\bullet\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H2ALME

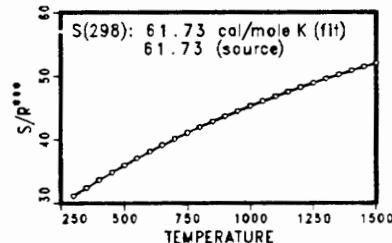
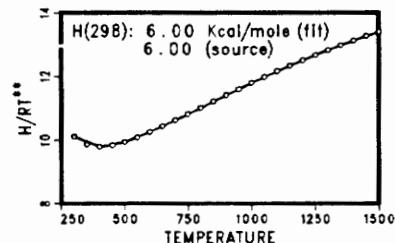
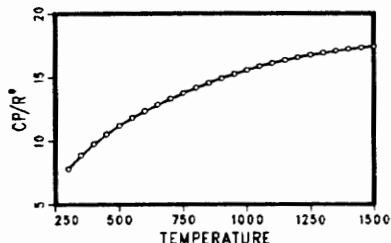
("ME" = CH<sub>3</sub>,METHYL)

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	-0.06283259E+01	0.03089530E+00	0.05774090E-04	-0.06488033E-06	0.0490711E-09	0.01889333E+05	0.02565779E+03
0600-1500K	0.04898410E+02	0.13582233E-01	0.02611458E-05	-0.04575170E-07	0.13848023E-11	0.08743072E+04	-0.11131169E+01



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet\bullet\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H2ASME

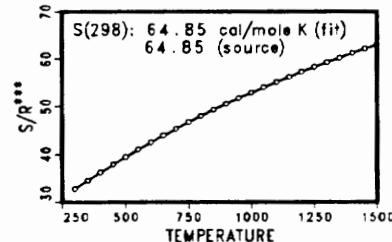
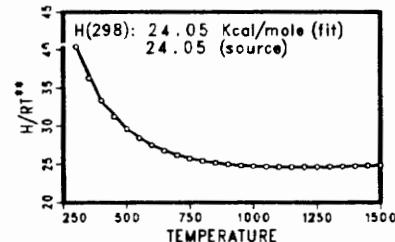
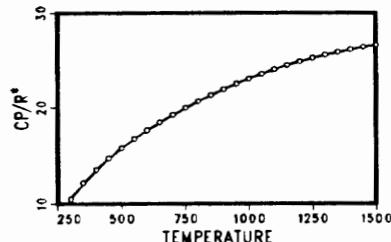
("ME" = CH<sub>3</sub>,METHYL)

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	-0.02113506E+02	0.04564229E+00	0.09983227E-04	-0.09399697E-06	0.07014021E-09	0.10771701E+05	0.03132610E+03
0600-1500K	0.05686213E+02	0.02154421E+00	0.08185247E-05	-0.07069951E-07	0.02101522E-10	0.09331084E+05	-0.06513957E+02



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

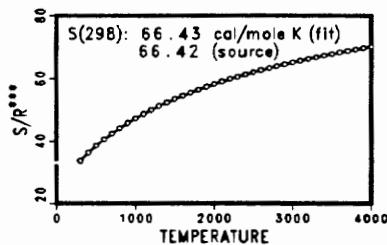
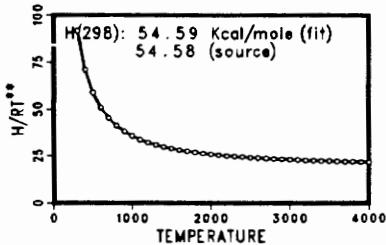
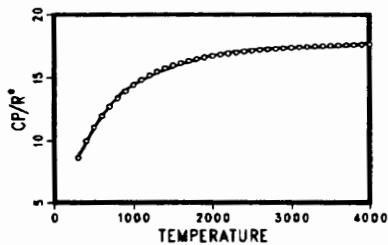
$$\bullet\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet\bullet\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H2C40 BUTADIENONE GAS As of: 12/01/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04810971E+02	0.13139988E-01	0.09865073E-05	-0.06120720E-07	0.16400028E-11	0.02545803E+06	0.02113424E+02
1000-4000K	0.10268878E+02	0.04896164E-01	-0.04885080E-05	-0.02708566E-08	0.05107013E-12	0.02346902E+06	-0.02815985E+03



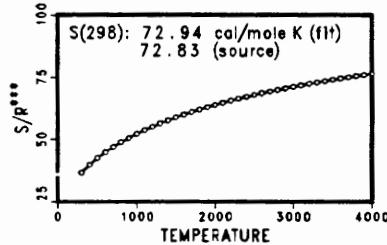
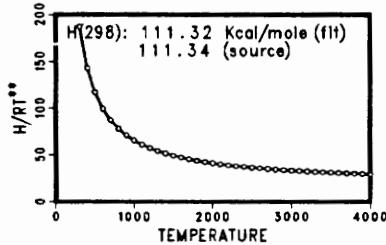
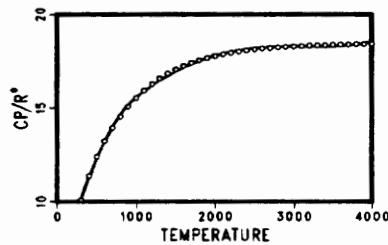
Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP}/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H}/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S}/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: H2CCCCH GAS As of: 8/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.06545799E+02	0.12424768E-01	0.05603226E-05	-0.05631141E-07	0.16652183E-11	0.05352502E+06	-0.04264082E+02
1000-4000K	0.11314095E+02	0.05014414E-01	-0.05350444E-05	-0.02825309E-08	0.05403279E-12	0.05181211E+06	-0.03062434E+03



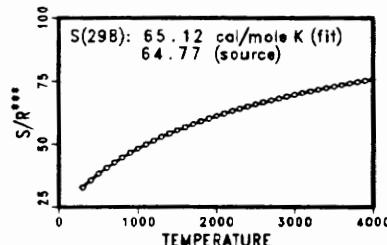
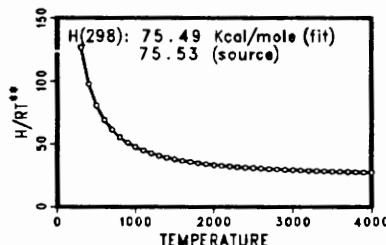
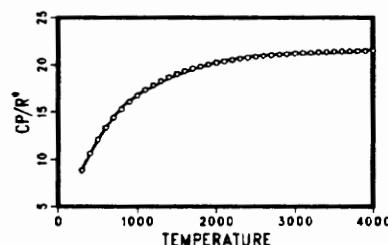
Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP}/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H}/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S}/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: H2CCCCH2 BUTATRIENE D2H GAS As of: 8/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03849007E+02	0.01713169E+00	0.16442703E-05	-0.07761590E-07	0.01947859E-10	0.03608372E+06	0.05732120E+02
1000-4000K	0.10620828E+02	0.07199370E-01	-0.06806234E-05	-0.04021185E-08	0.07378498E-12	0.03358797E+06	-0.03193583E+03



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP}/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H}/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S}/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: H<sub>2</sub>CCCH

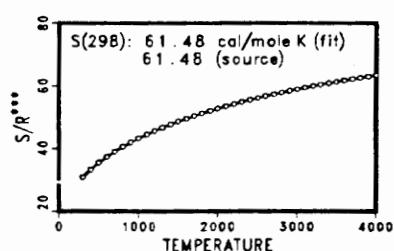
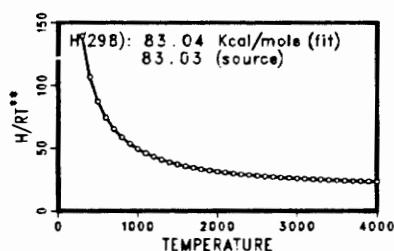
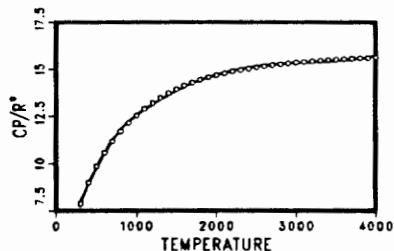
2-PROPYNYL C2V 2B2

GAS

As of: 8/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04754199E+02	0.11080277E-01	0.02793323E-05	-0.05479212E-07	0.01949629E-10	0.03988883E+06	0.05854549E+01
1000-4000K	0.08831047E+02	0.04357194E-01	-0.04109066E-05	-0.02368723E-08	0.04376520E-12	0.03847419E+06	-0.02177919E+03



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

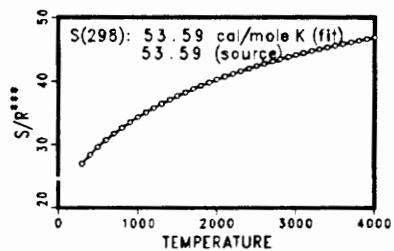
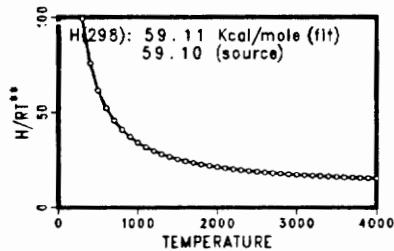
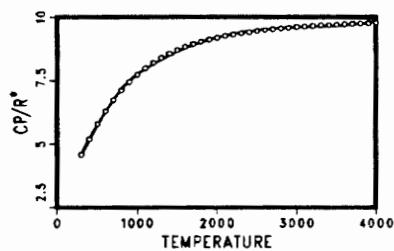
Species: H<sub>2</sub>CN

GAS

As of: 4/16/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02851661E+02	0.05695233E-01	0.10711403E-05	-0.16226120E-08	-0.02351108E-11	0.02863782E+06	0.08992751E+02
1000-4000K	0.05209703E+02	0.02969291E-01	-0.02855589E-05	-0.16355504E-09	0.03043259E-12	0.02767711E+06	-0.04444478E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

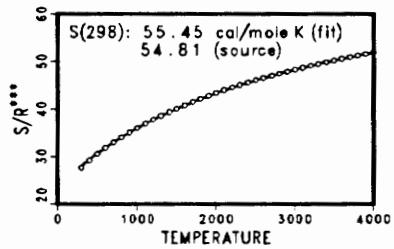
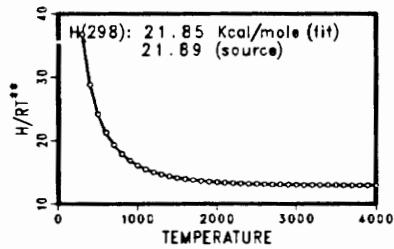
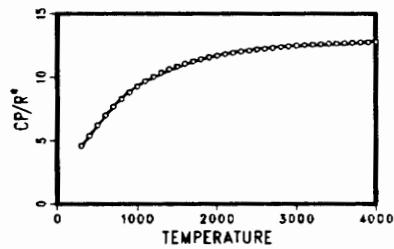
Species: H<sub>2</sub>CNH

GAS

As of: 4/16/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02365878E+02	0.06780570E-01	0.02422999E-04	-0.06157824E-08	-0.16150971E-11	0.09971141E+05	0.12307176E+02
1000-4000K	0.05221589E+02	0.04748525E-01	-0.04179158E-05	-0.02606612E-08	0.04703140E-12	0.08657219E+05	-0.04500776E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

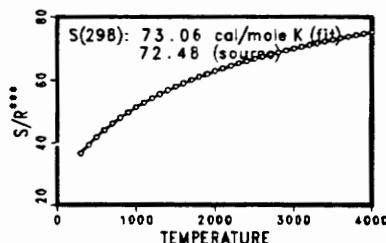
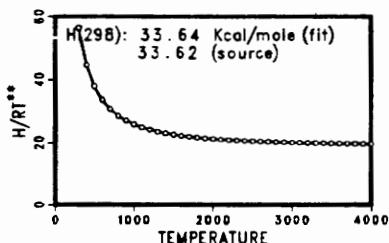
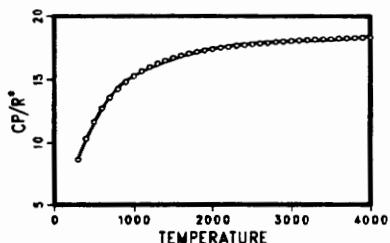
Species: H2CNNO2

GAS

As of: 4/16/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03534316E+02	0.01811271E+00	0.02394017E-05	-0.10800240E-07	0.04222725E-10	0.15090057E+05	0.11311378E+02
1000-4000K	0.11407942E+02	0.04564542E-01	-0.04600304E-05	-0.02513538E-08	0.04782211E-12	0.12421422E+05	-0.03165237E+03



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: H2GAET

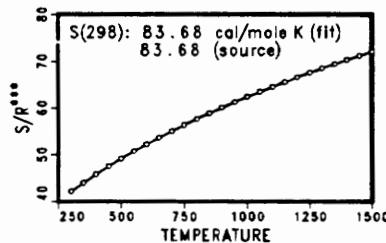
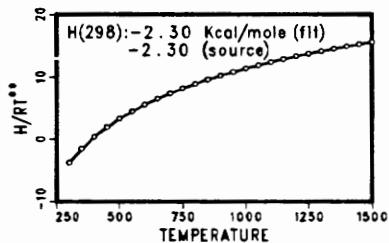
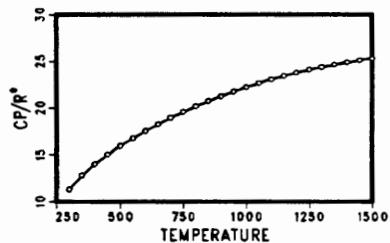
("ET" = C2H5, ETHYL)

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.04124020E+01	0.03972971E+00	0.07979140E-04	-0.08059233E-06	0.06040387E-09	-0.02983932E+05	0.02816147E+03
0600-1500K	0.07187273E+02	0.01867211E+00	0.06156157E-05	-0.06027763E-07	0.01797524E-10	-0.04232757E+05	-0.04686699E+02



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: H2GAME

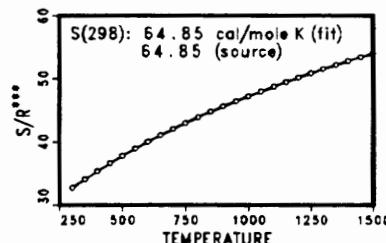
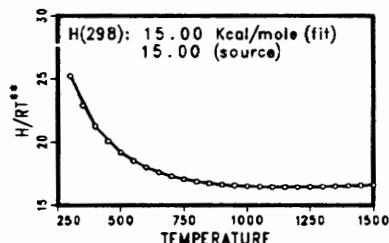
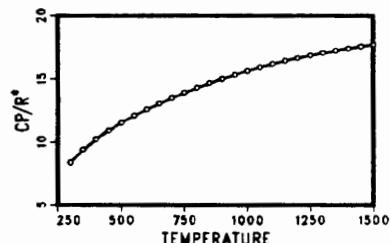
("ME" = CH3, METHYL)

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.05251130E+01	0.02904695E+00	0.04844148E-04	-0.06097646E-06	0.04672763E-09	0.06158712E+05	0.02122148E+03
0600-1500K	0.05831604E+02	0.12228715E-01	0.03033669E-05	-0.03956941E-07	0.12254516E-11	0.05189255E+05	-0.04446614E+02



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: H<sub>2</sub>NF

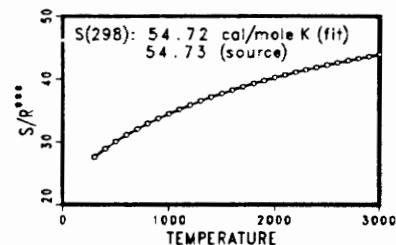
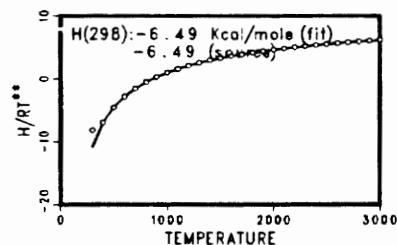
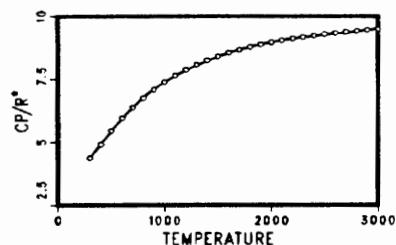
FLUOROAMMONIA

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02597862E+02	0.05882104E-01	0.04936351E-05	-0.01948600E-07	0.03634002E-11	-0.04301253E+05	0.10982895E+02
1000-3000K	0.04143658E+02	0.03805135E-01	-0.02771153E-05	-0.03589717E-08	0.07589549E-12	-0.04891486E+05	0.02309362E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: H<sub>2</sub>O

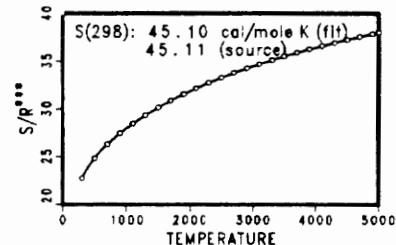
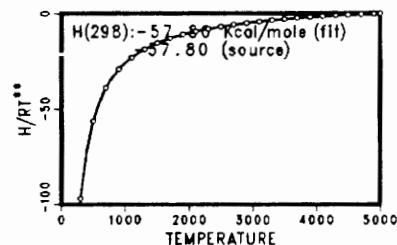
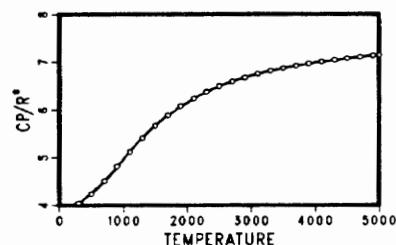
WATER

GAS

As of: 2/03/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03386842E+02	0.03474982E-01	-0.06354696E-04	0.06968581E-07	-0.02506588E-10	-0.03020811E+06	0.02590232E+02
1000-5000K	0.02672145E+02	0.03056293E-01	-0.08730260E-05	0.12009964E-09	-0.06391618E-13	-0.02989921E+06	0.06862817E+02



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: H<sub>2</sub>O(L)

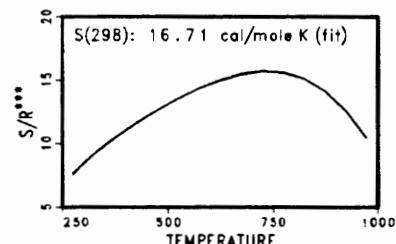
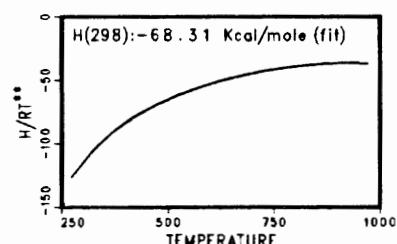
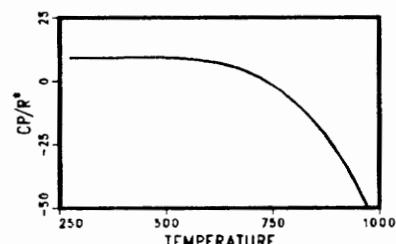
WATER

LIQUID

As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0273-1000K	0.12712782E+02	-0.01766279E+00	-0.02255666E-03	0.02082090E-05	-0.02407861E-08	-0.03748320E+06	-0.05911534E+03
1000-1000K	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00



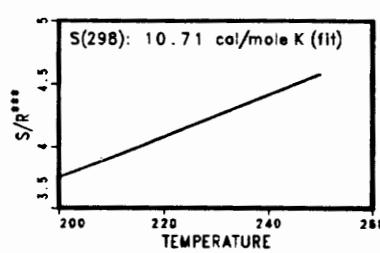
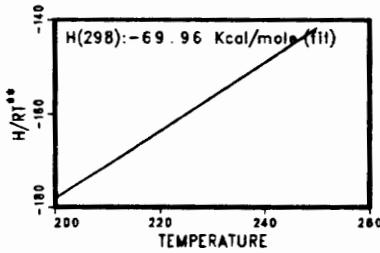
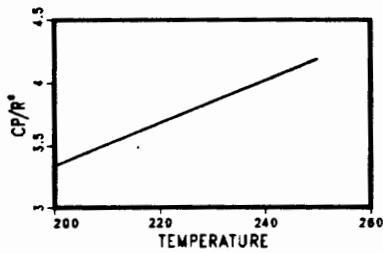
Source: NASA FIT TO NASA LEWIS DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: H<sub>2</sub>O(S) WATER SOLID As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0200-1000K	-0.03926933E+00	0.01692042E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	-0.03594958E+06	0.05693378E+01
1000-0273K	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00



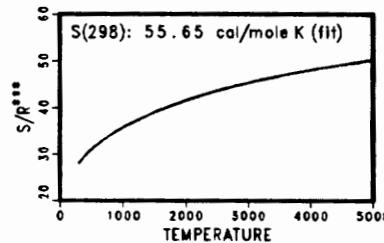
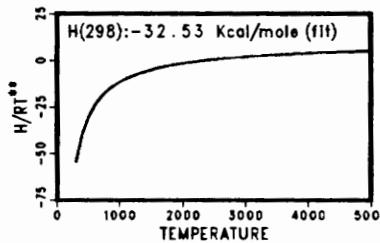
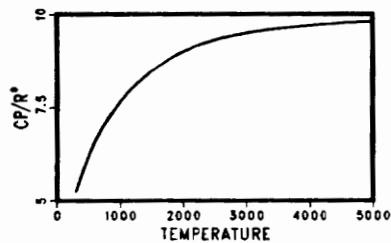
Source: NASA FIT TO NASA LEWIS DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: H<sub>2</sub>O<sub>2</sub> HYDROGEN PEROXIDE GAS As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03388753E+02	0.06569226E-01	-0.14850125E-06	-0.04625805E-07	0.02471514E-10	-0.01766314E+06	0.06785363E+02
1000-5000K	0.04573167E+02	0.04336136E-01	-0.14746888E-05	0.02348903E-08	-0.14316536E-13	-0.01800696E+06	0.05011369E+01



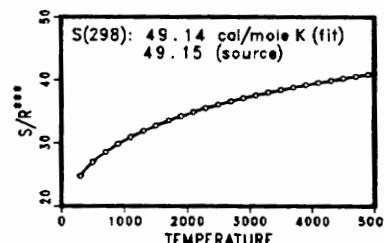
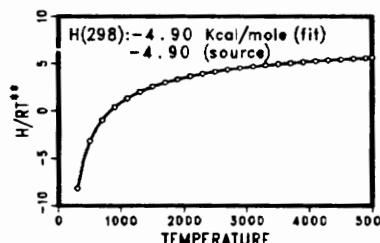
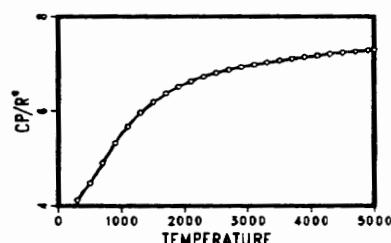
Source: NASA FIT TO NASA-LEWIS DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: H<sub>2</sub>S HYDROGEN SULFIDE GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03071029E+02	0.05578261E-01	-0.10309669E-04	0.12019529E-07	-0.04838369E-10	-0.03559826E+05	0.05935226E+02
1000-5000K	0.02883147E+02	0.03827835E-01	-0.14233978E-05	0.02497998E-08	-0.16602733E-13	-0.03480742E+05	0.07258161E+02



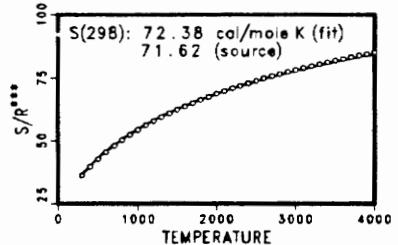
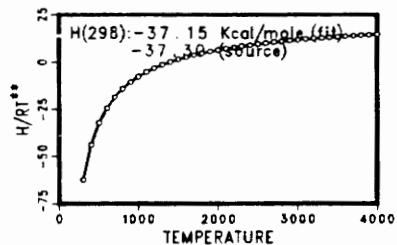
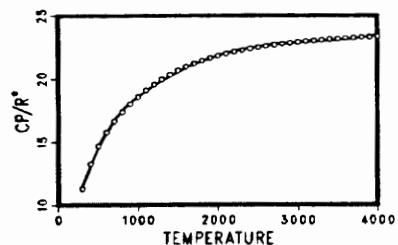
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: H<sub>2</sub>Si(NH<sub>2</sub>)<sub>2</sub> DIAMINOSILANE GAS As of: 2/27/90

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.05615307E+02	0.02079854E+00	-0.09999531E-05	-0.12885246E-07	0.06091865E-10	-0.02126283E+06	-0.16156578E+01
1000-4000K	0.13021791E+02	0.06465444E-01	-0.05816746E-05	-0.03484493E-08	0.06340675E-12	-0.02357070E+06	-0.04132569E+03



Source: SNL FIT TO BAC-MP4 DATA

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

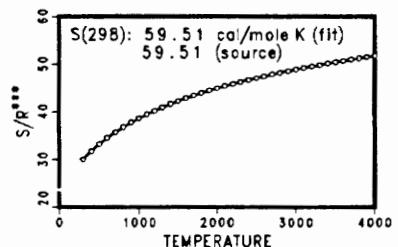
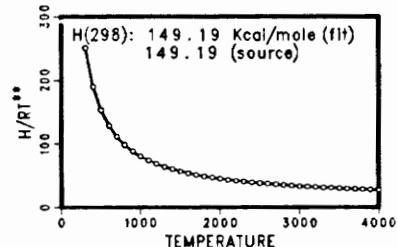
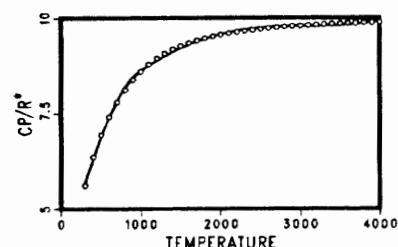
$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H<sub>2</sub>SIN GAS As of: 2/27/90

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03549344E+02	0.07311004E-01	0.03249025E-05	-0.03682945E-07	0.11215113E-11	0.07370656E+06	0.07565328E+02
1000-4000K	0.06826533E+02	0.02125460E-01	-0.02343131E-05	-0.11663394E-09	0.02277273E-12	0.07253672E+06	-0.10521624E+02



Source: SNL FIT TO BAC-MP4 DATA

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

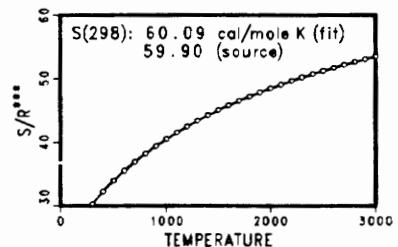
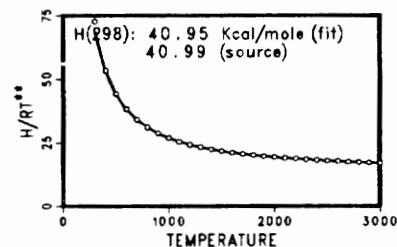
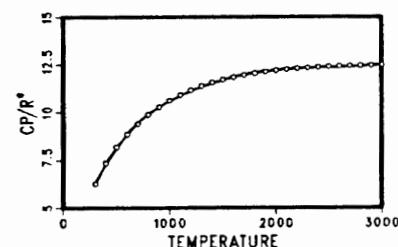
$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H<sub>2</sub>SINH GAS As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02822195E+02	0.12455182E-01	-0.08350819E-05	-0.07411813E-07	0.03579019E-10	0.01923616E+06	0.10547831E+02
1000-3000K	0.06588295E+02	0.04903194E-01	-0.04944719E-05	-0.05014630E-08	0.11394698E-12	0.01809794E+06	-0.09522970E+02



Source: SNL FIT TO BAC-MP4 DATA

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H2SINH2

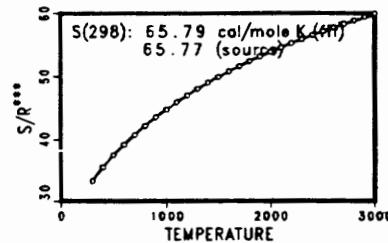
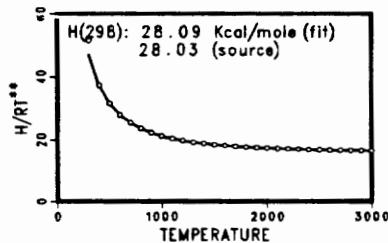
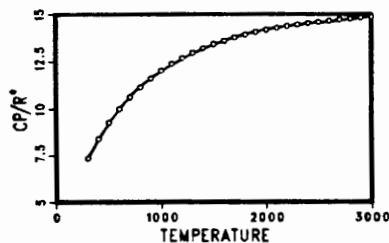
AMINOSILYL

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04053222E+02	0.11822311E-01	-0.04348128E-05	-0.06225818E-07	0.02798829E-10	0.12419705E+05	0.06562032E+02
1000-3000K	0.07392047E+02	0.05476841E-01	-0.04453276E-05	-0.05236661E-08	0.11383899E-12	0.11368581E+05	-0.11380495E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

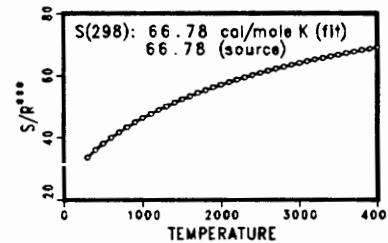
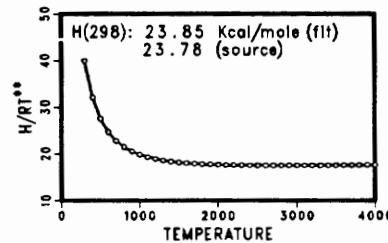
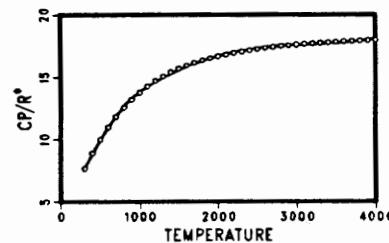
Species: H2SINH3

SILENE-AMMONIA TRANS STATE GAS

As of: 12/13/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04269729E+02	0.11252245E-01	0.01951721E-04	-0.03578372E-07	-0.08372202E-12	0.10222041E+05	0.05876735E+02
1000-4000K	0.08711392E+02	0.05909106E-01	-0.05436615E-05	-0.03248350E-08	0.05960257E-12	0.08441694E+05	-0.01933470E+03



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: H2SISIH2

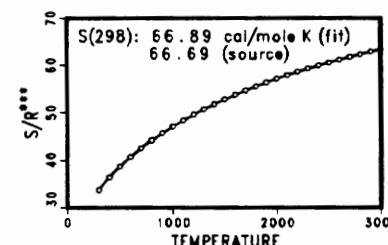
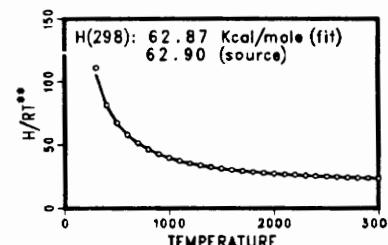
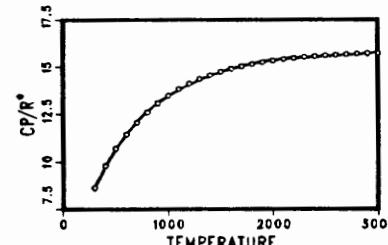
DISILENE

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.05133186E+02	0.12528548E-01	-0.04620421E-05	-0.06606075E-07	0.02864344E-10	0.02956915E+06	0.07605133E+01
1000-3000K	0.08986817E+02	0.05405047E-01	-0.05214021E-05	-0.05313742E-08	0.11887266E-12	0.02832747E+06	-0.02004478E+03



Source: SNLL FIT TO BAC-MP4 DATA

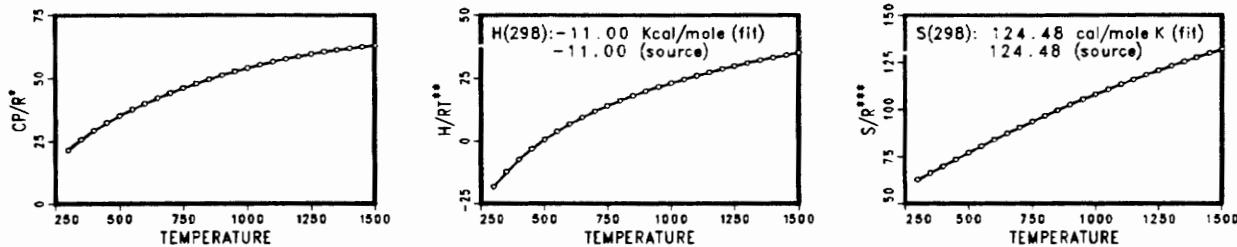
$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: H3ASGAET3 ("ET" = C2H5, ETHYL) GAS As of: 6/29/87

Fit  
 Coefficients       $a_1$        $a_2$        $a_3$        $a_4$        $a_5$        $a_6$        $a_7$   
 0300-0600K -0.08974745E+02 0.10905161E+00 0.02811457E-03 -0.02195513E-05 0.15997339E-09 -0.07592761E+05 0.08165459E+03  
 0600-1500K 0.08508501E+02 0.05632369E+00 0.02524140E-04 -0.01861451E-06 0.05372402E-10 -0.10855169E+05 -0.03399857E+02



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

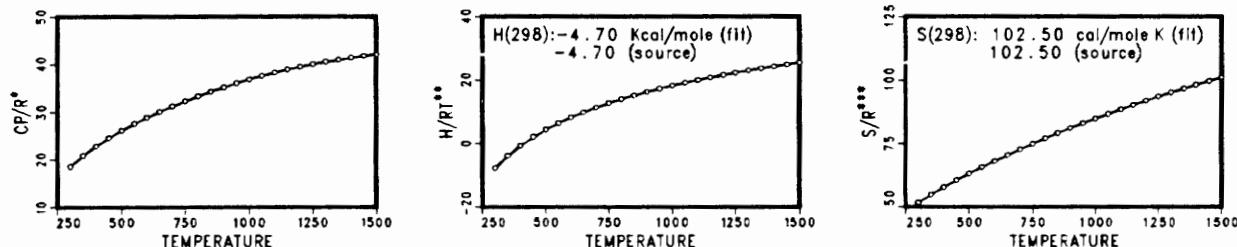
$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: H3ASGAME3 ("ME" = CH3,METHYL) GAS As of: 6/29/87

Fit  
 Coefficients       $a_1$        $a_2$        $a_3$        $a_4$        $a_5$        $a_6$        $a_7$   
 0300-0600K 0.12671606E+01 0.06214586E+00 0.13856307E-04 -0.12200444E-06 0.08982019E-09 -0.05425619E+05 0.02613306E+03  
 0600-1500K 0.11254990E+02 0.03159752E+00 0.11779036E-05 -0.10133524E-07 0.02947355E-10 -0.07280344E+05 -0.02238729E+03



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

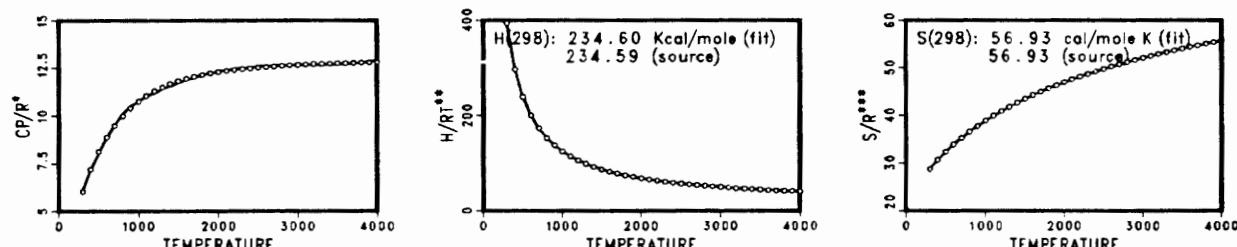
$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: H3SIN SILYLNITRENE GAS As of: 2/27/90

Fit  
 Coefficients       $a_1$        $a_2$        $a_3$        $a_4$        $a_5$        $a_6$        $a_7$   
 0300-1000K 0.02790628E+02 0.11345662E-01 0.08321879E-05 -0.05845045E-07 0.01685969E-10 0.11673571E+06 0.09384630E+02  
 1000-4000K 0.07964213E+02 0.03355633E-01 -0.03579695E-05 -0.01889818E-08 0.03650912E-12 0.11486972E+06 -0.01924110E+03



Source:

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

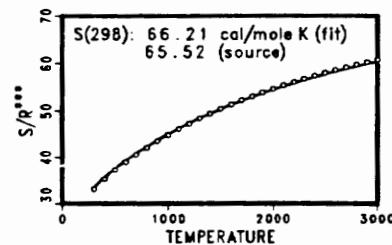
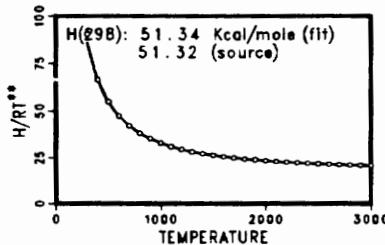
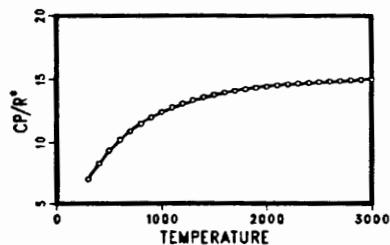
$$\bullet \text{H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: H<sub>3</sub>SINH                      SİYALAMİDOGEN                      GAS                      As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02778390E+02	0.15107111E-01	-0.06734260E-05	-0.08928515E-07	0.04115347E-10	0.02435913E+06	0.13093859E+02
1000-3000K	0.07697340E+02	0.05657943E-01	-0.05209306E-05	-0.05617966E-08	0.12635020E-12	0.02282005E+06	-0.13303793E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

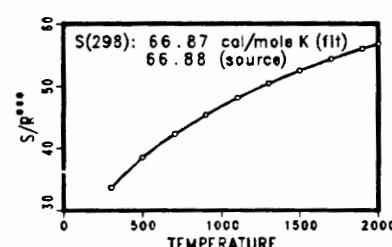
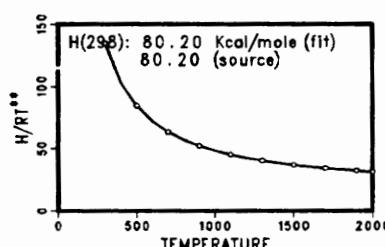
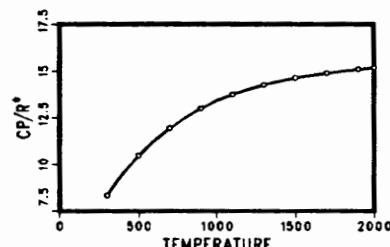
$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H<sub>3</sub>SISIH                      GAS                      As of: 9/05/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02774192E+02	0.02555302E+00	-0.02883836E-03	0.02000737E-06	-0.06100616E-10	0.03861801E+06	0.11350098E+02
1000-2000K	0.07778291E+02	0.07255418E-01	-0.08123265E-05	-0.11682818E-08	0.03425139E-11	0.03742600E+06	-0.13484629E+02



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

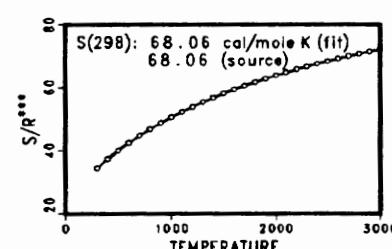
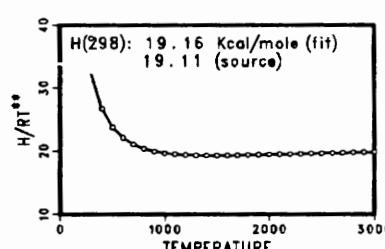
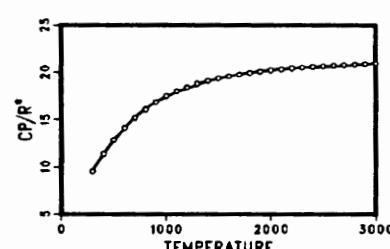
$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: H<sub>3</sub>SISIH<sub>3</sub>                      DISILANE                      GAS                      As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03898289E+02	0.01977415E+00	0.01791014E-05	-0.10331682E-07	0.03931698E-10	0.07621719E+05	0.06227022E+02
1000-3000K	0.10682729E+02	0.08221416E-01	-0.08096035E-05	-0.08337975E-08	0.01908205E-11	0.05316920E+05	-0.03082188E+03



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

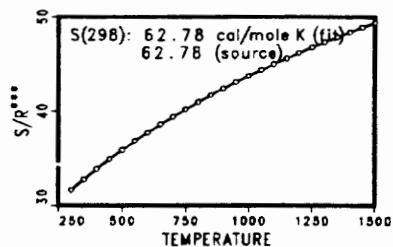
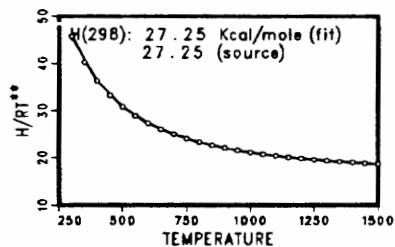
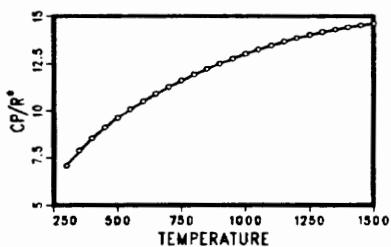
$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HALME ("ME" = CH<sub>3</sub>,METHYL) GAS As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.11187894E+01	0.02180038E+00	0.04120785E-04	-0.04366690E-06	0.03273825E-09	0.12447363E+05	0.01886107E+03
0600-1500K	0.04812273E+02	0.10296448E-01	0.02582807E-05	-0.03323596E-07	0.09884584E-11	0.11766730E+05	0.09557062E+01



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

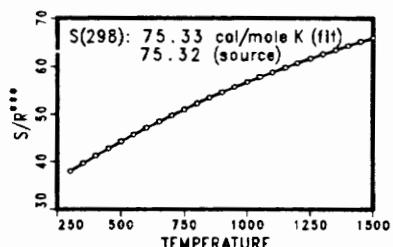
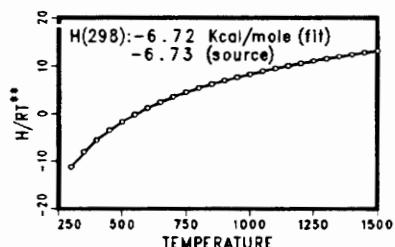
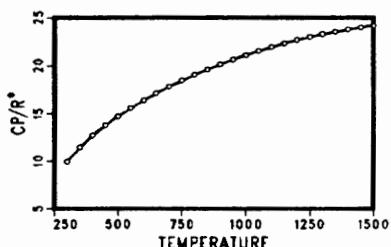
$$\bullet\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet\bullet\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HALME2 ("ME" = CH<sub>3</sub>,METHYL) GAS As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	-0.14942614E+01	0.04158567E+00	0.08686772E-04	-0.08604142E-06	0.06447652E-09	-0.04722516E+05	0.03427724E+03
0600-1500K	0.05705171E+02	0.01924317E+00	0.06377855E-05	-0.06346800E-07	0.01896799E-10	-0.06049864E+05	-0.06331378E+01



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

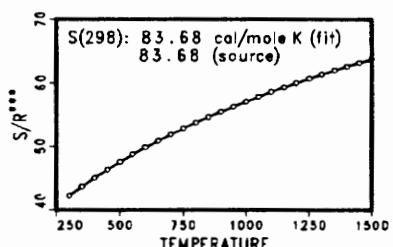
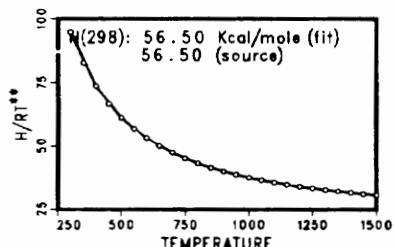
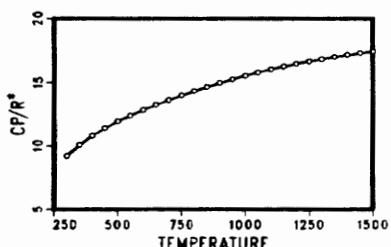
$$\bullet\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet\bullet\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HASALME ("ME" = CH<sub>3</sub>,METHYL) GAS As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.02544858E+02	0.02465794E+00	0.03677807E-04	-0.05008893E-06	0.03848383E-09	0.02663010E+06	0.02046858E+03
0600-1500K	0.06956538E+02	0.10612781E-01	0.02440153E-05	-0.03297737E-07	0.10200039E-11	0.02582505E+06	-0.08625792E+01



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

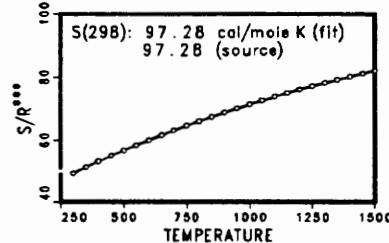
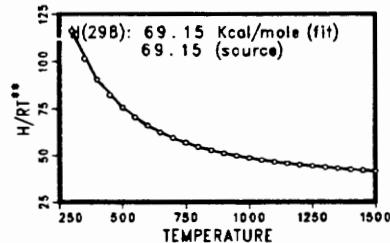
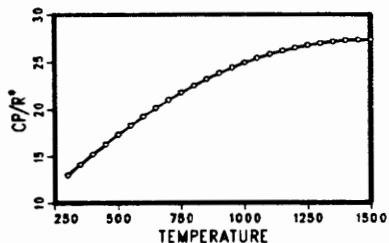
$$\bullet\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet\bullet\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HASGAET ("ET" = C2H5, ETHYL) GAS As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.05642723E+02	0.02296738E+00	0.10948674E-04	-0.02449038E-06	0.09602700E-10	0.03204717E+06	0.09675533E+02
0600-1500K	0.06336445E+02	0.02340603E+00	0.09066638E-05	-0.07519059E-07	0.01828115E-10	0.03184605E+06	0.05812180E+02



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HASGAME

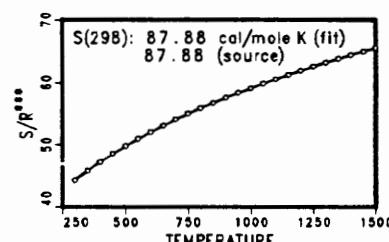
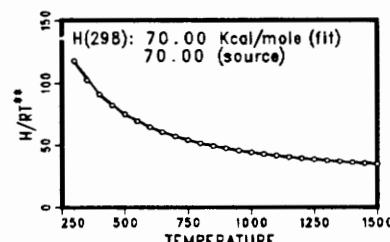
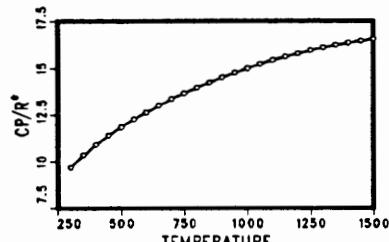
("ME" = CH3,METHYL)

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.04859126E+02	0.01750423E+00	0.02831995E-04	-0.03107936E-06	0.02299468E-09	0.03302941E+06	0.11429521E+02
0600-1500K	0.07507970E+02	0.09277900E-01	0.01891931E-05	-0.02769886E-07	0.07996069E-11	0.03253907E+06	-0.14226081E+01



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HASME

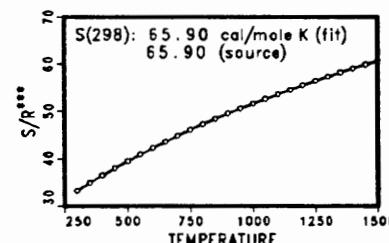
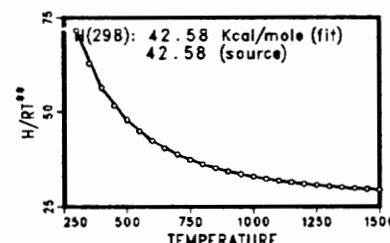
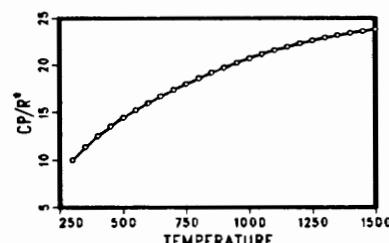
("ME" = CH3,METHYL)

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	-0.15750948E+00	0.03649094E+00	0.08332939E-04	-0.07234666E-06	0.05330928E-09	0.01989791E+06	0.02335316E+03
0600-1500K	0.05753261E+02	0.01841813E+00	0.07493312E-05	-0.05919916E-07	0.01726246E-10	0.01880057E+06	-0.05360325E+02



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

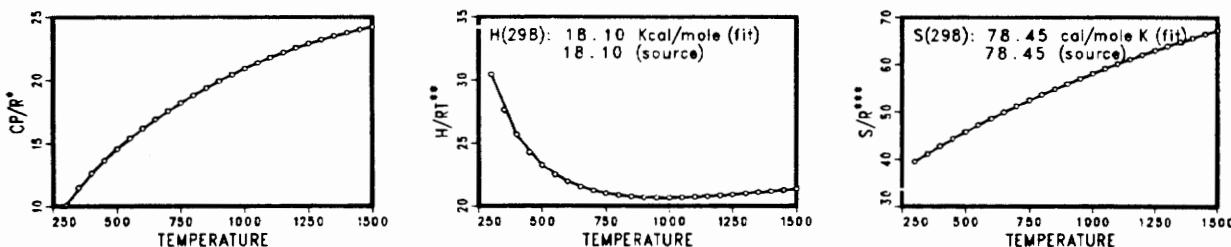
$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: HASME2 ("ME" = CH<sub>3</sub>,METHYL) GAS As of: 6/29/87

Fit  
 Coefficients      a<sub>1</sub>      a<sub>2</sub>      a<sub>3</sub>      a<sub>4</sub>      a<sub>5</sub>      a<sub>6</sub>      a<sub>7</sub>  
 0300-0600K -0.02908405E+01 0.03729576E+00 0.08335854E-04 -0.07455611E-06 0.055278B1E-09 0.07587765E+05 0.03020451E+03  
 0600-1500K 0.05850436E+02 0.01841765E+00 0.08066844E-05 -0.05868715E-07 0.01726428E-10 0.06450535E+05 0.03909152E+01

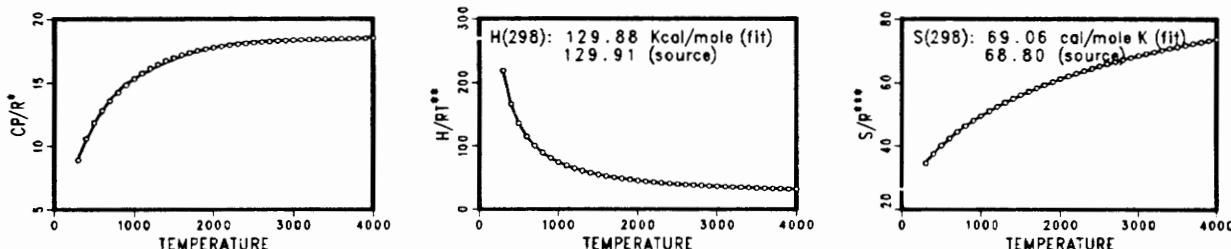


Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
 Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: HCCHCCH HCCH CIS GAS As of: 8/24/89

Fit  
 Coefficients      a<sub>1</sub>      a<sub>2</sub>      a<sub>3</sub>      a<sub>4</sub>      a<sub>5</sub>      a<sub>6</sub>      a<sub>7</sub>  
 0300-1000K 0.04153881E+02 0.01726287E+00 -0.02389374E-05 -0.10187000E-07 0.04340504E-10 0.06338070E+06 0.06036506E+02  
 1000-4000K 0.010752738E+02 0.05381153E-01 -0.05549637E-05 -0.03052266E-08 0.05761740E-12 0.06121419E+06 -0.02973025E+03

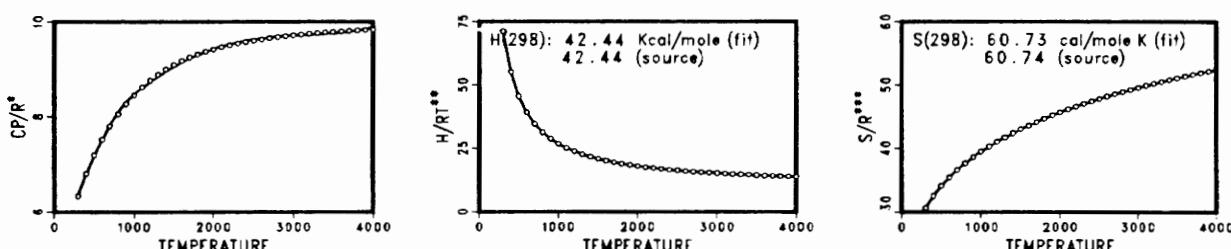


Source: SNLL FIT TO BURCAT DATA

$$\begin{aligned} * \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: HCCO KETYL GAS As of: 3/23/87

Fit  
 Coefficients      a<sub>1</sub>      a<sub>2</sub>      a<sub>3</sub>      a<sub>4</sub>      a<sub>5</sub>      a<sub>6</sub>      a<sub>7</sub>  
 0300-1000K 0.05047965E+02 0.04453478E-01 0.02268282E-05 -0.14820945E-08 0.02250741E-11 0.01965891E+06 0.04818439E+01  
 1000-4000K 0.06758073E+02 0.02000400E-01 -0.02027607E-05 -0.10411318E-09 0.01965164E-12 0.01901513E+06 -0.09071262E+02



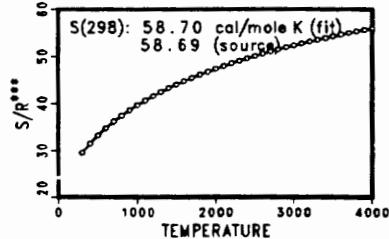
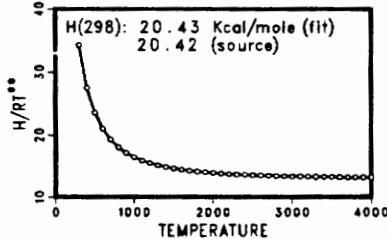
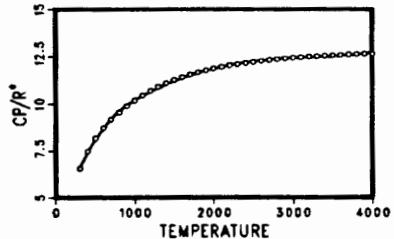
Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: HCCOH                    ETHYNOL                    GAS                    As of: 3/23/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03899465E+02	0.09701075E-01	-0.03119309E-05	-0.05537732E-07	0.02465732E-10	0.08701190E+05	0.04491874E+02
1000-4000K	0.07328324E+02	0.03336416E-01	-0.03024705E-05	-0.01781106E-08	0.03245168E-12	0.07598258E+05	-0.14012140E+02



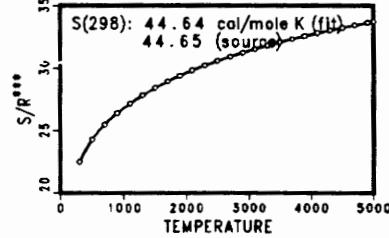
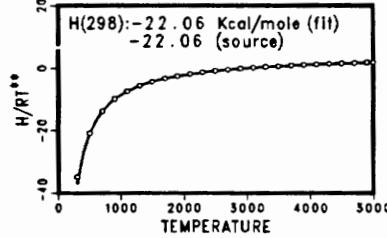
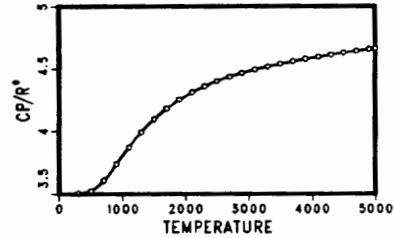
Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: HCl                    HYDROGEN CHLORIDE                    GAS                    As of: 4/21/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03338534E+02	0.12682066E-02	-0.03666916E-04	0.04703992E-07	-0.01836011E-10	-0.12131511E+05	0.03193555E+02
1000-5000K	0.02755335E+02	0.14735811E-02	-0.04971254E-05	0.08108658E-09	-0.05072063E-13	-0.11918058E+05	0.06515116E+02



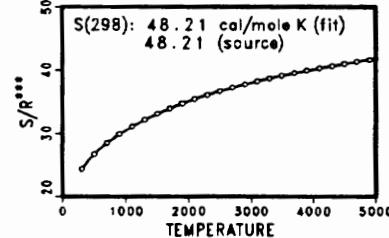
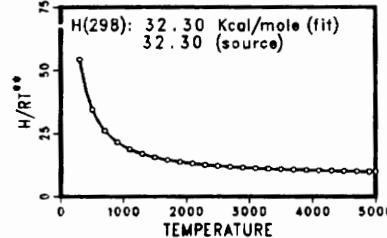
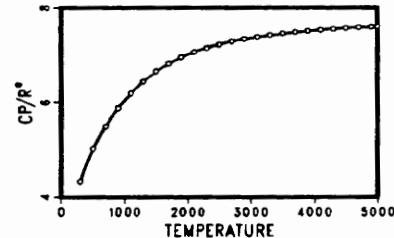
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: HCN                    HYDROGEN CYANIDE                    GAS                    As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02490462E+02	0.08611280E-01	-0.10310342E-04	0.07481498E-07	-0.02229109E-10	0.15208344E+05	0.07904981E+02
1000-5000K	0.03650077E+02	0.03460998E-01	-0.12742788E-05	0.02217655E-08	-0.14771774E-13	0.14983916E+05	0.02393220E+02



Source: SNLL FIT TO JANAF TABLES (CHN)

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

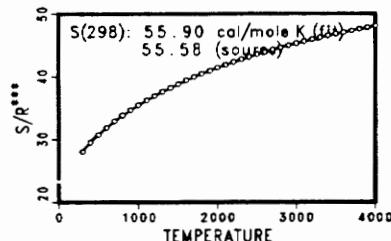
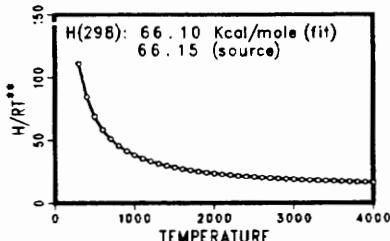
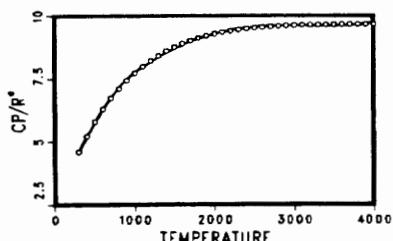
Species: HCNH

GAS

As of: 4/16/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02759456E+02	0.06103386E-01	0.07713149E-05	-0.02063093E-07	0.01931919E-11	0.03217247E+06	0.10574895E+02
1000-4000K	0.04923292E+02	0.03332897E-01	-0.03370896E-05	-0.01901619E-08	0.03531825E-12	0.03132669E+06	-0.16325088E+01



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

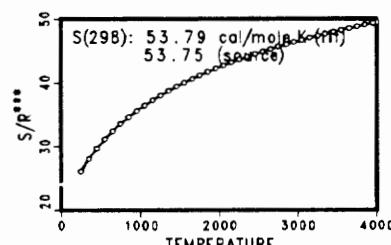
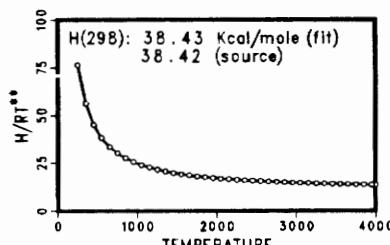
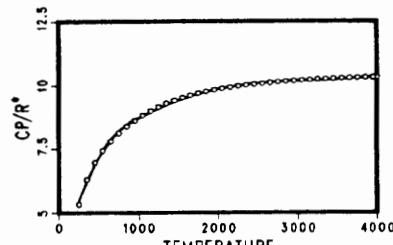
Species: HCNO

GAS

As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0250-1000K	0.03184858E+02	0.09752316E-01	-0.12802028E-05	-0.06163104E-07	0.03226275E-10	0.01797907E+06	0.06123843E+02
1000-4000K	0.06692412E+02	0.02368360E-01	-0.02371510E-05	-0.12755033E-09	0.02407137E-12	0.01694736E+06	-0.12454345E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: HCO

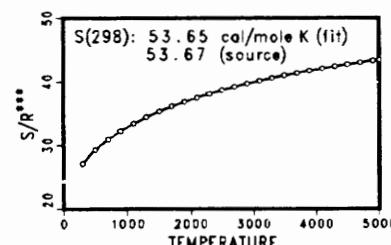
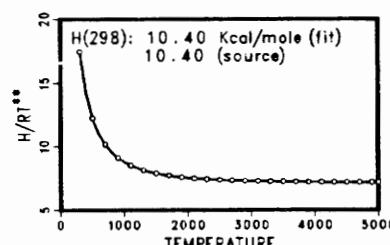
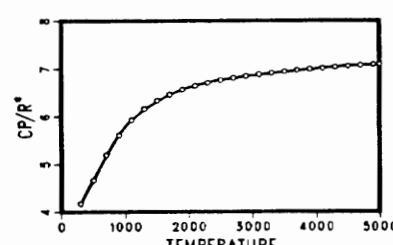
FORMYL

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02898329E+02	0.06199146E-01	-0.09623084E-04	0.10898249E-07	-0.04574885E-10	0.04159922E+05	0.08983614E+02
1000-5000K	0.03557271E+02	0.03345572E-01	-0.13350060E-05	0.02470572E-08	-0.01713850E-12	0.03916324E+05	0.05552299E+02



Source: SNLL FIT TO JANAF TABLES (CHO)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: HCO+

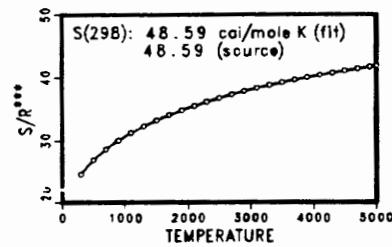
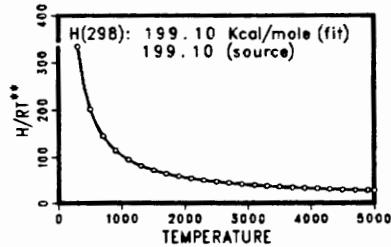
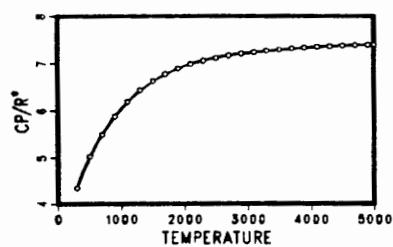
FORMYL, UNIPOSITIVE ION

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02496483E+02	0.08690658E-01	-0.10604453E-04	0.07882791E-07	-0.02418385E-10	0.09915097E+06	0.08048177E+02
1000-5000K	0.03692074E+02	0.03454732E-01	-0.13165244E-05	0.02323551E-08	-0.15541321E-13	0.09890941E+06	0.02330722E+02



Source: SNLL FIT TO JANAF TABLES (CHO+)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: HE

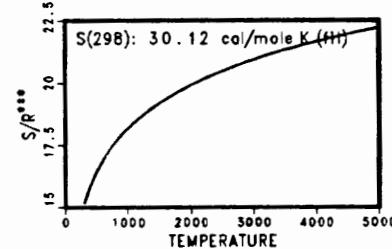
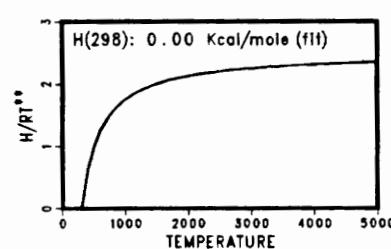
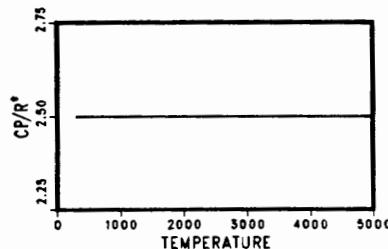
HELUM, MONATOMIC (REF ST)

GAS

As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	-0.07453750E+04	0.09153488E+01
1000-5000K	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	-0.07453750E+04	0.09153489E+01



Source: NASA FIT TO NASA-LEWIS DATA

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: HE+

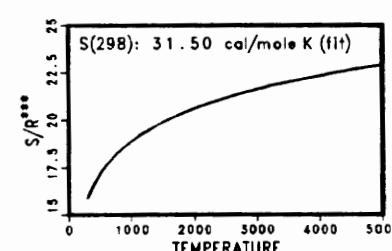
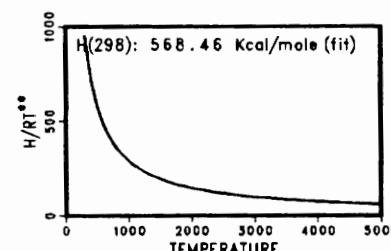
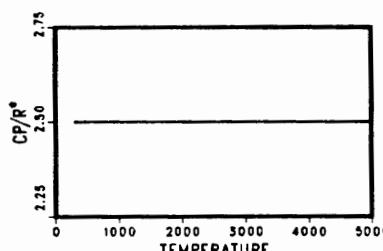
HELUM, UNIPOSITIVE ION

GAS

As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.02853426E+07	0.16084046E+01
1000-5000K	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.02853426E+07	0.16084045E+01



Source: NASA FIT TO NASA-LEWIS DATA

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: HF

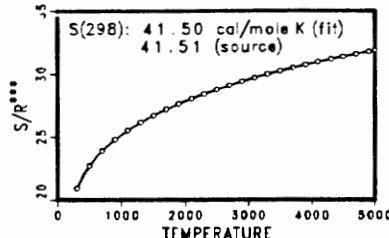
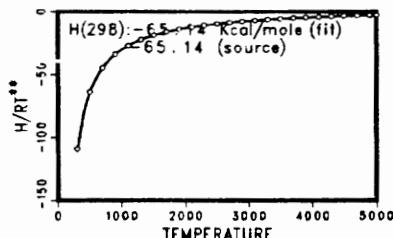
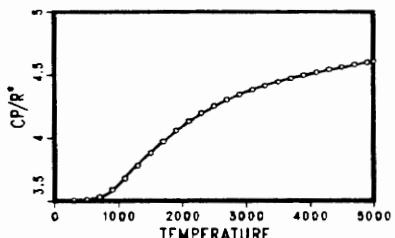
## HYDROGEN FLUORIDE

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03431841E+02	0.04404165E-02	-0.08828452E-05	0.06574516E-08	-0.02055909E-12	-0.03381977E+06	0.12382699E+01
1000-5000K	0.02956767E+02	0.07721015E-02	-0.09899834E-06	-0.04993520E-10	0.14293306E-14	-0.03361061E+06	0.04016731E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: HGAET

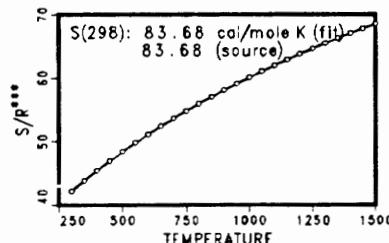
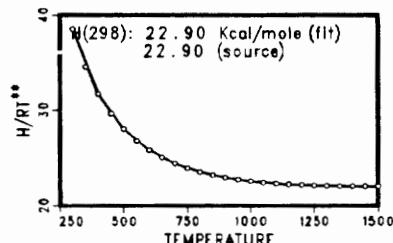
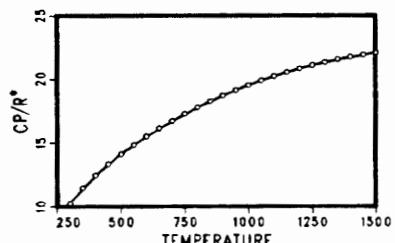
("ET" = C<sub>2</sub>H<sub>5</sub>, ETHYL)

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	0.11632838E+01	0.03282212E+00	0.06765717E-04	-0.06509541E-06	0.04835806E-09	0.09767174E+05	0.02588269E+03
0600-1500K	0.06580151E+02	0.16101323E-01	0.05009545E-05	-0.05185148E-07	0.15240853E-11	0.08765131E+05	-0.04046067E+01



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: HGAET2

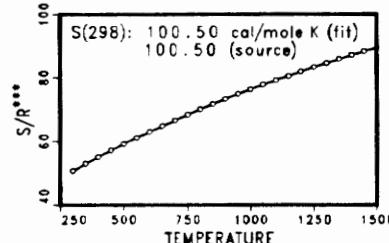
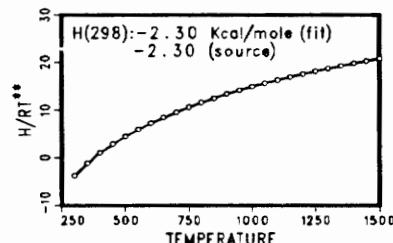
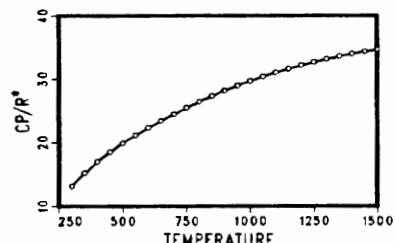
("ET" = C<sub>2</sub>H<sub>5</sub>, ETHYL)

GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	-0.14865759E+01	0.05217640E+00	0.13563420E-04	-0.10119820E-06	0.07319853E-09	-0.02985242E+05	0.04364749E+03
0600-1500K	0.06511306E+02	0.02819753E+00	0.14187506E-05	-0.09000947E-07	0.02572894E-10	-0.04482180E+05	0.04709021E+02



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

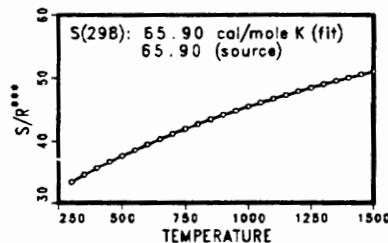
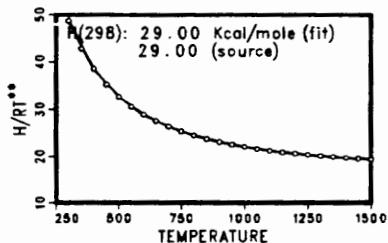
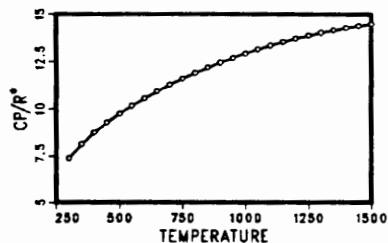
$$\bullet \text{H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: HGAME ("ME" = CH<sub>3</sub>,METHYL) GAS As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-600K	0.01784749E+02	0.02058861E+00	0.03548509E-04	-0.04111927E-06	0.03108978E-09	0.13184225E+05	0.01700701E+03
0600-1500K	0.05318279E+02	0.09490931E-01	0.02277164E-05	-0.03005070E-07	0.09037830E-11	0.12535338E+05	-0.10657105E+00



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

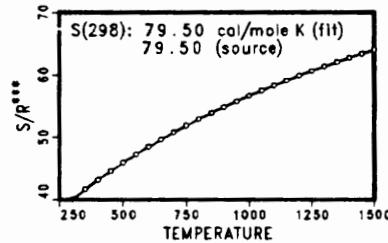
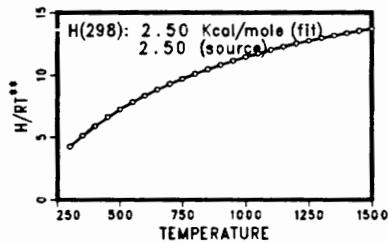
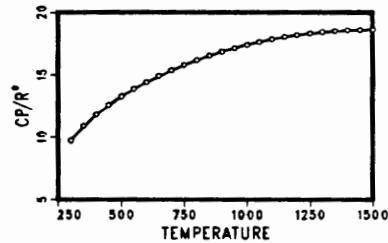
$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: HGAME2 ("ME" = CH<sub>3</sub>,METHYL) GAS As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-600K	0.09039155E+01	0.03264779E+00	0.05389243E-04	-0.06814504E-06	0.05150323E-09	-0.03978242E+04	0.02539304E+03
0600-1500K	0.06759397E+02	0.14261030E-01	-0.11740239E-06	-0.05001401E-07	0.15027851E-11	-0.14732646E+04	-0.02967135E+02



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

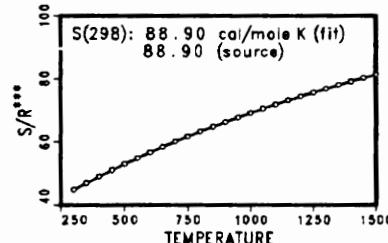
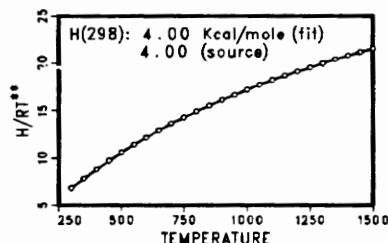
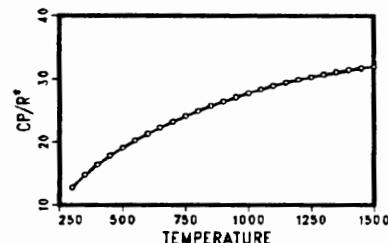
$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: HMEGAET ("ME"=CH<sub>3</sub>,METHYL; "ET"=C<sub>2</sub>H<sub>5</sub>,ETHYL) GAS As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-600K	-0.02079142E+02	0.05373076E+00	0.11810364E-04	-0.10998548E-06	0.08189554E-09	0.03216961E+04	0.04086070E+03
0600-1500K	0.07025463E+02	0.02564787E+00	0.09619100E-05	-0.08403699E-07	0.02488960E-10	-0.13613768E+04	-0.03319484E+02



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

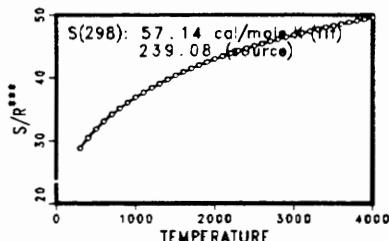
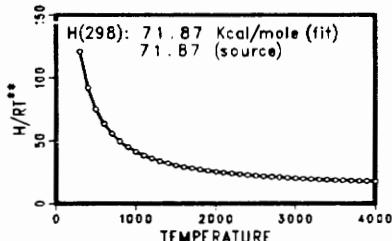
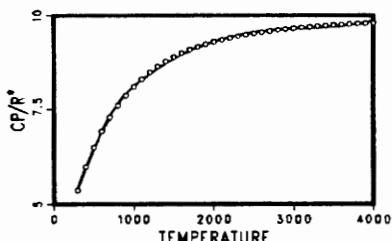
$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: HN3 HYDRAZOIC ACID GAS As of: 8/26/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03621003E+02	0.06030785E-01	0.04054460E-05	-0.02545270E-07	0.06174280E-11	0.03482373E+06	0.06333769E+02
1000-4000K	0.06023015E+02	0.02454362E-01	-0.02404279E-05	-0.13229726E-09	0.02474146E-12	0.03394051E+06	-0.07015537E+02



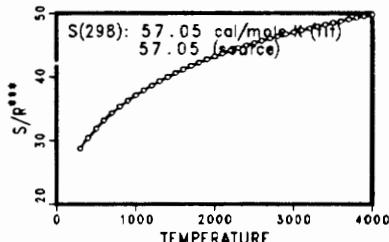
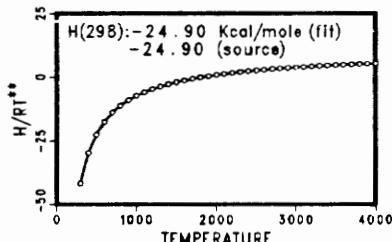
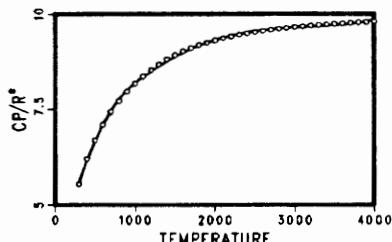
Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: HNCO ISOCYANIC ACID GAS As of: 3/12/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03694059E+02	0.06657236E-01	-0.05054468E-06	-0.03473411E-07	0.13605694E-11	-0.13919758E+05	0.05712742E+02
1000-4000K	0.06211867E+02	0.02297137E-01	-0.02216128E-05	-0.12220438E-09	0.02272406E-12	-0.14770725E+05	-0.08016633E+02



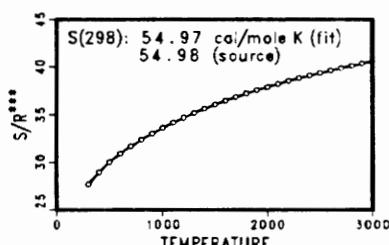
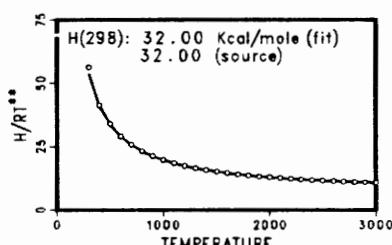
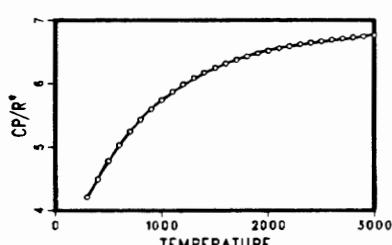
Source: FIT TO BAC-MP4 DATA WITH H298=-24.9 PER MILLER

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: HNF MONOFLUOROAMIDOGEN GAS As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03249760E+02	0.03261817E-01	0.04355642E-06	-0.11002765E-08	0.02926757E-11	0.14991264E+05	0.08187434E+02
1000-3000K	0.04133219E+02	0.01912056E-01	-0.16253301E-06	-0.01726461E-08	0.03743691E-12	0.14670521E+05	0.03292122E+02



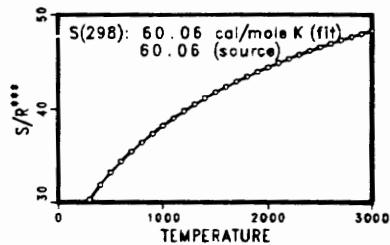
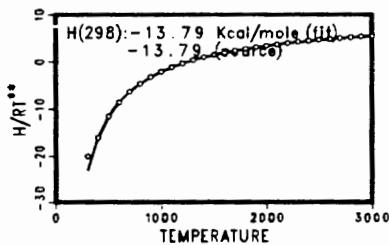
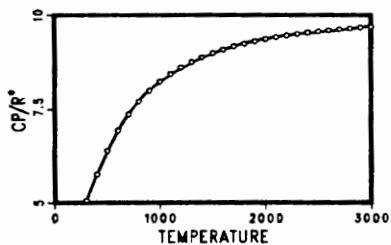
Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: HNF2 DIFLUOROAMMONIA GAS As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02572812E+02	0.08762144E-01	-0.02326921E-05	-0.05000826E-07	0.02143837E-10	-0.08086760E+05	0.13006810E+02
1000-3000K	0.05704866E+02	0.03049897E-01	-0.02826802E-05	-0.02923184E-08	0.06551055E-12	-0.09107488E+05	-0.03941331E+02



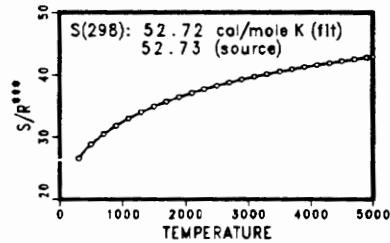
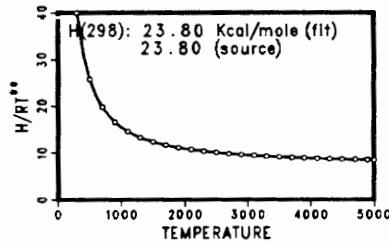
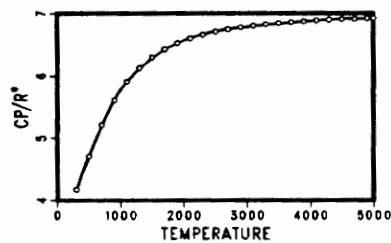
Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6 T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: HNO NITROXYL GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02784402E+02	0.06609646E-01	-0.09300223E-04	0.09437980E-07	-0.03753146E-10	0.10918779E+05	0.09035629E+02
1000-5000K	0.03615144E+02	0.03212485E-01	-0.12603370E-05	0.02267297E-08	-0.15362358E-13	0.10661911E+05	0.04810263E+02



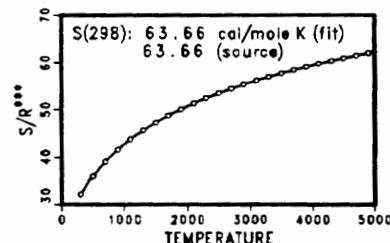
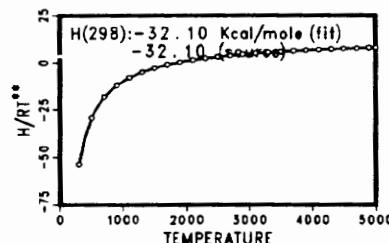
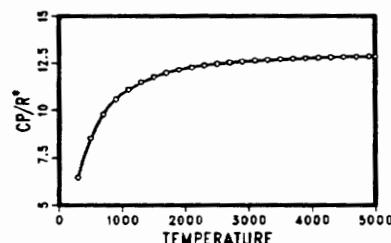
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6 T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: HNO3 NITRIC ACID GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.13531850E+01	0.02220024E+00	-0.01978811E-03	0.08773908E-07	-0.16583844E-11	-0.01738562E+06	0.01851868E+03
1000-5000K	0.07003844E+02	0.05811493E-01	-0.02333788E-04	0.04288814E-08	-0.02959385E-12	-0.01889952E+06	-0.10478628E+02



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6 T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: HO<sub>2</sub>

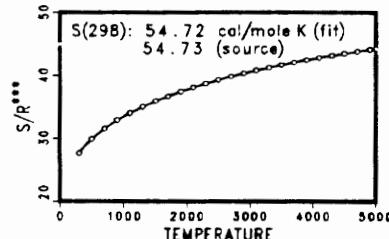
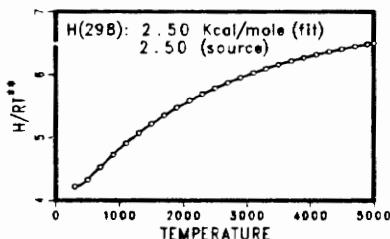
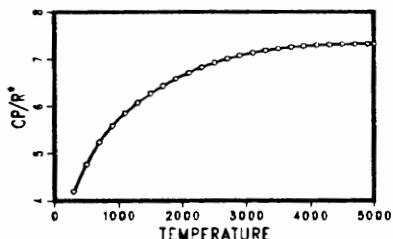
## HYDROPEROXYL

GAS

As of: 2/03/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02979963E+02	0.04996697E-01	-0.03790997E-04	0.02354192E-07	-0.08089024E-11	0.01762273E+04	0.09222724E+02
1000-5000K	0.04072191E+02	0.02131296E-01	-0.05308145E-05	0.06112269E-09	-0.02841164E-13	-0.15797270E+03	0.03476029E+02



Source: SNLL FIT TO JANAF TABLES WITH H298=2.5 PER MILLER

\*  $CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$   
\*\*  $H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6 T^5/6 + a_7 T^6/7$   
\*\*\*  $S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_6 T^5/5 + a_7 T^6/6$

Species: HOCl

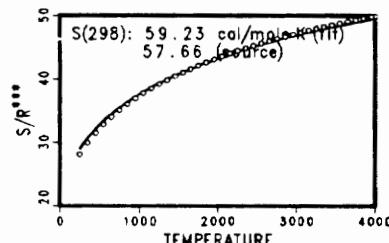
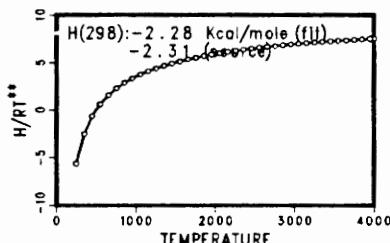
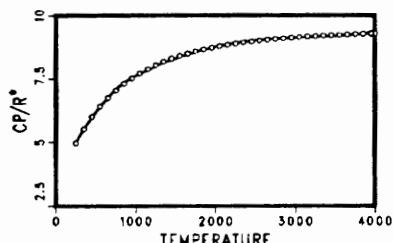
## CYANIC ACID TRANS

GAS

As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0250-1000K	0.03628292E+02	0.05664184E-01	-0.11702056E-06	-0.02348638E-07	0.08016402E-11	-0.02475925E+05	0.07476825E+02
1000-4000K	0.05645607E+02	0.02298206E-01	-0.02162629E-05	-0.12148014E-09	0.02238636E-12	-0.03178109E+05	-0.03590263E+02



Source: SNLL FIT TO BAC-MP4 DATA

\*  $CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$   
\*\*  $H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6 T^5/6 + a_7 T^6/7$   
\*\*\*  $S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_6 T^5/5 + a_7 T^6/6$

Species: HONO

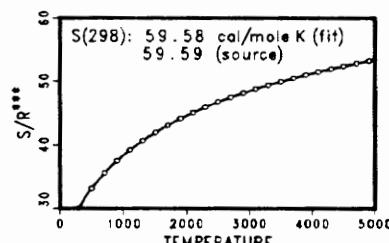
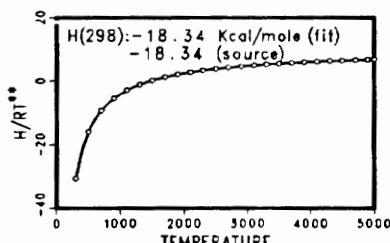
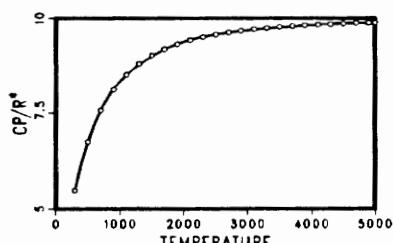
## NITROUS ACID, CIS-

GAS

As of: 3/17/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02290413E+02	0.14099223E-01	-0.13678717E-04	0.07498780E-07	-0.01876905E-10	-0.10431945E+05	0.13280769E+02
1000-5000K	0.05486892E+02	0.04218064E-01	-0.16491426E-05	0.02971876E-08	-0.02021148E-12	-0.11268646E+05	-0.02997002E+02

Source: SNLL FIT TO JANAF TABLES (HNO<sub>2</sub>)

\*  $CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$   
\*\*  $H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6 T^5/6 + a_7 T^6/7$   
\*\*\*  $S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_6 T^5/5 + a_7 T^6/6$

Species: HSi(NH<sub>2</sub>)<sub>2</sub>

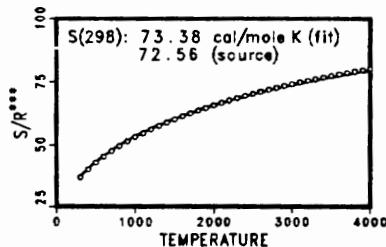
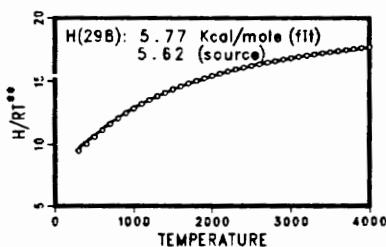
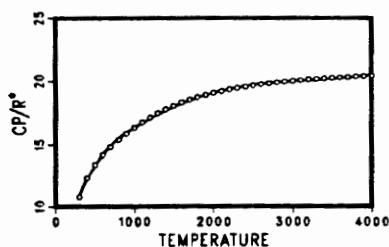
## DIAMINOSILANE

## GAS

As of: 2/27/90

Fit

Coefficients	$\alpha_1$	$\alpha_2$	$\alpha_3$	$\alpha_4$	$\alpha_5$	$\alpha_6$	$\alpha_7$
0300-1000K	0.0628969E+02	0.16750596E-01	-0.15208775E-05	-0.10700650E-07	0.05538640E-10	0.03154770E+04	-0.03746008E+02
1000-4000K	0.11716773E+02	0.05339021E-01	-0.04667823E-05	-0.02824087E-08	0.05080915E-12	-0.12641686E+04	-0.03245117E+03



Source: SNL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= \alpha_1 + \alpha_2 T + \alpha_3 T^2 + \alpha_4 T^3 + \alpha_5 T^4 \\ ** \text{H/RT} &= \alpha_1 + \alpha_2 T / 2 + \alpha_3 T^2 / 3 + \alpha_4 T^3 / 4 + \alpha_5 T^4 / 5 + \alpha_6 T \\ *** \text{S/R} &= \alpha_1 \ln(T) + \alpha_2 T + \alpha_3 T^2 / 2 + \alpha_4 T^3 / 3 + \alpha_5 T^4 / 4 + \alpha_7 \end{aligned}$$

Species: HSi(NH<sub>2</sub>)<sub>3</sub>

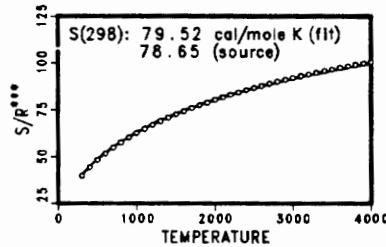
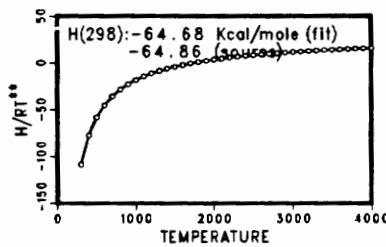
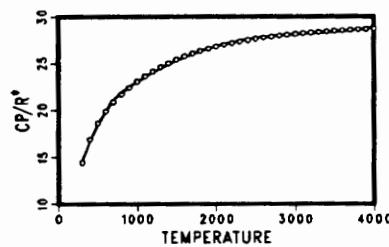
## TRIAMINOSILANE

## GAS

As of: 2/27/90

Fit

Coefficients	$\alpha_1$	$\alpha_2$	$\alpha_3$	$\alpha_4$	$\alpha_5$	$\alpha_6$	$\alpha_7$
0300-1000K	0.07070983E+02	0.02754435E+00	-0.02603669E-04	-0.01874567E-06	0.09778511E-10	-0.03582658E+06	-0.08209675E+02
1000-4000K	0.16614058E+02	0.07395874E-01	-0.06440009E-05	-0.03918887E-08	0.07045959E-12	-0.03859547E+06	-0.05865317E+03



Source: SNL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= \alpha_1 + \alpha_2 T + \alpha_3 T^2 + \alpha_4 T^3 + \alpha_5 T^4 \\ ** \text{H/RT} &= \alpha_1 + \alpha_2 T / 2 + \alpha_3 T^2 / 3 + \alpha_4 T^3 / 4 + \alpha_5 T^4 / 5 + \alpha_6 T \\ *** \text{S/R} &= \alpha_1 \ln(T) + \alpha_2 T + \alpha_3 T^2 / 2 + \alpha_4 T^3 / 3 + \alpha_5 T^4 / 4 + \alpha_7 \end{aligned}$$

Species: HSiCl

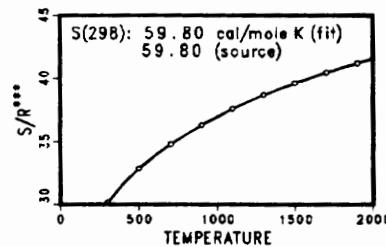
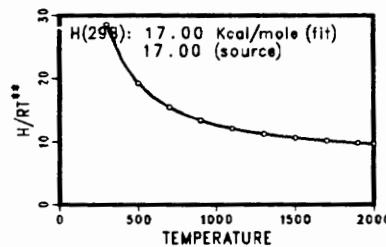
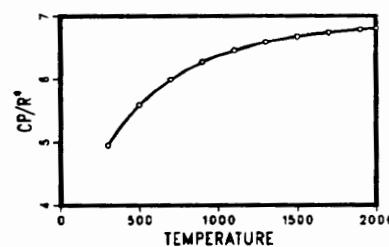
## CHLOROSILYLENE

## GAS

As of: 12/19/86

Fit

Coefficients	$\alpha_1$	$\alpha_2$	$\alpha_3$	$\alpha_4$	$\alpha_5$	$\alpha_6$	$\alpha_7$
0300-1000K	0.03072747E+02	0.09057843E-01	-0.11591338E-04	0.08310476E-07	-0.02482999E-10	0.07324210E+05	0.10334904E+02
1000-2000K	0.04900627E+02	0.01981752E-01	-0.03634646E-05	-0.02285211E-08	0.07633527E-12	0.06914634E+05	0.13770041E+01



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$\begin{aligned} * \text{CP/R} &= \alpha_1 + \alpha_2 T + \alpha_3 T^2 + \alpha_4 T^3 + \alpha_5 T^4 \\ ** \text{H/RT} &= \alpha_1 + \alpha_2 T / 2 + \alpha_3 T^2 / 3 + \alpha_4 T^3 / 4 + \alpha_5 T^4 / 5 + \alpha_6 T \\ *** \text{S/R} &= \alpha_1 \ln(T) + \alpha_2 T + \alpha_3 T^2 / 2 + \alpha_4 T^3 / 3 + \alpha_5 T^4 / 4 + \alpha_7 \end{aligned}$$

Species: HSIN

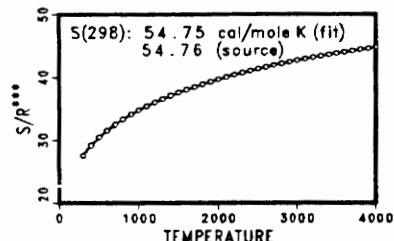
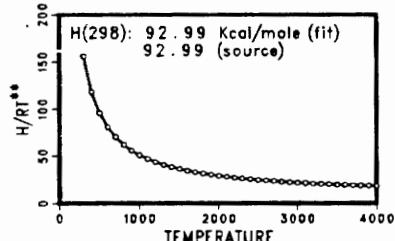
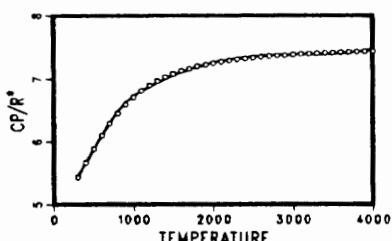
## SILANITRILE

GAS

As of: 2/27/90

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04865176E+02	0.01775119E-01	0.04890869E-05	0.03922382E-08	-0.07913276E-11	0.04526352E+06	-0.07134509E+01
1000-4000K	0.05746590E+02	0.11671186E-02	-0.13607424E-06	-0.05908616E-09	0.11746961E-13	0.04484671E+06	-0.05931788E+02



Source: SNL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP}/\text{R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H}/\text{RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S}/\text{R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

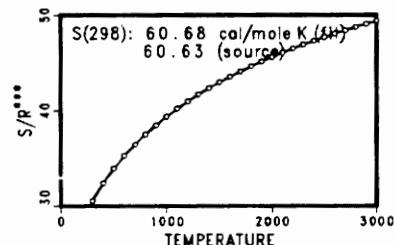
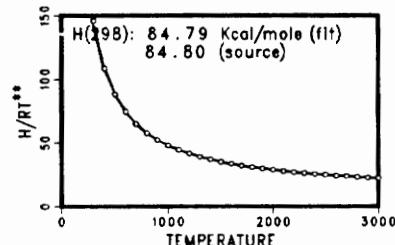
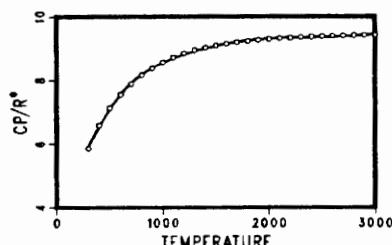
Species: HSINH

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03566343E+02	0.08446736E-01	-0.07699952E-05	-0.05270970E-07	0.02581065E-10	0.04124903E+06	0.07780791E+02
1000-3000K	0.06493435E+02	0.02567980E-01	-0.03126526E-05	-0.02577467E-08	0.06216479E-12	0.04035934E+06	-0.07830112E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP}/\text{R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H}/\text{RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S}/\text{R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: HSINH2

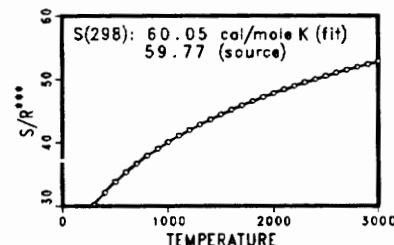
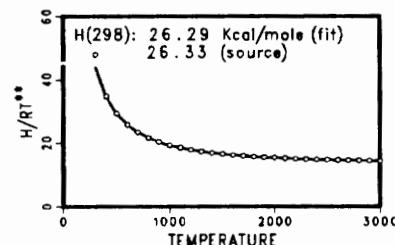
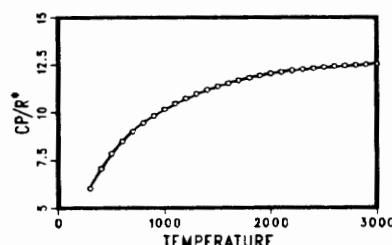
## AMINOSILYLENE

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02716144E+02	0.12042781E-01	-0.09827195E-05	-0.07408477E-07	0.03789792E-10	0.11907715E+05	0.11262523E+02
1000-3000K	0.06177894E+02	0.04689964E-01	-0.03583293E-05	-0.04457980E-08	0.09379187E-12	0.10912773E+05	-0.07006672E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP}/\text{R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H}/\text{RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S}/\text{R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species:  $\text{^1C3H}_7$ 

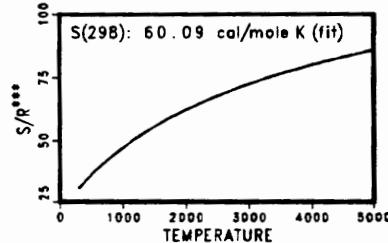
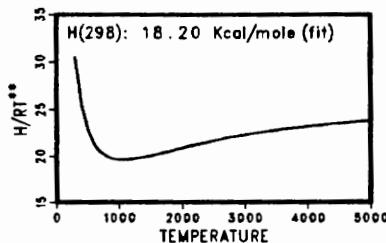
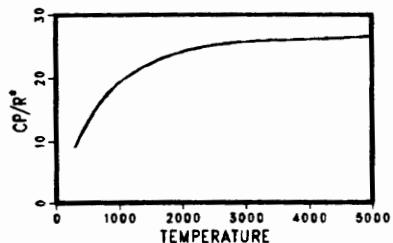
ISOPROPYL RAD

GAS

As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.01713299E+02	0.02542616E+00	0.15808083E-05	-0.01821286E-06	0.08827710E-10	0.07535808E+05	0.12979008E+02
1000-5000K	0.08063369E+02	0.15744876E-01	-0.05182391E-04	0.07477245E-08	-0.03854422E-12	0.05313871E+05	-0.02192646E+03



Source: BURCAT (TECHNION REPORTS)

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

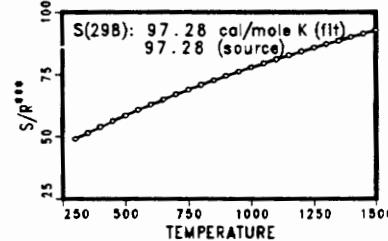
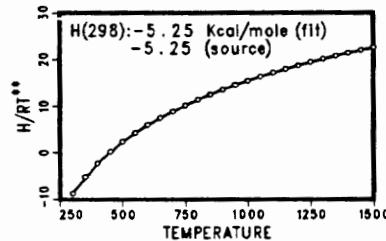
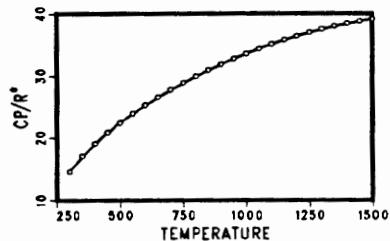
Species: ME2GAET

("ME"=CH<sub>3</sub>,METHYL; "ET"=C<sub>2</sub>H<sub>5</sub>,ETHYL) GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	-0.03218207E+02	0.06398884E+00	0.15545521E-04	-0.12847095E-06	0.09441259E-09	-0.04451897E+05	0.04848091E+03
0600-1500K	0.07174541E+02	0.03235532E+00	0.14951986E-05	-0.10482260E-07	0.03053961E-10	-0.06383914E+05	-0.02026765E+02



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

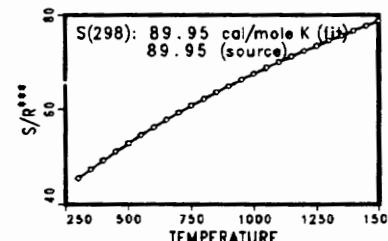
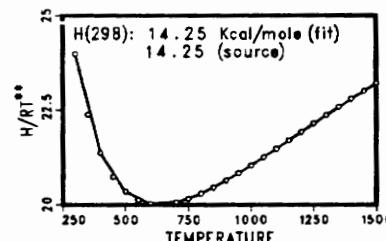
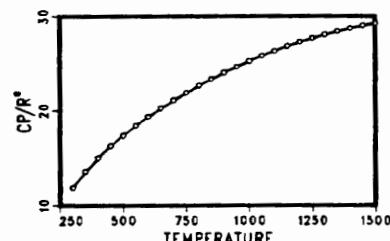
Species: MEGAET

("ME"=CH<sub>3</sub>,METHYL; "ET"=C<sub>2</sub>H<sub>5</sub>,ETHYL) GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	-0.08169937E+01	0.04554296E+00	0.10531326E-04	-0.09079987E-06	0.06700563E-09	0.05448005E+05	0.03655501E+03
0600-1500K	0.06600990E+02	0.02284791E+00	0.10133754E-05	-0.07318045E-07	0.02140196E-10	0.04071592E+05	0.05239051E+01



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT

Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

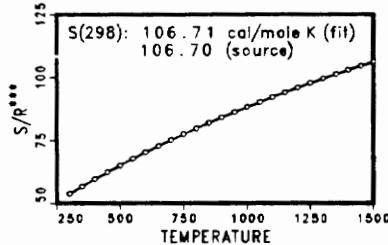
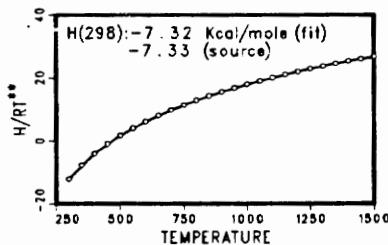
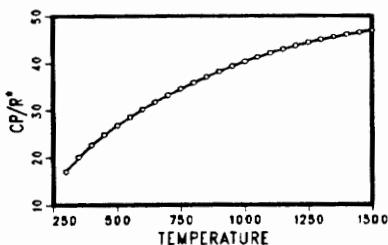
Species: MEGAET2

("ME"=CH<sub>3</sub>,METHYL; "ET"=C<sub>2</sub>H<sub>5</sub>,ETHYL) GAS

As of: 6/29/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0600K	-0.05607498E+02	0.08187357E+00	0.01920530E-03	-0.01678978E-05	0.12433538E-09	-0.05546687E+05	0.06163371E+03
0600-1500K	0.08123155E+02	0.03978908E+00	0.01690979E-04	-0.13084149E-07	0.03852598E-10	-0.08091056E+05	-0.05039992E+02



Source: SNLL FIT TO DATA GENERATED FROM POLLARD FIT  
Comments: R. POLLARD, J. CRYSTAL GROW., V.77, P.200 (1986)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: N

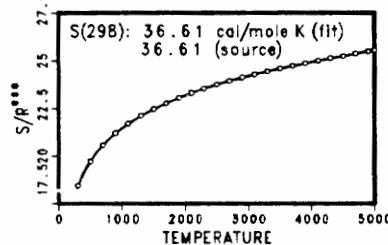
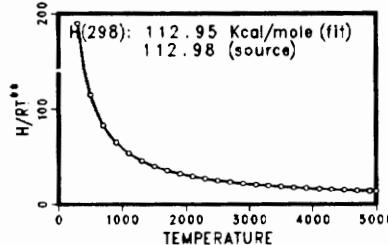
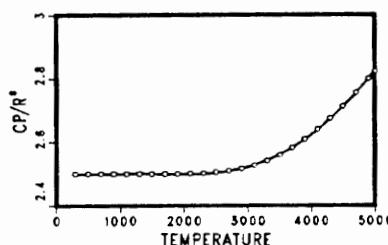
NITROGEN, MONATOMIC

GAS

As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02503071E+02	-0.02180018E-03	0.05420529E-06	-0.05647560E-09	0.02099904E-12	0.05609890E+06	0.04167566E+02
1000-5000K	0.02450268E+02	0.10661458E-03	-0.07465337E-06	0.01879652E-09	-0.10259839E-14	0.05611604E+06	0.04448758E+02



Source: NASA FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: N\*C3H7

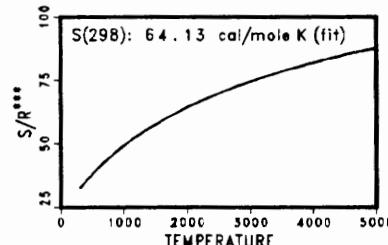
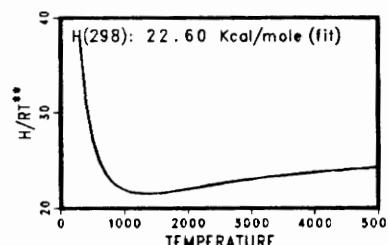
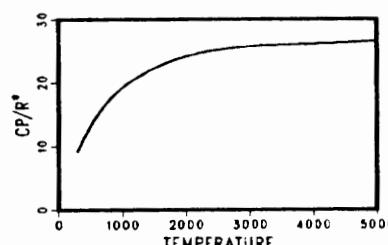
N-PROPYL RAD

GAS

As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.01922536E+02	0.02478927E+00	0.01810249E-04	-0.01783265E-06	0.08582996E-10	0.09713281E+05	0.13992715E+02
1000-5000K	0.07978290E+02	0.15761134E-01	-0.05173243E-04	0.07443892E-08	-0.03824978E-12	0.07579402E+05	-0.01935611E+03



Source: BURCAT (TECHNION REPORTS)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

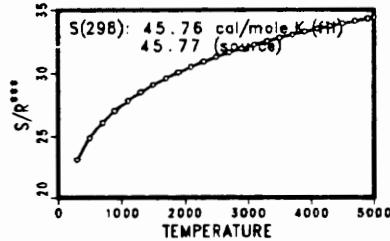
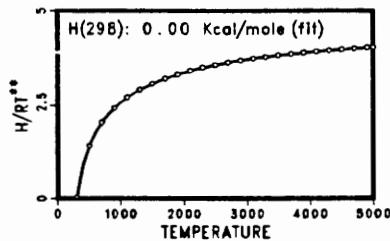
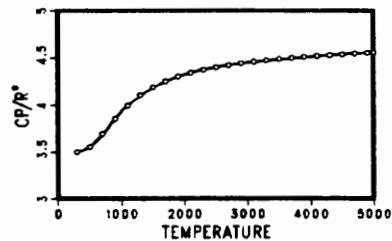
Species: N<sub>2</sub>

NITROGEN, DIATOMIC (REF ST) GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03298677E+02	0.14082404E-02	-0.03963222E-04	0.05641515E-07	-0.02444854E-10	-0.10208999E+04	0.03950372E+02
1000-5000K	0.02926640E+02	0.14879768E-02	-0.05684760E-05	0.10097038E-09	-0.06753351E-13	-0.09227977E+04	0.05980528E+02



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: N<sub>2</sub>H<sub>2</sub>

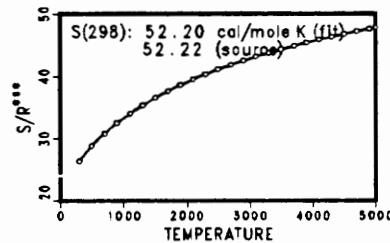
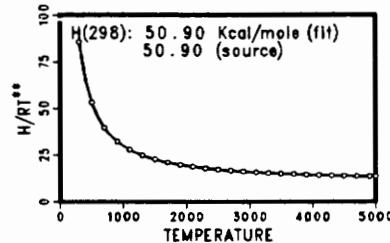
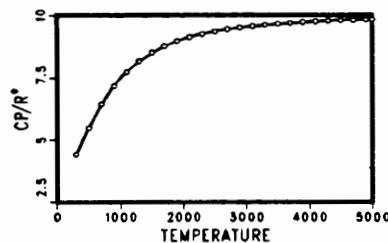
DI-IMIDE

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.16179994E+01	0.13063122E-01	-0.0171571E-03	0.16056079E-07	-0.06093638E-10	0.02467526E+06	0.13794670E+02
1000-5000K	0.03371185E+02	0.06039968E-01	-0.02303853E-04	0.04062789E-08	-0.02713144E-12	0.02418172E+06	0.04980585E+02



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

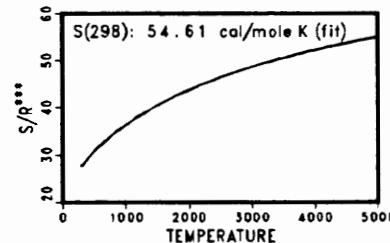
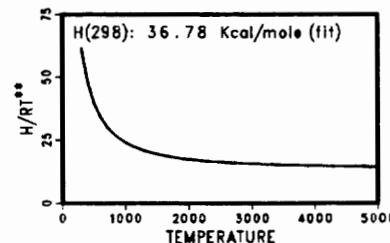
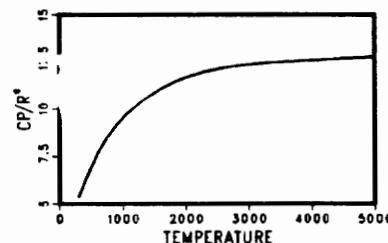
Species: N<sub>2</sub>H<sub>3</sub>

GAS

As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03174203E+02	0.04715907E-01	0.13348671E-04	-0.01919684E-06	0.07487563E-10	0.01727269E+06	0.07557224E+02
1000-5000K	0.04441846E+02	0.07214270E-01	-0.02495684E-04	0.03920564E-08	-0.02298949E-12	0.16642211E+05	-0.04275204E+01



Source: SNLL FIT TO BAHN DATA OF 1973

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: N2H4

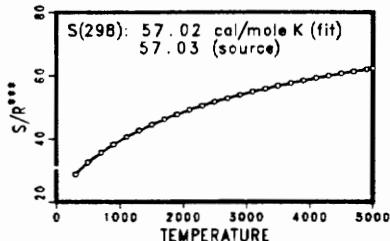
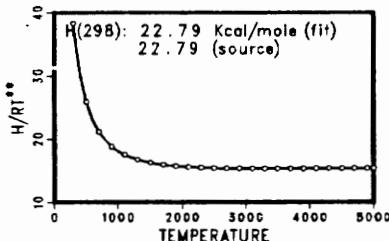
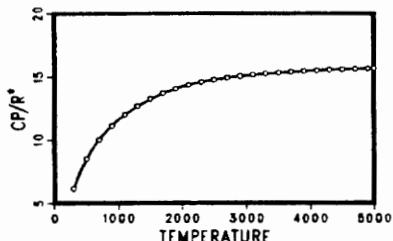
## HYDRAZINE

## GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.06442605E+00	0.02749729E+00	-0.02899451E-03	0.01745239E-06	-0.04422282E-10	0.10451917E+05	0.02127789E+03
1000-5000K	0.04977317E+02	0.09595519E-01	-0.03547639E-04	0.06124299E-08	-0.04029795E-12	0.09341219E+05	-0.02962989E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: N2H4(L)

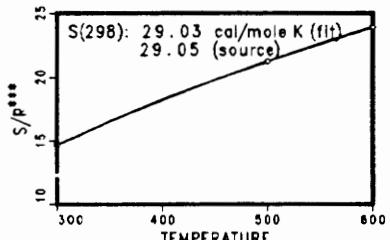
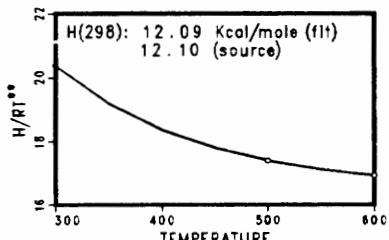
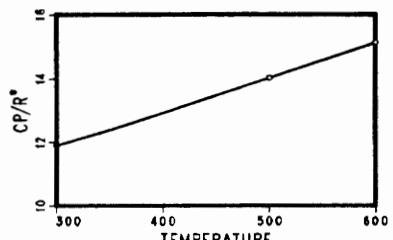
## HYDRAZINE

## LIQUID

As of: 9/05/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-0450K	0.09047444E+02	0.09241592E-01	0.02263547E-04	-0.08952247E-07	0.14868629E-10	0.02970392E+05	-0.03974033E+03
0450-0600K	0.08890683E+02	0.08330343E-01	0.04945549E-04	-0.04909251E-08	-0.03355824E-10	0.03032250E+05	-0.03871433E+03



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: N2O

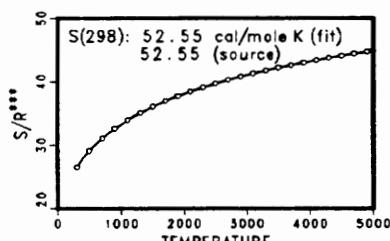
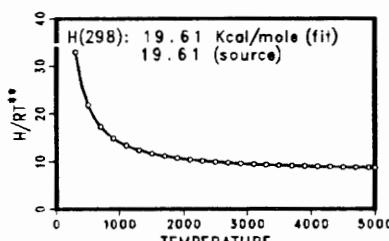
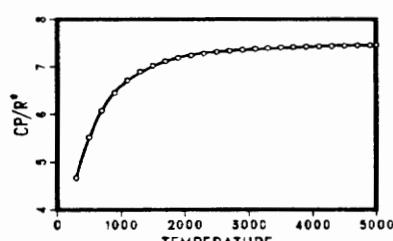
## DINITROGEN MONOXIDE

## GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02543057E+02	0.09492193E-01	-0.09792775E-04	0.06263844E-07	-0.01901825E-10	0.08765100E+05	0.09511222E+02
1000-5000K	0.04718977E+02	0.02873713E-01	-0.11974958E-05	0.02250551E-08	-0.15753370E-13	0.08165811E+05	-0.16572504E+01



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

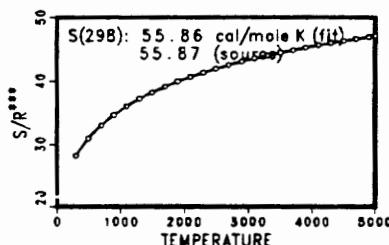
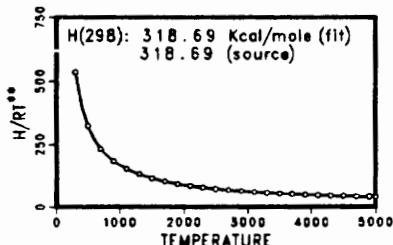
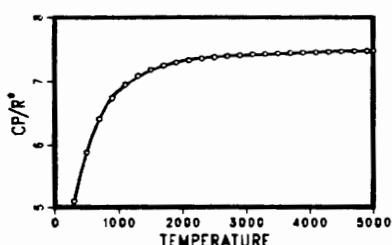
Species: N2O+

## DINITROGEN MONOXIDE, UNIPOSITIVE IONGAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03187228E+02	0.08350714E-01	-0.07894548E-04	0.04597444E-07	-0.13810748E-11	0.15912794E+06	0.07779425E+02
1000-5000K	0.05398516E+02	0.02249478E-01	-0.09577056E-05	0.01823192E-08	-0.12844222E-13	0.15848513E+06	-0.03733146E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: N2O4

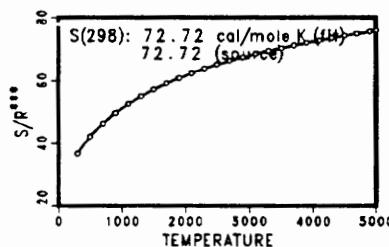
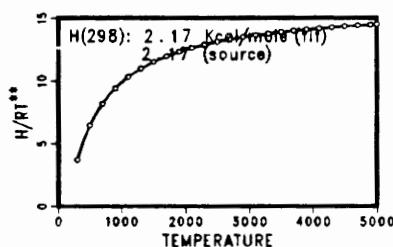
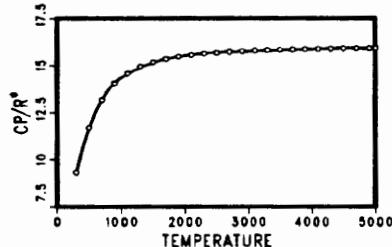
## NITROGEN TETROXIDE

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03624592E+02	0.02474708E+00	-0.02172874E-03	0.09927103E-07	-0.02222817E-10	-0.09128241E+04	0.09457174E+02
1000-5000K	0.10482201E+02	0.05972272E-01	-0.02564043E-04	0.04916885E-08	-0.03490969E-12	-0.02849988E+05	-0.02612289E+03



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: N3

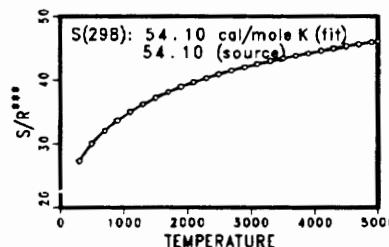
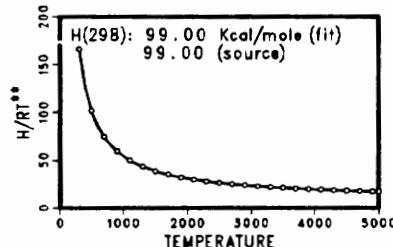
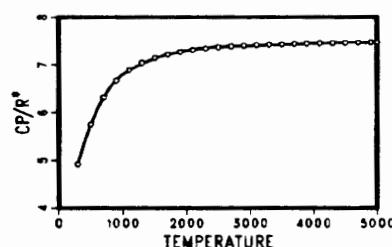
## AZIDE

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02882218E+02	0.08930338E-01	-0.08539038E-04	0.05045585E-07	-0.15212480E-11	0.04863468E+06	0.08481757E+02
1000-5000K	0.05208505E+02	0.02444507E-01	-0.10389415E-05	0.01977416E-08	-0.13956436E-13	0.04796178E+06	-0.03612755E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: NCO

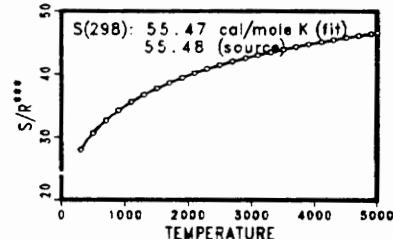
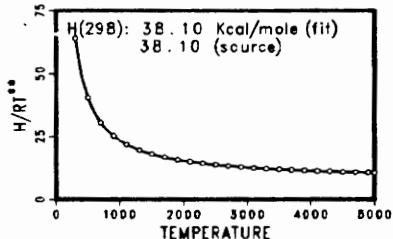
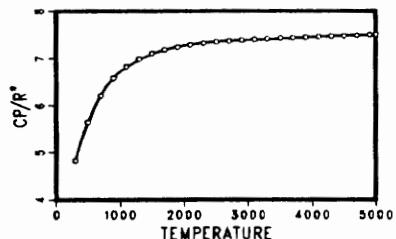
## NCO RADICAL

## GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02830320E+02	0.08871490E-01	-0.08945636E-04	0.05876918E-07	-0.01907734E-10	0.01800543E+06	0.09498831E+02
1000-5000K	0.05012045E+02	0.02626773E-01	-0.11082433E-05	0.02093860E-08	-0.14603470E-13	0.01737185E+06	-0.01830075E+02



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: NF

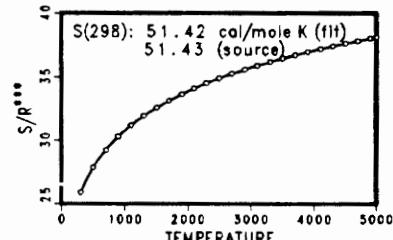
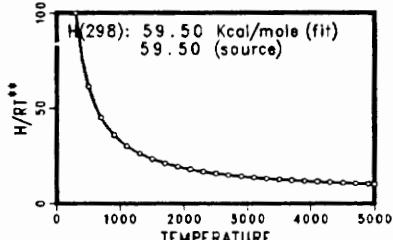
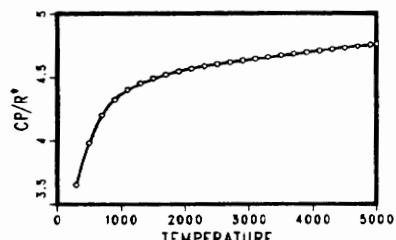
## NITROGEN MONOFLUORIDE

## GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02871947E+02	0.03312192E-01	-0.02691158E-04	0.11219514E-08	-0.02475130E-11	0.02896257E+06	0.08640247E+02
1000-5000K	0.03862176E+02	0.07551806E-02	-0.03044942E-05	0.05874447E-09	-0.04187479E-13	0.02867242E+06	0.03457232E+02



Source: SNLL FIT TO JANAF TABLES (FN)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: NFO

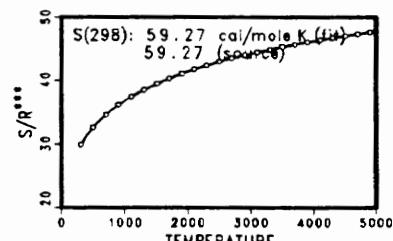
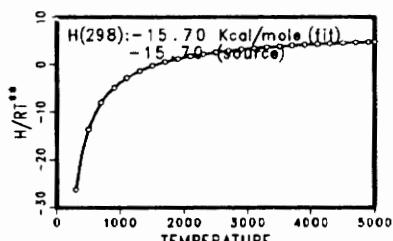
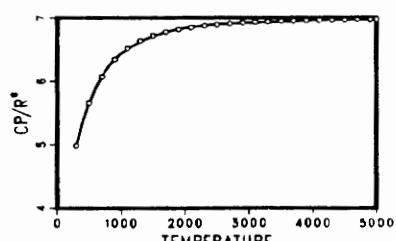
## NITROSYL FLUORIDE

## GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03352307E+02	0.07229966E-01	-0.06951136E-04	0.03828526E-07	-0.10235582E-11	-0.09167035E+05	0.08854189E+02
1000-5000K	0.05174520E+02	0.01938472E-01	-0.08222701E-05	0.15642909E-09	-0.11044974E-13	-0.09670935E+05	-0.05352460E+01



Source: SNLL FIT TO JANAF TABLES (FNO)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: NF02

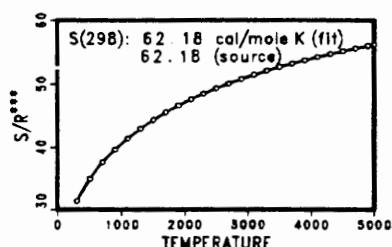
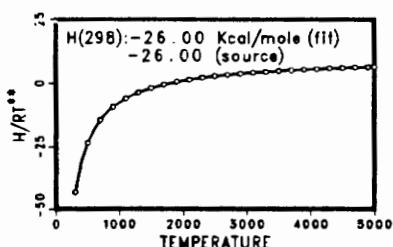
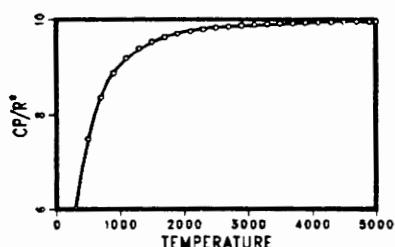
NITRYL FLUORIDE

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02447528E+02	0.15441095E-01	-0.13005952E-04	0.04856383E-07	-0.06852266E-11	-0.14393999E+05	0.13283804E+02
1000-5000K	0.06816857E+02	0.03462639E-01	-0.14922156E-05	0.02869665E-08	-0.02041856E-12	-0.15602619E+05	-0.09320129E+02



Source: SNLL FIT TO JANAF TABLES (FN02)

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: NH

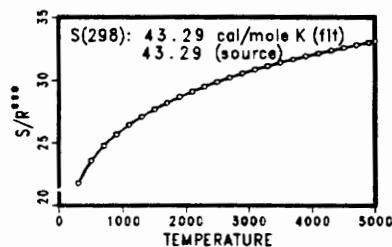
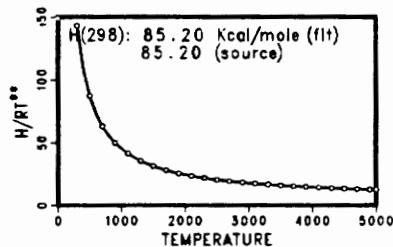
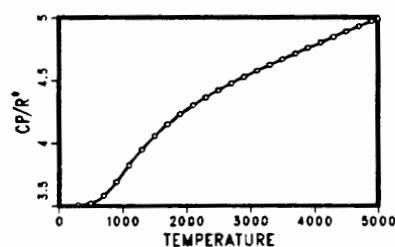
IMIDOGEN

GAS

As of: 3/13/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03339758E+02	0.12530086E-02	-0.03491645E-04	0.04218812E-07	-0.15576179E-11	0.04185047E+06	0.02507180E+02
1000-5000K	0.02760249E+02	0.13753463E-02	-0.04451914E-05	0.07692791E-09	-0.05017592E-13	0.04207828E+06	0.05857199E+02



Source: FIT JANAF TABLES WITH H298=85.2 PER MILLER

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: NH2

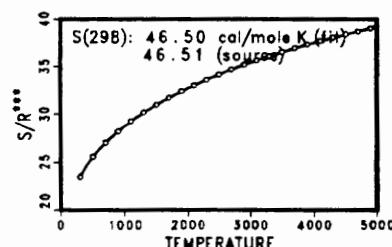
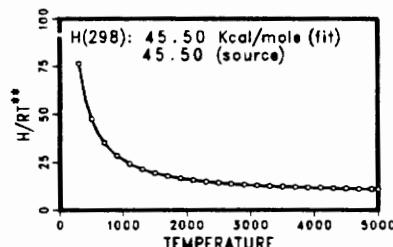
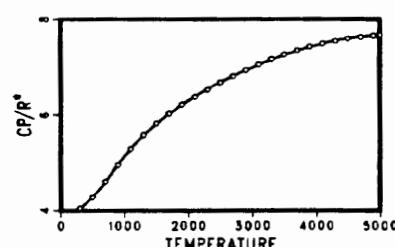
AMIDOGEN

GAS

As of: 12/16/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03432493E+02	0.03299540E-01	-0.06613600E-04	0.08590947E-07	-0.03572046E-10	0.02177227E+06	0.03090110E+02
1000-5000K	0.02961311E+02	0.02932699E-01	-0.09063600E-05	0.16172575E-09	-0.12042003E-13	0.02191976E+06	0.05777878E+02

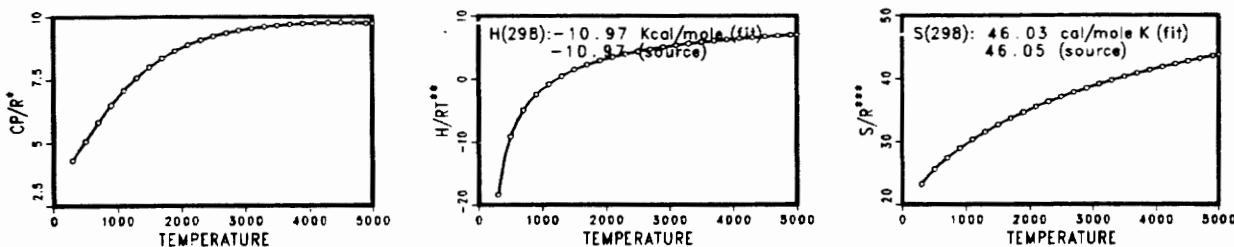


Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: NH<sub>3</sub> AMMONIA GAS As of: 12/13/86

Fit Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02204351E+02	0.10114765E-01	-0.14652648E-04	0.14472350E-07	-0.05328509E-10	-0.06525488E+05	0.08127138E+02
1000-5000K	0.02461904E+02	0.06059166E-01	-0.02004976E-04	0.03136003E-08	-0.01938317E-12	-0.06493269E+05	0.07472097E+02

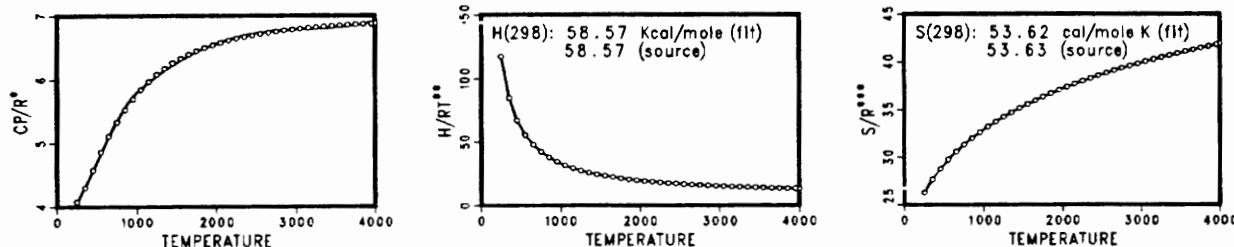


Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \quad & CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \quad & H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \quad & S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: NNH GAS As of: 12/01/86

Fit Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0250-1000K	0.03501344E+02	0.02053586E-01	0.07170409E-05	0.04921348E-08	-0.09671170E-11	0.02833347E+06	0.06391837E+02
1000-4000K	0.04415342E+02	0.16143879E-02	-0.16328943E-06	-0.08559846E-09	0.16147909E-13	0.02788029E+06	0.09042888E+01

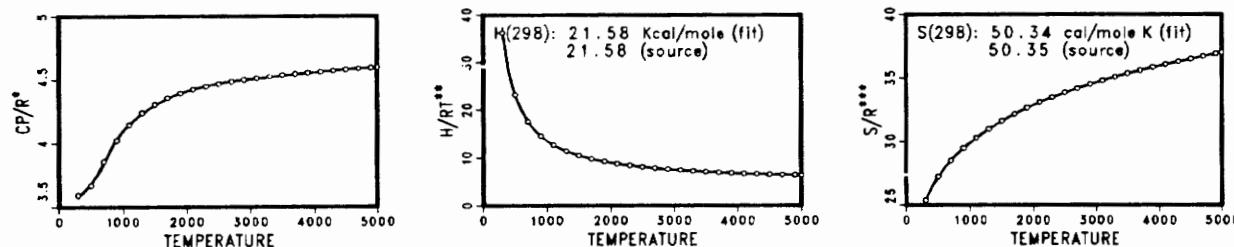


Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} \bullet \quad & CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \quad & H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \quad & S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: NO GAS As of: 12/12/86

Fit Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03376541E+02	0.12530634E-02	-0.03302750E-04	0.05217810E-07	-0.02446262E-10	0.09817961E+05	0.05829590E+02
1000-5000K	0.03245435E+02	0.12691383E-02	-0.05015890E-05	0.09169283E-09	-0.06275419E-13	0.09800840E+05	0.06417293E+02



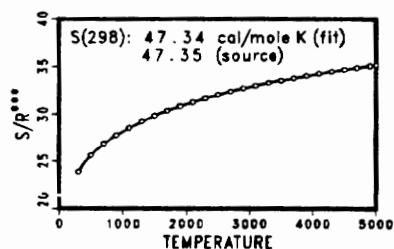
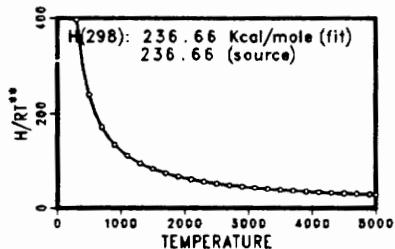
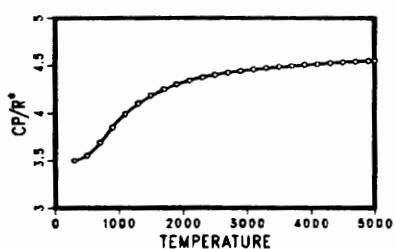
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \quad & CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \quad & H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \quad & S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: NO+ NITRIC OXIDE, UNIPOSITIVE ION GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03297349E+02	0.14228899E-02	-0.04007441E-04	0.05670551E-07	-0.02446971E-10	0.11808338E+06	0.04749948E+02
1000-5000K	0.02914888E+02	0.14993349E-02	-0.05727972E-05	0.10177767E-09	-0.06825390E-13	0.11818688E+06	0.06844346E+02



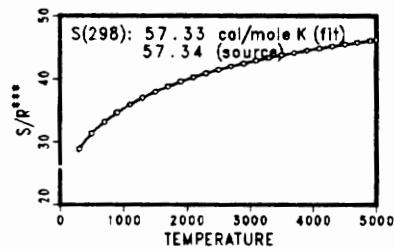
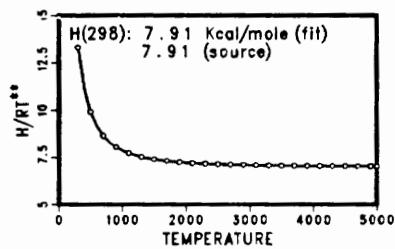
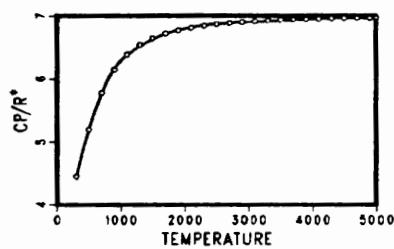
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: NO2 NITROGEN DIOXIDE GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02670600E+02	0.07838500E-01	-0.08063864E-04	0.06161714E-07	-0.02320150E-10	0.02896290E+05	0.11612071E+02
1000-5000K	0.04682859E+02	0.02462429E-01	-0.10422585E-05	0.01976902E-08	-0.13917168E-13	0.02261292E+05	0.09885985E+01



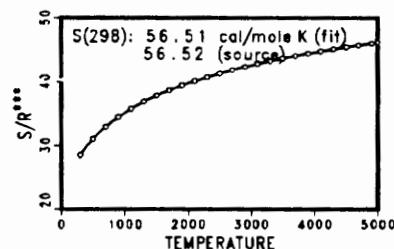
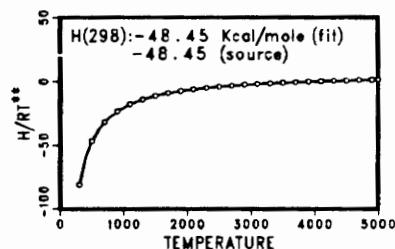
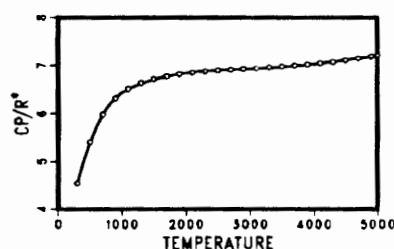
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: NO2- NITROGEN DIOXIDE, UNINEGATIVE ION GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02448586E+02	0.08982507E-01	-0.07853431E-04	0.03927276E-07	-0.10716939E-11	-0.02545097E+06	0.12130600E+02
1000-5000K	0.05043114E+02	0.02166427E-01	-0.09455454E-05	0.01816313E-08	-0.12383945E-13	-0.02621553E+06	-0.14459051E+01



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * CP/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** H/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** S/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: N03

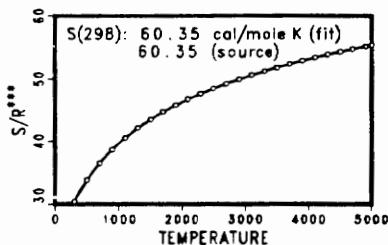
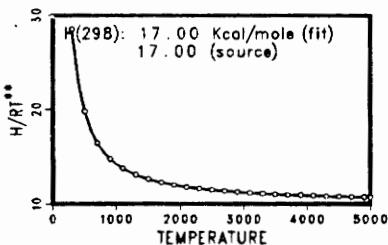
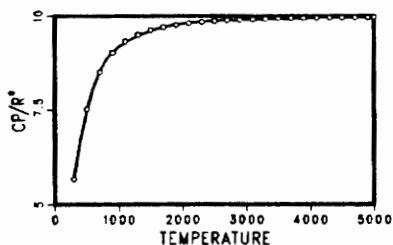
NITROGEN TRIOXIDE

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.12210763E+01	0.01878797E+00	-0.13443212E-04	0.12746013E-08	0.13540601E-11	0.07473144E+05	0.01840202E+03
1000-5000K	0.07120307E+02	0.03246228E-01	-0.14316134E-05	0.02797053E-08	-0.02013007E-12	0.05864479E+05	-0.12137301E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: O

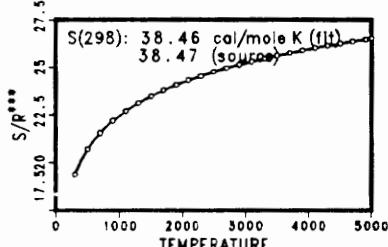
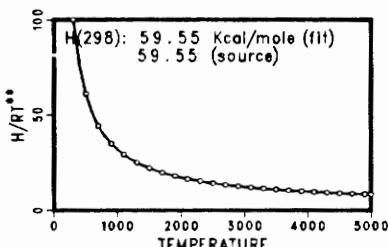
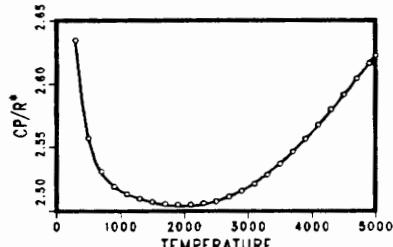
OXYGEN, MONATOMIC

GAS

As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02946428E+02	-0.16381665E-02	0.02421031E-04	-0.16028431E-08	0.03890696E-11	0.02914764E+06	0.02963995E+02
1000-5000K	0.02542059E+02	-0.02755061E-03	-0.03102803E-07	0.04551067E-10	-0.04368051E-14	0.02923080E+06	0.04920308E+02



Source: NASA FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: O+

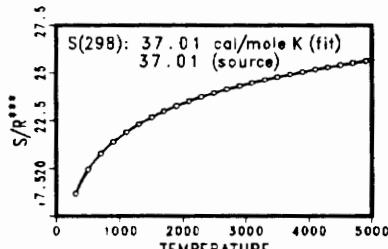
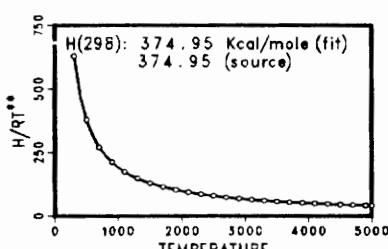
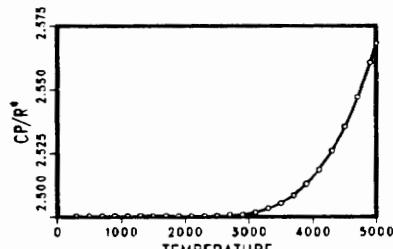
OXYGEN, UNIPOSITIVE ION

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02499272E+02	0.05820598E-04	-0.11209219E-07	0.08232108E-10	-0.01916378E-13	0.01879556E+07	0.04384825E+02
1000-5000K	0.02501869E+02	-0.06107262E-04	0.07324307E-07	-0.03438353E-10	0.05506407E-14	0.01879552E+07	0.04372826E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: O-

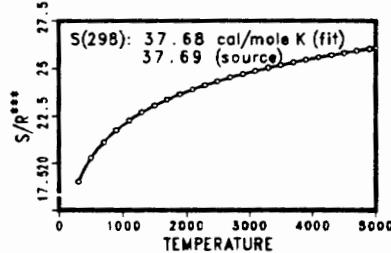
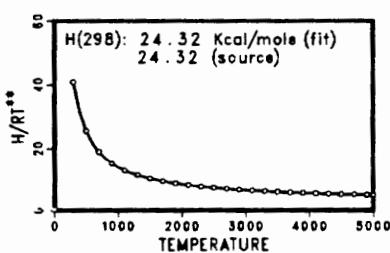
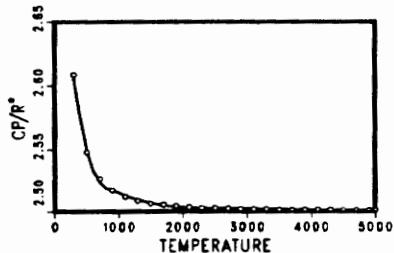
## OXYGEN, UNINEGATIVE ION

GAS

As of: 9/05/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02747263E+02	-0.05724860E-02	0.02712548E-05	0.02691511E-08	-0.02002357E-11	0.11443947E+05	0.03469852E+02
1000-5000K	0.02559580E+02	-0.07147887E-03	0.03301804E-06	-0.06660944E-10	0.04900726E-14	0.11489346E+05	0.04426186E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: O2

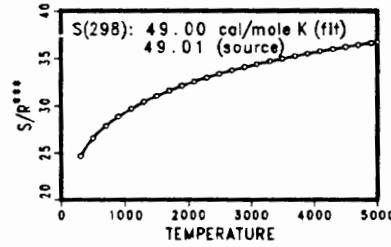
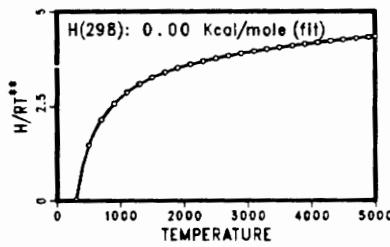
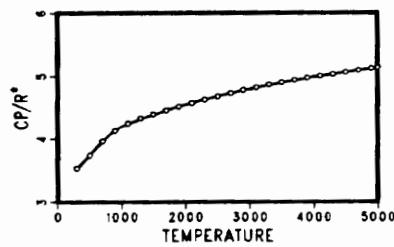
## OXYGEN, DIATOMIC (REF ST)

GAS

As of: 12/13/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03212936E+02	0.11274864E-02	-0.05756150E-05	0.13138773E-08	-0.08768554E-11	-0.10052490E+04	0.06034737E+02
1000-5000K	0.03697578E+02	0.06135197E-02	-0.12588420E-06	0.01775281E-09	-0.11364354E-14	-0.12339301E+04	0.03189165E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: O2-

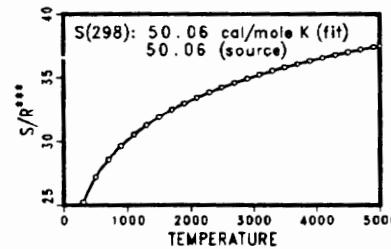
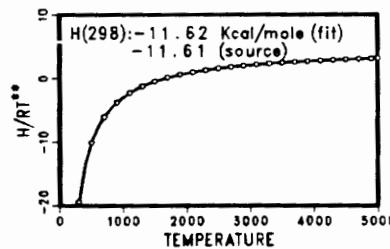
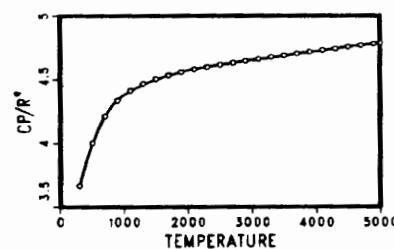
## OXYGEN, DIATOMIC, UNINEGATIVE ION

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02872291E+02	0.03359716E-01	-0.02664886E-04	0.09807524E-08	-0.16709571E-12	-0.06829094E+05	0.07938372E+02
1000-5000K	0.03883013E+02	0.07407872E-02	-0.02961776E-05	0.05724304E-09	-0.04086547E-13	-0.07121644E+05	0.02658211E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

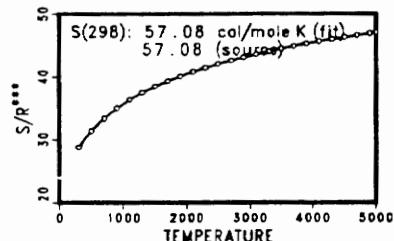
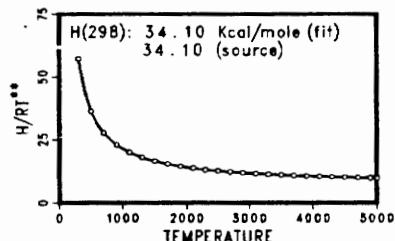
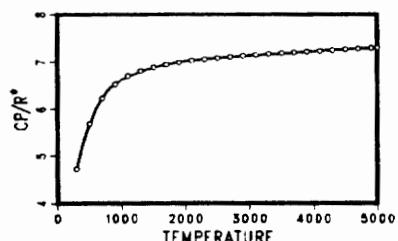
$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: O<sub>3</sub> OZONE GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02462608E+02	0.09582781E-01	-0.07087359E-04	0.13633683E-08	0.02969647E-11	0.16061522E+05	0.12141870E+02
1000-5000K	0.05429371E+02	0.01820380E-01	-0.07705607E-05	0.14992929E-09	-0.10755629E-13	0.15235267E+05	-0.03266386E+02



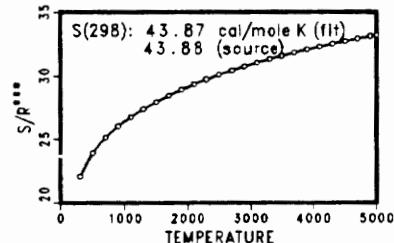
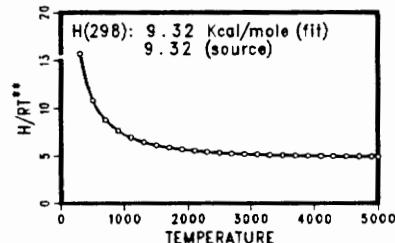
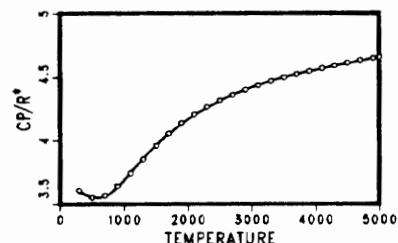
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: OH HYDROXYL GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03637266E+02	0.01850910E-02	-0.16761646E-05	0.02387202E-07	-0.08431442E-11	0.03606781E+05	0.13588605E+01
1000-5000K	0.02882730E+02	0.10139743E-02	-0.02276877E-05	0.02174683E-09	-0.05126305E-14	0.03886888E+05	0.05595712E+02



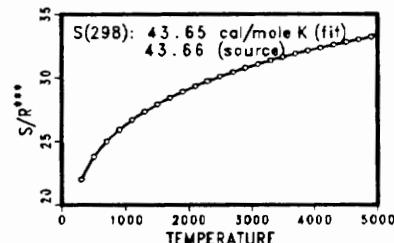
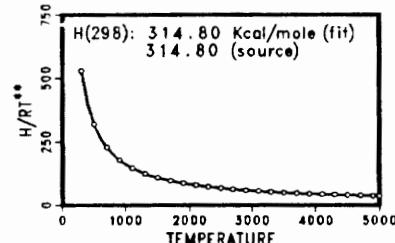
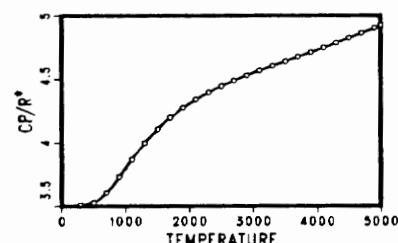
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: OH+ HYDROXYL, UNIPOSITIVE ION GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03326978E+02	0.13457859E-02	-0.03777167E-04	0.04687749E-07	-0.01780982E-10	0.15740294E+06	0.02744042E+02
1000-5000K	0.02719058E+02	0.15085714E-02	-0.05029369E-05	0.08261951E-09	-0.04947452E-13	0.15763414E+06	0.06234536E+02



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

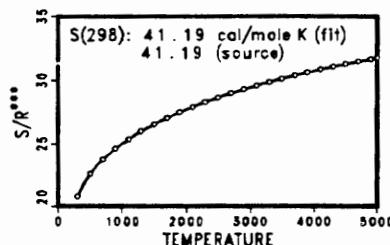
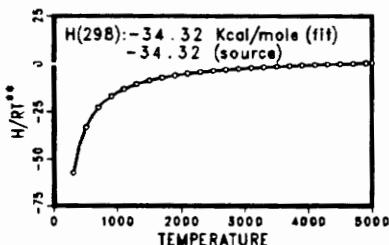
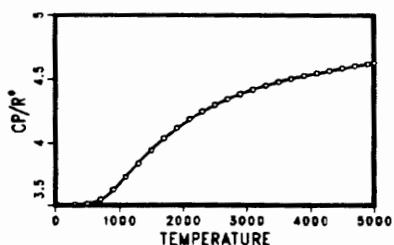
Species: OH-

HYDROXYL, UNINEGATIVE ION GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03390037E+02	0.07922381E-02	-0.01943429E-04	0.02001769E-07	-0.05702087E-11	-0.01830493E+06	0.12498923E+01
1000-5000K	0.02846204E+02	0.10418347E-02	-0.02416850E-05	0.02483215E-09	-0.07775605E-14	-0.01807280E+06	0.04422712E+02



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: S

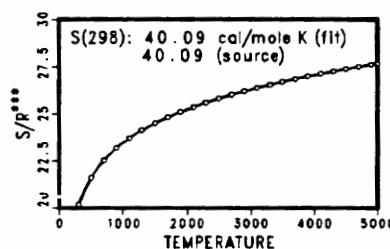
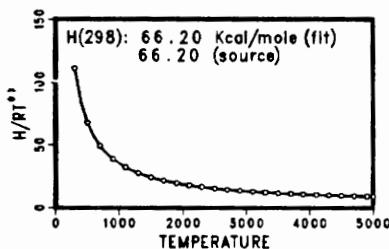
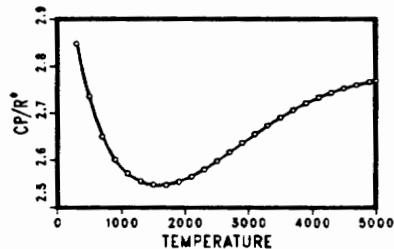
SULFUR, MONATOMIC

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03187329E+02	-0.15957763E-02	0.02005531E-04	-0.15070814E-08	0.04931282E-11	0.03242259E+06	0.02414441E+02
1000-5000K	0.02902148E+02	-0.05484546E-02	0.02764576E-05	-0.05017114E-09	0.03150684E-13	0.03249423E+06	0.03838471E+02



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: S(L)

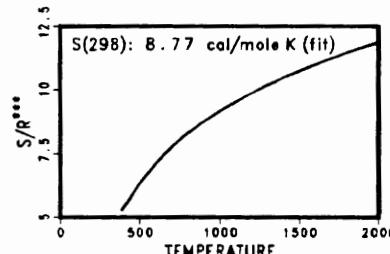
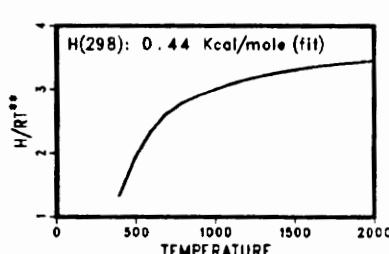
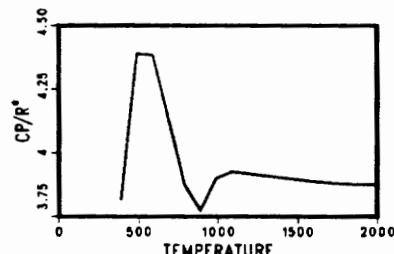
SULFUR

LIQUID

As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0388-1000K	-0.12706310E+02	0.09072521E+00	-0.01695178E-02	0.13070636E-06	-0.03527615E-09	0.12346069E+04	0.05621016E+03
1000-2000K	0.03603667E+02	0.09903341E-02	-0.10114410E-05	0.04053632E-08	-0.05667913E-12	-0.08453839E+04	-0.16344708E+02



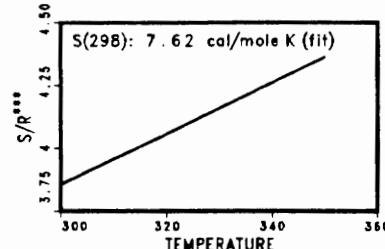
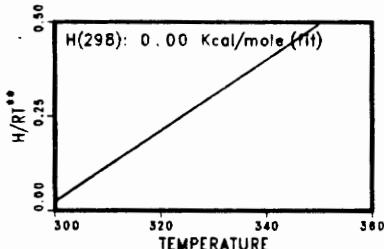
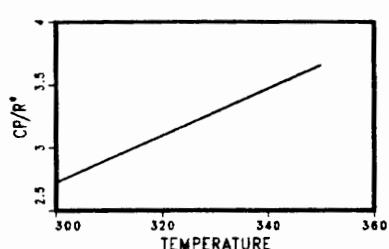
Source: NASA FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: S(S) SULFUR SOLID As of: 12/01/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	-0.05063702E+02	0.02881935E-01	-0.02133020E-03	0.08478786E-05	-0.01734496E-07	0.07148263E+04	0.02871407E+03
1000-388K	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00



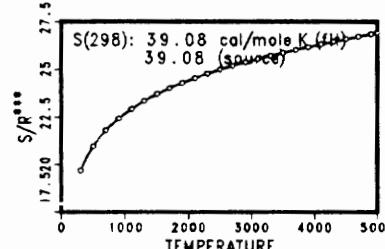
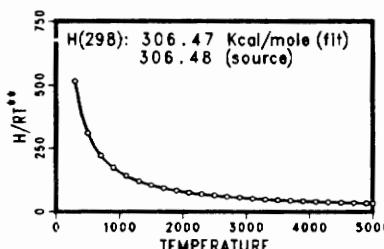
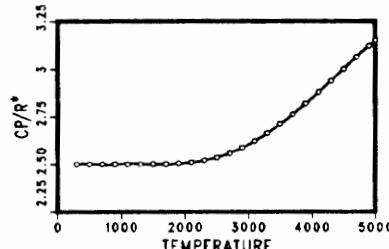
Source: NASA FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: S+ SULFUR, MONATOMIC, UNIPOSITIVE ION GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02366100E+02	0.09130767E-02	-0.02140283E-04	0.02076177E-07	-0.07133859E-11	0.15350910E+06	0.05993094E+02
1000-5000K	0.02404600E+02	0.02410908E-02	-0.02041779E-05	0.06592945E-09	-0.05756939E-13	0.15352225E+06	0.05924256E+02



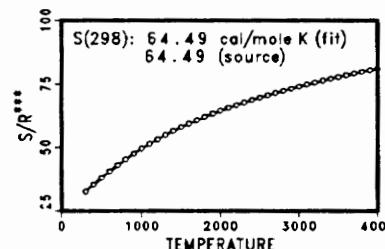
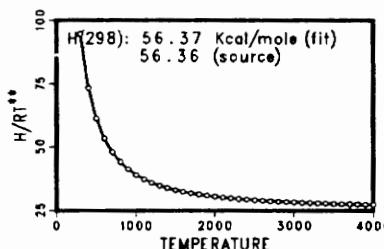
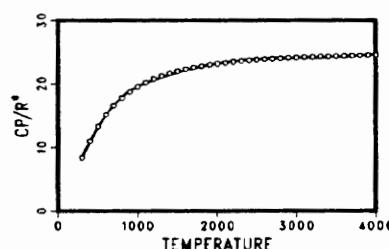
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: S-TRIAZINE GAS As of: 4/16/87

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04493492E+01	0.02728306E+00	0.02309304E-04	-0.14968443E-07	0.04546753E-10	0.02703032E+06	0.02178518E+03
1000-4000K	0.13036170E+02	0.07711820E-01	-0.07724374E-05	-0.04385191E-08	0.08298992E-12	0.02251663E+06	-0.04777676E+03



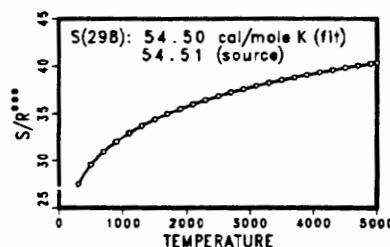
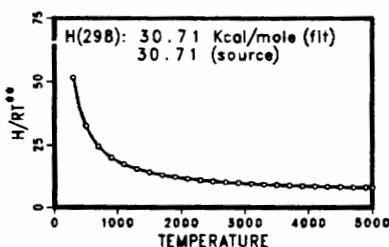
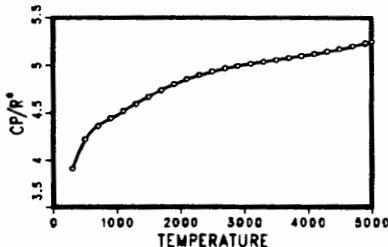
Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: S2 SULFUR, DIATOMIC GAS As of: 12/13/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03157672E+02	0.03099480E-01	-0.15607465E-05	-0.13578905E-08	0.11374435E-11	0.14391873E+05	0.08596062E+02
1000-5000K	0.03904443E+02	0.06925733E-02	-0.12330970E-06	0.08783809E-11	0.13746621E-14	0.14256933E+05	0.04956834E+02



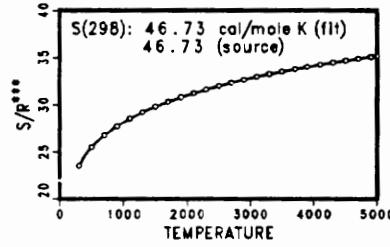
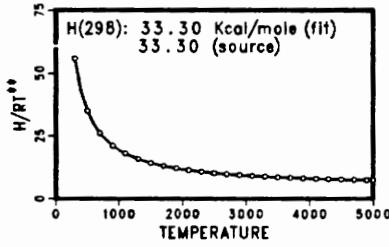
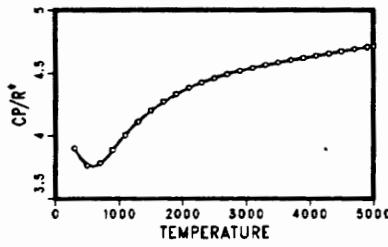
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP}/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H}/\text{RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6 T \\ *** \text{S}/\text{R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: SH SULFUR MONOHYDRID GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04133326E+02	-0.03787893E-02	-0.02777854E-04	0.05370112E-07	-0.02394006E-10	0.15558623E+05	0.16115348E+00
1000-5000K	0.03053810E+02	0.12588843E-02	-0.04249169E-05	0.06929591E-09	-0.04281691E-13	0.15882250E+05	0.05973551E+02



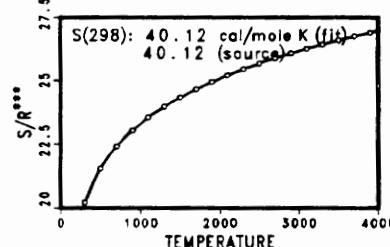
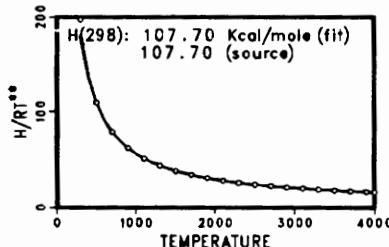
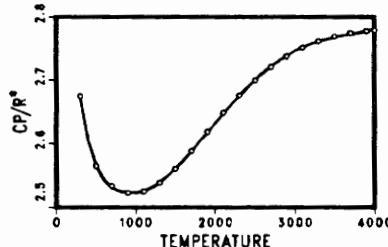
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP}/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H}/\text{RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6 T \\ *** \text{S}/\text{R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: SI SILICON, MONATOMIC GAS As of: 3/29/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03113515E+02	-0.02330991E-01	0.03518530E-04	-0.02417573E-07	0.06391902E-11	0.05335061E+06	0.03009718E+02
1000-4000K	0.02775845E+02	-0.06213257E-02	0.04843696E-05	-0.12756146E-09	0.11344818E-13	0.05339790E+06	0.04543298E+02



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP}/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H}/\text{RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6 T \\ *** \text{S}/\text{R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: Si(L)

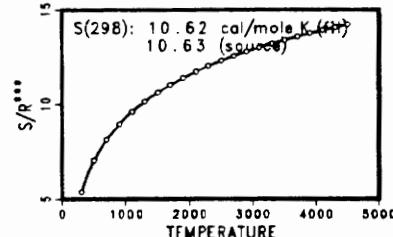
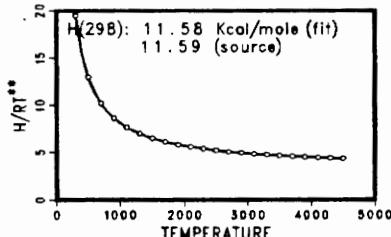
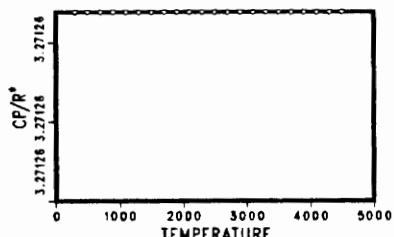
SILICON

LIQUID

As of: 9/05/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03271263E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.04855058E+05	-0.13290542E+02
1000-4500K	0.03271263E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.04855057E+05	-0.13290542E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: Si(NH<sub>2</sub>)<sub>3</sub>

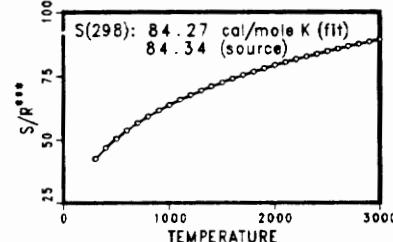
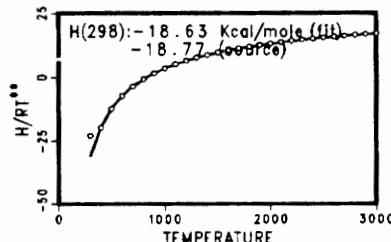
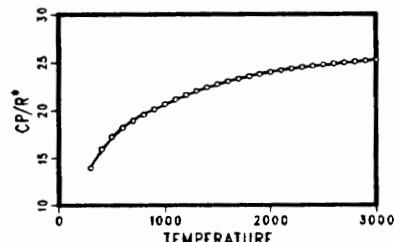
TRIAMINOSILYL

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.07598413E+02	0.02435266E+00	-0.04296202E-04	-0.01756006E-06	0.10501017E-10	-0.12653434E+05	-0.07808647E+02
1000-3000K	0.14065501E+02	0.07581744E-01	-0.05168510E-05	-0.06743626E-08	0.13979258E-12	-0.14144028E+05	-0.04063873E+03



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: Si(NH<sub>2</sub>)<sub>4</sub>

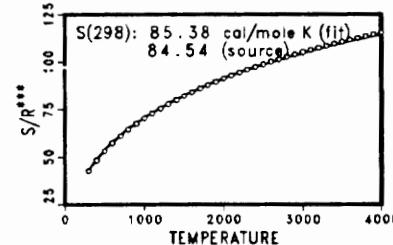
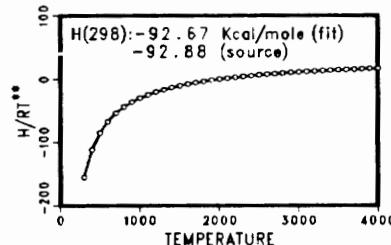
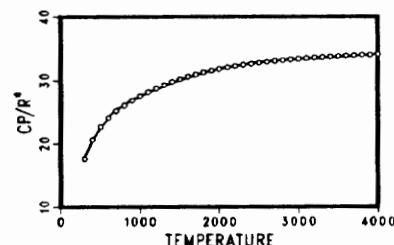
TETRAAMINOSILANE

GAS

As of: 2/27/90

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.08454529E+02	0.03465772E+00	-0.04266782E-04	-0.02495363E-06	0.13654663E-10	-0.05061518E+06	-0.15143013E+02
1000-4000K	0.02032107E+03	0.08289798E-01	-0.07077612E-05	-0.04340724E-08	0.07747068E-12	-0.05389855E+06	-0.07730464E+03



Source: SNL FIT TO BAC-MP4 DATA

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

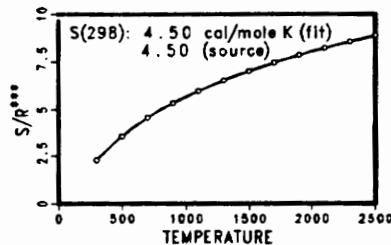
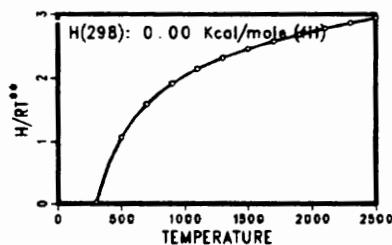
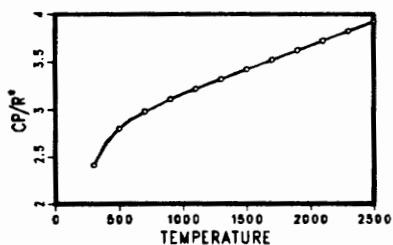
$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: Si(S) SILICON SOLID As of: 9/05/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.05746418E+01	0.10264855E-01	-0.01775345E-03	0.14575000E-07	-0.04491292E-10	-0.04969951E+04	-0.03400242E+02
1000-2500K	0.02530275E+02	0.08522433E-02	-0.03223468E-05	0.12808208E-09	-0.01850849E-12	-0.08395197E+04	-0.12514782E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

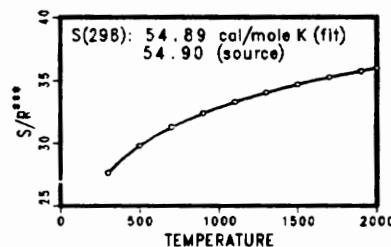
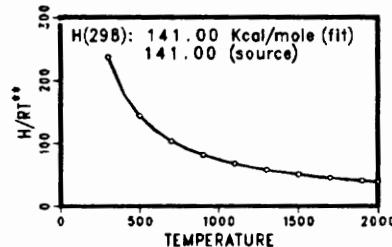
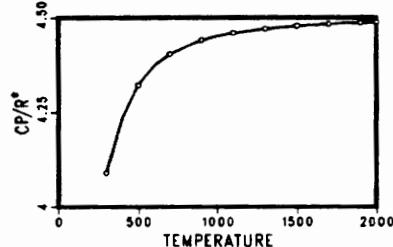
$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: Si2 SILICON, DIATOMIC GAS As of: 9/05/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02993750E+02	0.06053689E-01	-0.10158575E-04	0.07909737E-07	-0.02346083E-10	0.06987498E+06	0.09151741E+02
1000-2000K	0.0432196E+02	0.04315355E-02	-0.02964833E-05	0.09823294E-09	-0.12962688E-13	0.06964651E+06	0.03308527E+02



Source: SNLL FIT TO DATA GENERATE USING VIBRATIONAL FREQUENCIES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

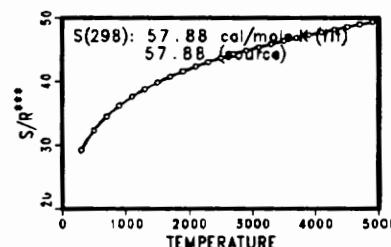
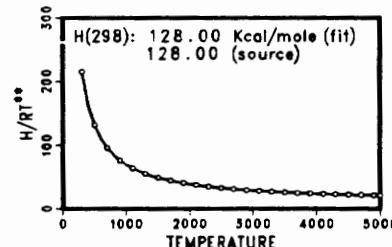
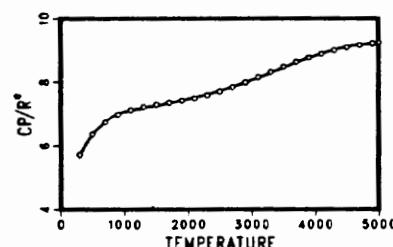
$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: Si2C DISILICON CARBIDE GAS As of: 11/29/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04157246E+02	0.07031825E-01	-0.07263033E-04	0.04633583E-07	-0.14934475E-11	0.06292421E+06	0.03635125E+02
1000-5000K	0.06334110E+02	0.12102520E-02	-0.06798289E-05	0.02244432E-08	-0.02280177E-12	0.06227189E+06	-0.07770097E+02



Source: SNLL FIT TO JANAF DATA

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: Si2F6

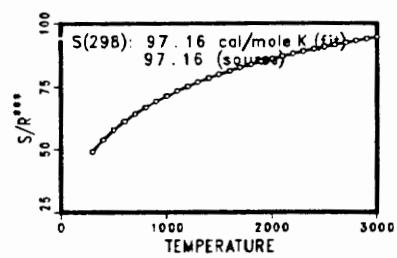
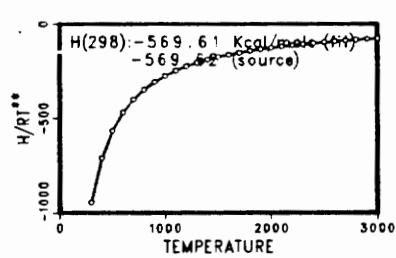
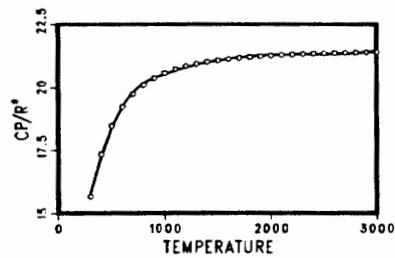
HEXAFLUORODISILANE

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.09998134E+02	0.02170313E+00	-0.03875091E-04	-0.16702523E-07	0.09407529E-10	-0.02905482E+07	-0.14228863E+02
1000-3000K	0.01830047E+03	0.02868752E-01	-0.04545576E-05	-0.02497900E-08	0.06630658E-12	-0.02928185E+07	-0.05760425E+03



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

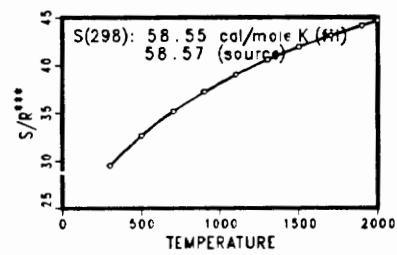
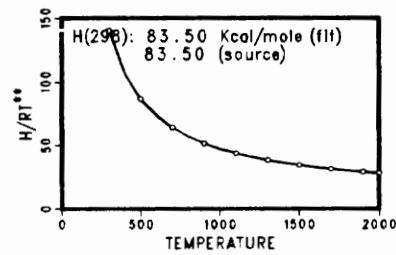
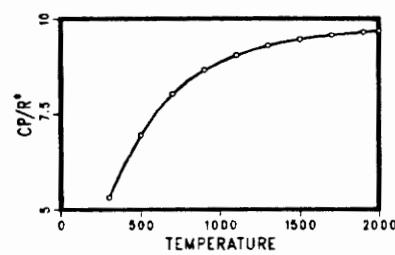
Species: Si2H2

GAS

As of: 9/05/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.16247229E+01	0.14871029E-01	-0.08707160E-04	-0.01699554E-09	0.10972211E-11	0.04095325E+06	0.16165730E+02
1000-2000K	0.05778180E+02	0.04070596E-01	-0.04259125E-05	-0.07920228E-08	0.02379752E-11	0.03980520E+06	-0.05392375E+02



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

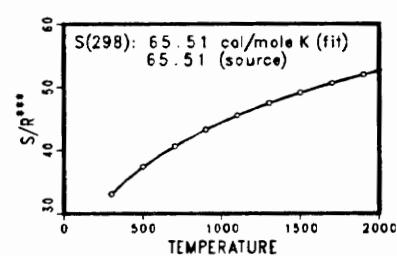
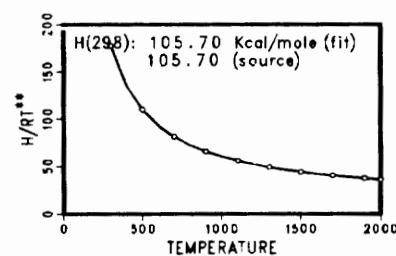
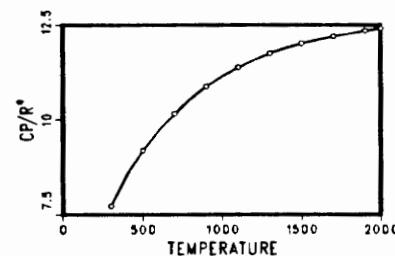
Species: Si2H3

GAS

As of: 9/05/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03335404E+02	0.02155614E+00	-0.02933937E-03	0.02287784E-06	-0.07272827E-10	0.05146157E+06	0.08656853E+02
1000-2000K	0.07257627E+02	0.05123859E-01	-0.07633465E-05	-0.06662471E-08	0.02053052E-11	0.05062055E+06	-0.10314127E+02



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

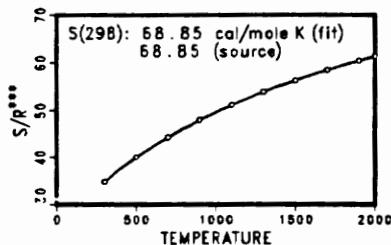
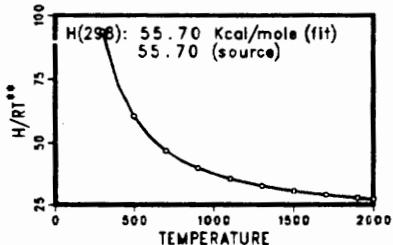
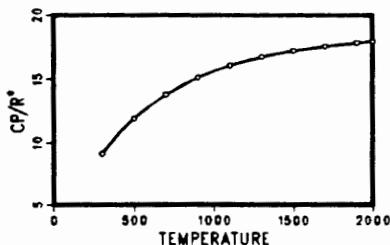
Species: Si2H5

GAS

As of: 9/05/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.15788481E+01	0.03549382E+00	-0.04267511E-03	0.03059177E-06	-0.09360425E-10	0.02630549E+06	0.16720734E+02
1000-2000K	0.08451010E+02	0.09286371E-01	-0.10911831E-05	-0.14423673E-08	0.04250824E-11	0.02472718E+06	-0.01710331E+03



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$\begin{aligned} * \text{CP}/\text{R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H}/\text{RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S}/\text{R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

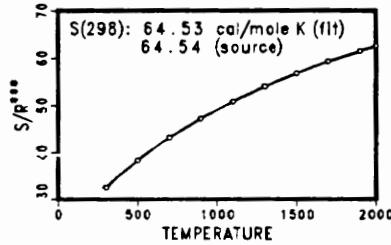
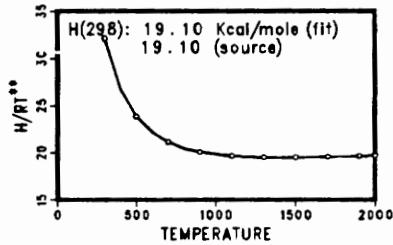
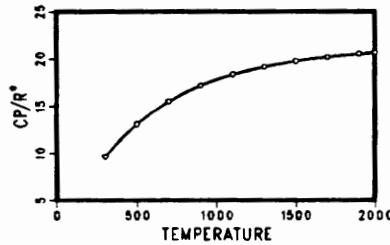
Species: Si2H6

GAS

As of: 9/05/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.05301921E+01	0.04184055E+00	-0.04685249E-03	0.03179525E-06	-0.09484526E-10	0.07950597E+05	0.01880453E+03
1000-2000K	0.08882090E+02	0.11513955E-01	-0.12162159E-05	-0.01905085E-07	0.05542379E-11	0.05967241E+05	-0.02265611E+03



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$\begin{aligned} * \text{CP}/\text{R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H}/\text{RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S}/\text{R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: Si3

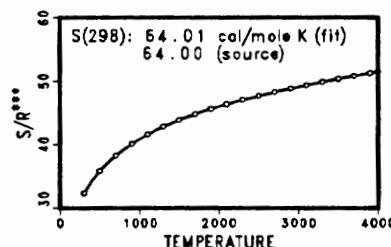
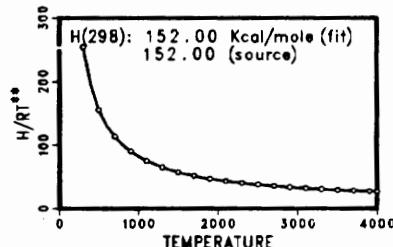
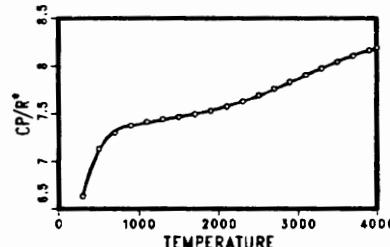
SILICON, TRIATOMIC

GAS

As of: 3/29/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.05312161E+02	0.05920180E-01	-0.05075224E-04	0.05303866E-08	0.07031630E-11	0.07469501E+06	0.04036452E+01
1000-4000K	0.07021584E+02	0.06981538E-02	-0.04818729E-05	0.01720754E-08	-0.01927024E-12	0.07429956E+06	-0.08179232E+02



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} * \text{CP}/\text{R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H}/\text{RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S}/\text{R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

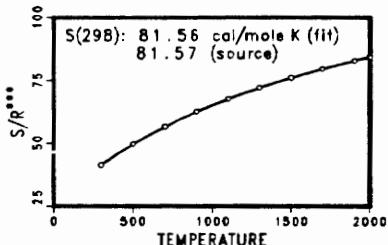
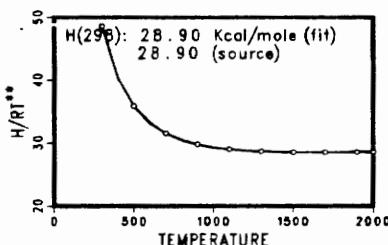
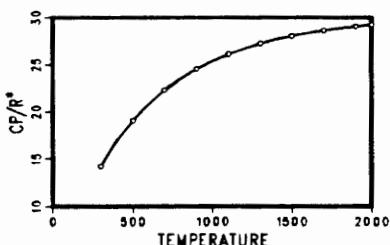
Species: Si3H8

GAS

As of: 9/05/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.06319791E+01	0.06412995E+00	-0.0772444E-03	0.05486969E-06	-0.16460971E-10	0.12092580E+05	0.02133318E+03
1000-2000K	0.13422770E+02	0.15636323E-01	-0.01936565E-04	-0.02388329E-07	0.07120030E-11	0.09165887E+05	-0.04163000E+03



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: Si3N4(A)

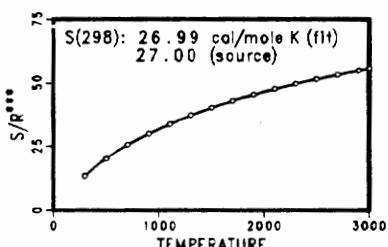
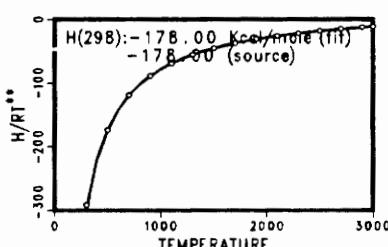
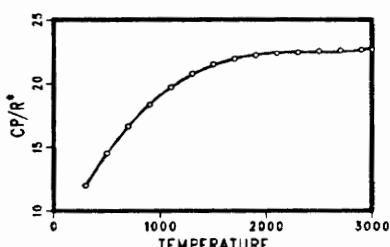
SILICON NITRIDE, ALPHA

SOLID

As of: 4/25/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.06631384E+02	0.02293928E+00	-0.02152875E-03	0.01766237E-06	-0.06632214E-10	-0.09241684E+06	-0.03021795E+03
1000-3000K	0.09667453E+02	0.11927212E-01	-0.01709281E-04	-0.10846074E-08	0.02713018E-11	-0.09324734E+06	-0.04556492E+03



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: SiC

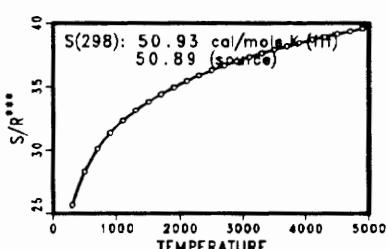
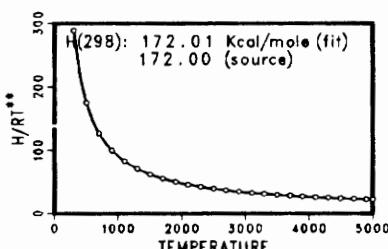
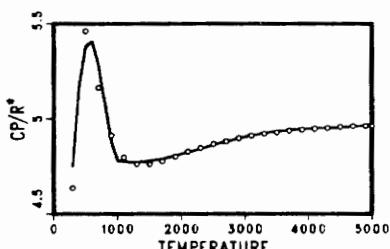
SILICON CARBIDE

GAS

As of: 11/29/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02427812E+02	0.09551934E-01	-0.02796633E-04	-0.13600122E-07	0.09196322E-10	0.08546512E+06	0.09179253E+02
1000-5000K	0.05024270E+02	-0.04920894E-02	0.03109315E-05	-0.06901344E-09	0.05215735E-13	0.08531026E+06	-0.02478798E+02



Source: SNLL FIT TO JANNAF DATA

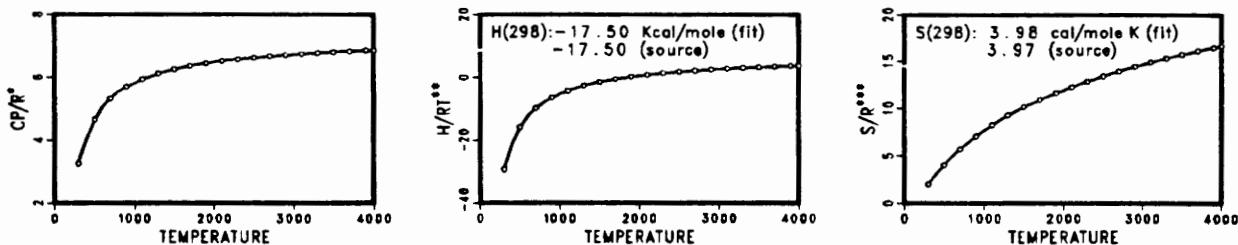
$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: SIC(B) SILICON CARBIDE, BETA SOLID As of: 11/29/89

Fit  
 Coefficients       $a_1$        $a_2$        $a_3$        $a_4$        $a_5$        $a_6$        $a_7$   
 0300-1000K -0.03551395E+01 0.15998806E-01 -0.13933268E-04 0.03314914E-07 0.07825957E-11 -0.09294352E+05 -0.15153885E+00  
 1000-4000K 0.03548056E+02 0.03636817E-01 -0.01734872E-04 0.03912869E-08 -0.03337952E-12 -0.10188585E+05 -0.01967253E+03



Source: SNLL FIT TO JANNAF DATA

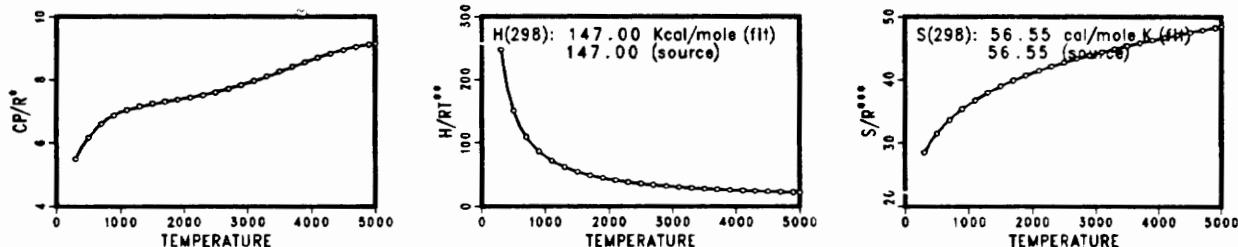
$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: SIC2 SILICON DICARBIDE GAS As of: 11/29/89

Fit  
 Coefficients       $a_1$        $a_2$        $a_3$        $a_4$        $a_5$        $a_6$        $a_7$   
 0300-1000K 0.03647724E+02 0.08765100E-01 -0.10798686E-04 0.07974287E-07 -0.02617042E-10 0.07258578E+06 0.05481049E+02  
 1000-5000K 0.05753725E+02 0.02067546E-01 -0.11325346E-05 0.03106456E-08 -0.02799936E-12 0.07200461E+06 -0.05294926E+02



Source: SNLL FIT TO JANNAF DATA

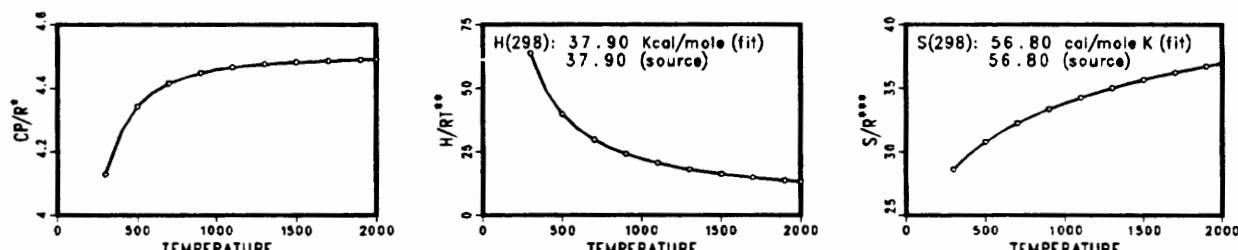
$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: SiCl SILICON MONOCHLORIDE GAS As of: 12/19/86

Fit  
 Coefficients       $a_1$        $a_2$        $a_3$        $a_4$        $a_5$        $a_6$        $a_7$   
 0300-1000K 0.03096406E+02 0.05738623E-01 -0.09740903E-04 0.07643597E-07 -0.02279178E-10 0.01796794E+06 0.09603212E+02  
 1000-2000K 0.04258459E+02 0.04020317E-02 -0.02888145E-05 0.10097771E-09 -0.14110117E-13 0.01775613E+06 0.04134521E+02



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: SICL2

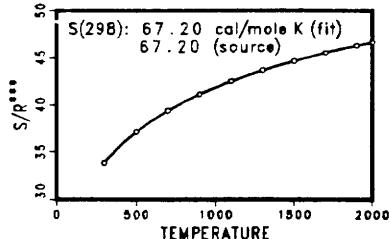
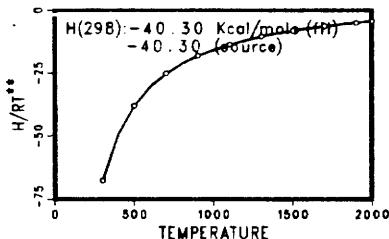
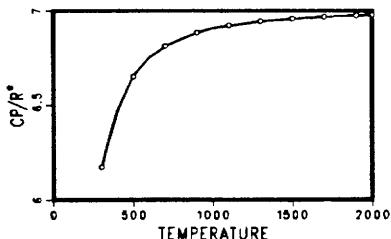
## DICHLOROSILYLENE

## GAS

As of: 12/19/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03826666E+02	0.13082964E-01	-0.02234087E-03	0.01760741E-06	-0.05267404E-10	-0.02183869E+06	0.08965448E+02
1000-2000K	0.06491204E+02	0.08242384E-02	-0.05767737E-05	0.01972405E-08	-0.02713757E-12	-0.02232408E+06	-0.03570531E+02



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SICL2H2

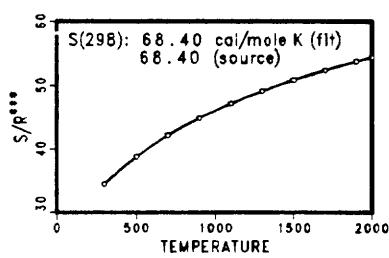
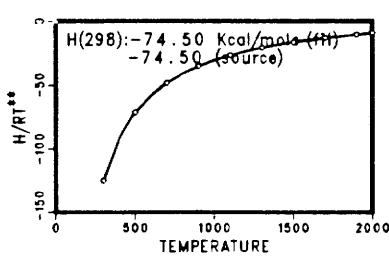
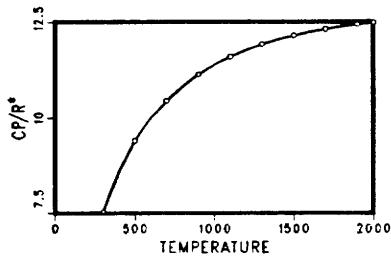
## DICHLOROSILANE

## GAS

As of: 12/19/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.11002086E+01	0.03262361E+00	-0.04691994E-03	0.03494565E-06	-0.10362847E-10	-0.03892086E+06	0.02022693E+03
1000-2000K	0.07727079E+02	0.05034188E-01	-0.10957459E-05	-0.04419587E-08	0.16311241E-12	-0.04028605E+06	-0.11708156E+02



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SICL3

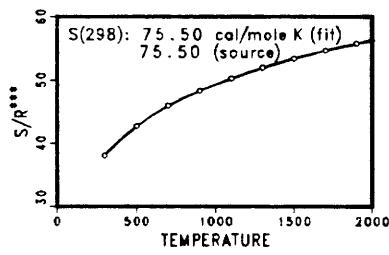
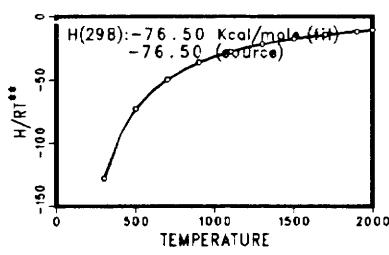
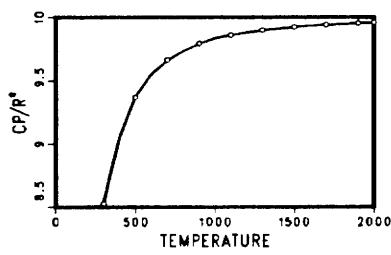
## TRICHLOROSILYL RADICAL

## GAS

As of: 12/19/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04485690E+02	0.02241754E+00	-0.03794196E-03	0.02973183E-06	-0.08861335E-10	-0.04055264E+06	0.07198771E+02
1000-2000K	0.09098097E+02	0.14053526E-02	-0.09317005E-05	0.02982296E-08	-0.03822010E-12	-0.04140193E+06	-0.14550117E+02



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SiCl<sub>3</sub>H

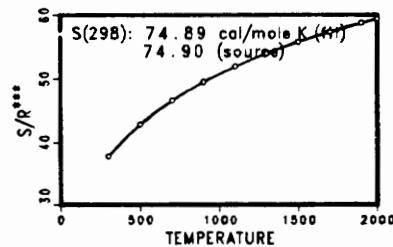
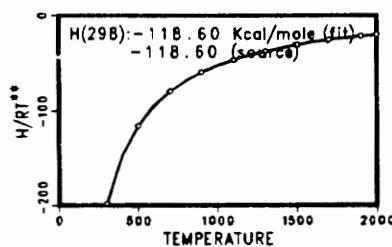
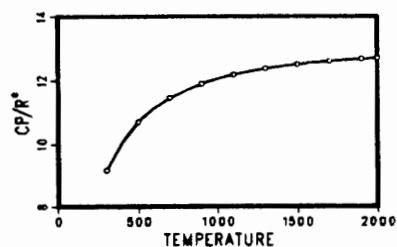
TRICHLOROSILANE

GAS

As of: 12/19/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02883769E+02	0.03308240E+00	-0.05169241E-03	0.03949918E-06	-0.11721043E-10	-0.06163323E+06	0.13374664E+02
1000-2000K	0.09663121E+02	0.03563367E-01	-0.12149114E-05	-0.16090094E-10	0.05641710E-12	-0.06295557E+06	-0.01894777E+03



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet\bullet\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: SiCl<sub>4</sub>

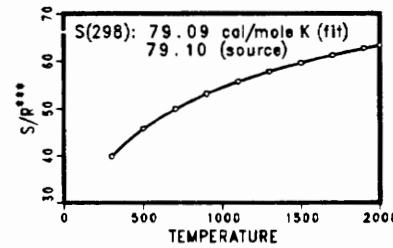
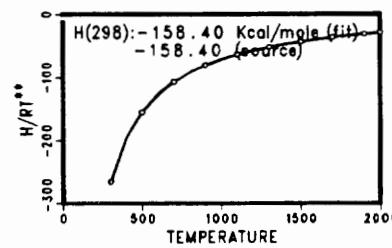
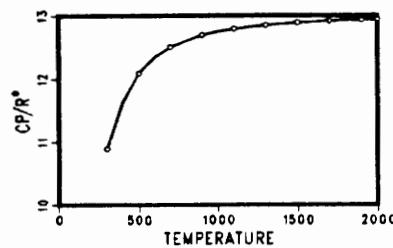
TETRACHLOROSILANE

GAS

As of: 12/19/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.05252110E+02	0.03122067E+00	-0.05254593E-03	0.04102707E-06	-0.12199071E-10	-0.08228177E+06	0.02575727E+02
1000-2000K	0.11709377E+02	0.01972091E-01	-0.12690771E-05	0.03900188E-08	-0.04756468E-12	-0.08347808E+06	-0.02791153E+03



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet\bullet\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: SiClH<sub>3</sub>

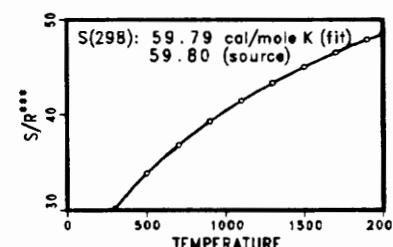
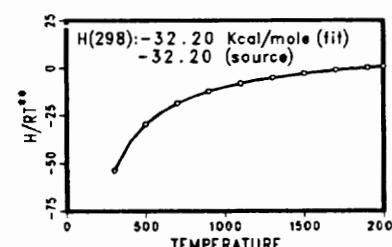
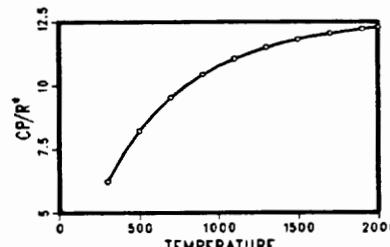
CHLOROSILANE

GAS

As of: 12/19/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.05057173E+01	0.02703377E+00	-0.03301474E-03	0.02302732E-06	-0.06778703E-10	-0.01730819E+06	0.02043167E+03
1000-2000K	0.05964237E+02	0.06278087E-01	-0.08205634E-05	-0.09280558E-08	0.02796642E-11	-0.01854309E+06	-0.06395305E+02



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet\bullet \text{ H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet\bullet\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: SIF

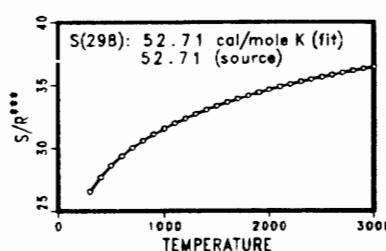
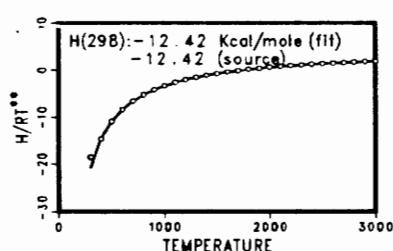
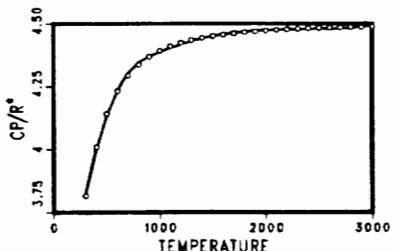
FLUOROSILYLIDYNE

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03144947E+02	0.02588557E-01	-0.05795912E-05	-0.01807278E-07	0.10411718E-11	-0.07294439E+05	0.07876774E+02
1000-3000K	0.04120066E+02	0.03548820E-02	-0.07200222E-06	-0.02190434E-09	0.06764591E-13	-0.07561378E+05	0.02784246E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: SIF(NH<sub>2</sub>)<sub>2</sub>

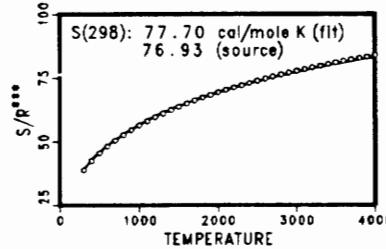
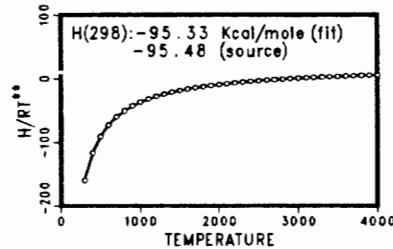
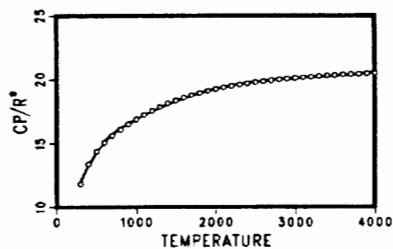
DIAMINOFLUOROSILYL RADICAL

GAS

As of: 2/27/90

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.07210094E+02	0.01764697E+00	-0.02542059E-04	-0.12422138E-07	0.06989787E-10	-0.05086706E+06	-0.07024622E+02
1000-4000K	0.12879436E+02	0.04598535E-01	-0.04004440E-05	-0.02374189E-08	0.04255211E-12	-0.05238278E+06	-0.03653418E+03



Source: SNL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: SIF(NH<sub>2</sub>)<sub>3</sub>

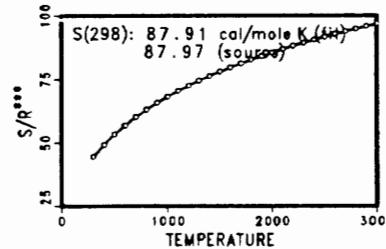
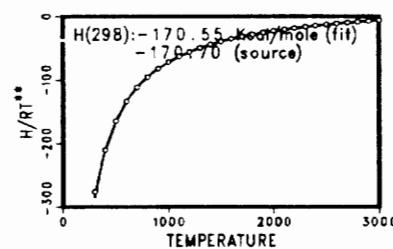
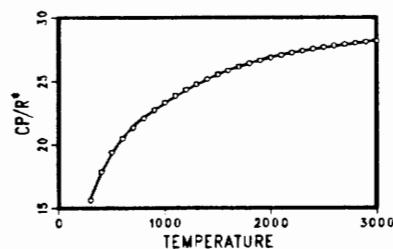
TRIAMINOFLUOROSILANE

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.08388268E+02	0.02746622E+00	-0.04455674E-04	-0.01955732E-06	0.11407210E-10	-0.08947806E+06	-0.11381777E+02
1000-3000K	0.16111795E+02	0.08329222E-01	-0.06023787E-05	-0.07470125E-08	0.15707311E-12	-0.09137007E+06	-0.05098123E+03



Source: SNL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: SIF2

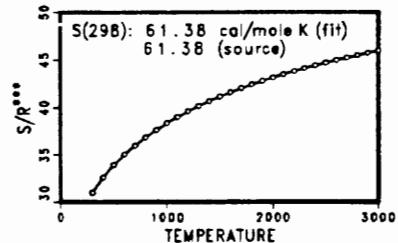
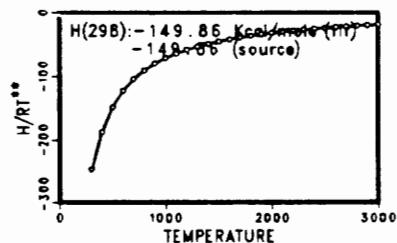
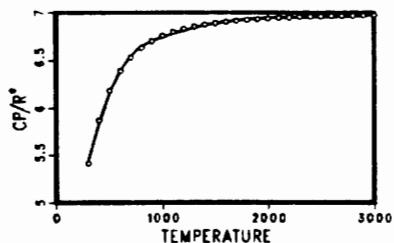
DIFLUOROSIYLENE

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03845345E+02	0.06038465E-01	-0.11677323E-05	-0.04579553E-07	0.02607414E-10	-0.07681633E+06	0.07272983E+02
1000-3000K	0.06142470E+02	0.07807974E-02	-0.13393119E-06	-0.06264839E-09	0.01725138E-12	-0.07744042E+06	-0.04712327E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: SIF2(NH2)2

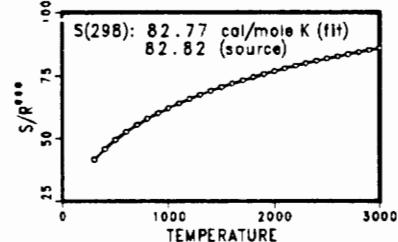
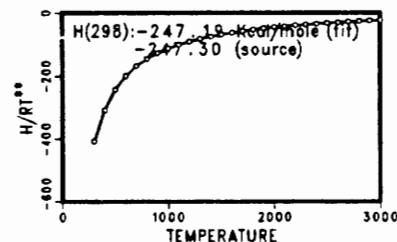
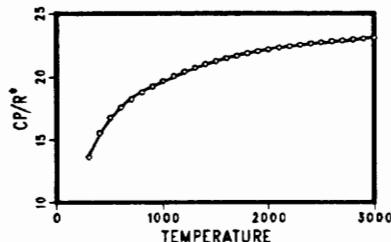
DIFLUORODIAMINOSILANE

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.07634268E+02	0.02315843E+00	-0.04193827E-04	-0.01715350E-06	0.10164619E-10	-0.12764102E+06	-0.08419031E+02
1000-3000K	0.14414775E+02	0.06110646E-01	-0.04871145E-05	-0.05455935E-08	0.11727140E-12	-0.12927572E+06	-0.04308682E+03



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

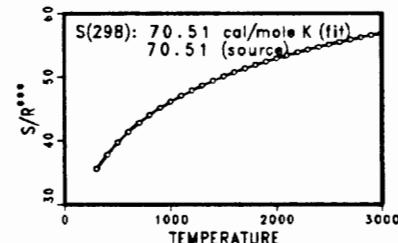
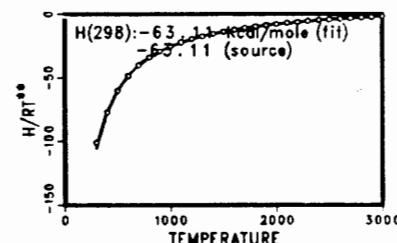
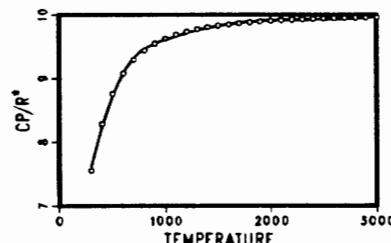
Species: SIF2N

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.05102583E+02	0.09456606E-01	-0.01819383E-04	-0.07309616E-07	0.04178902E-10	-0.03367293E+06	0.03734423E+02
1000-3000K	0.08687337E+02	0.11934885E-02	-0.01992660E-05	-0.09951333E-09	0.02704383E-12	-0.03463832E+06	-0.14940526E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: SIF2NH2

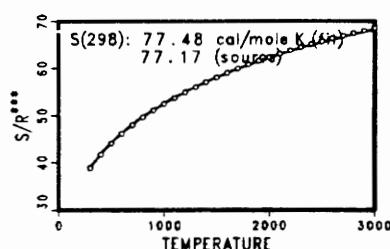
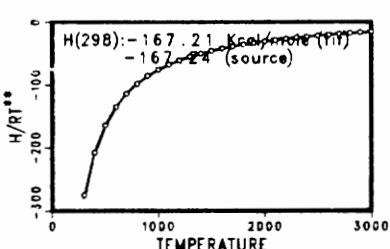
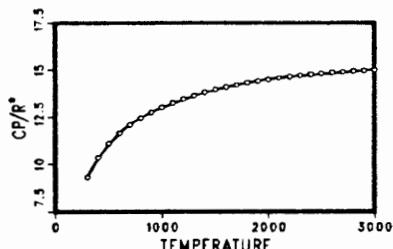
DIFLUOROAMINOSILYL

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.05890444E+02	0.12851282E-01	-0.01863556E-04	-0.08718963E-07	0.04848951E-10	-0.08644527E+06	0.01756162E+02
1000-3000K	0.09872415E+02	0.03722112E-01	-0.03271338E-05	-0.03321674E-08	0.07293692E-12	-0.08751628E+06	-0.01899095E+03



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP}/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H}/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S}/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: SIF3

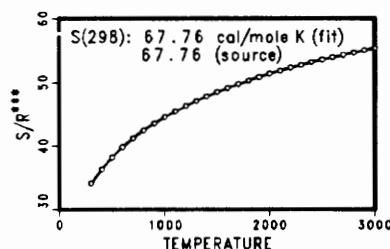
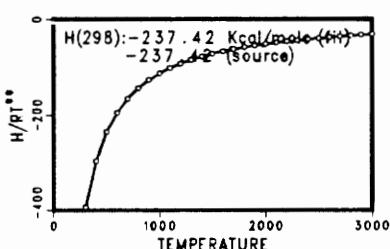
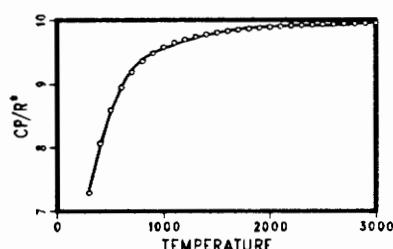
TRIFLUOROSILYL

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04662868E+02	0.10087878E-01	-0.01805544E-04	-0.07769299E-07	0.04377851E-10	-0.12129652E+06	0.04672966E+02
1000-3000K	0.08524790E+02	0.13237924E-02	-0.02104278E-05	-0.11495040E-09	0.03055301E-12	-0.12235223E+06	-0.15502343E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP}/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H}/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S}/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: SIF3NH

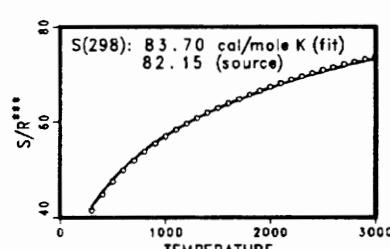
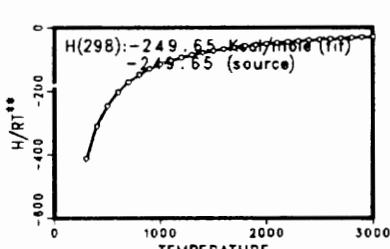
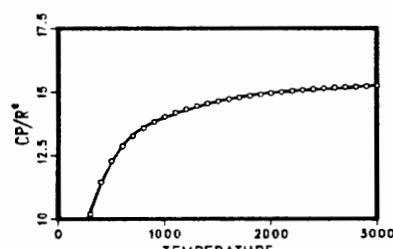
TRIFLUOROSILYLAMIDOGEN

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.06013822E+02	0.15977294E-01	-0.02791466E-04	-0.12141200E-07	0.06927415E-10	-0.12809741E+06	0.03316770E+02
1000-3000K	0.11637665E+02	0.02880768E-01	-0.03357310E-05	-0.02584594E-08	0.06162371E-12	-0.12958909E+06	-0.02590717E+03



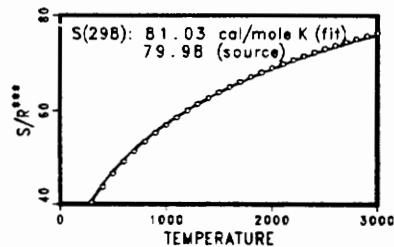
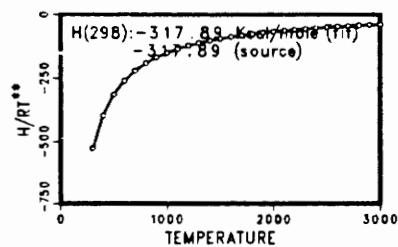
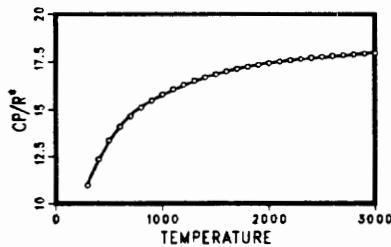
Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP}/R &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H}/RT &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ *** \text{S}/R &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: SIF3NH2 TRIFLUOROSILYLAMINE GAS As of: 4/24/89

fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.06229403E+02	0.01778015E+00	-0.02612304E-04	-0.12672434E-07	0.07044556E-10	-0.16258489E+06	0.02045440E+01
1000-3000K	0.12109636E+02	0.04383282E-01	-0.04142245E-05	-0.03989090E-08	0.08958954E-12	-0.16417679E+06	-0.03046928E+03



Source: SNLL FIT TO BAC-MP4 DATA

$$CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

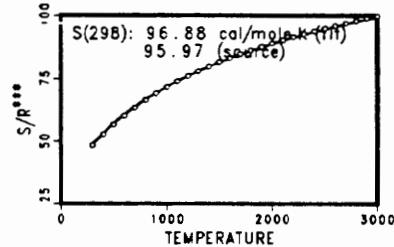
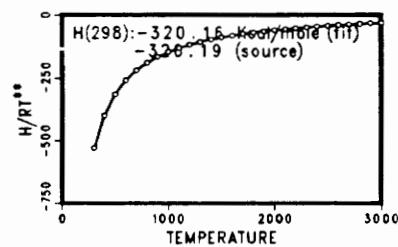
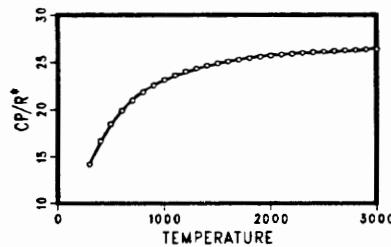
$$\bullet \bullet H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: SIF3NHSIH3                    TRIFLUOROSILYL-SILYLAMINE            GAS                    As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.06216046E+02	0.02939330E+00	-0.02717745E-04	-0.01982877E-06	0.10027676E-10	-0.16422818E+06	0.04858261E+02
1000-3000K	0.16699406E+02	0.07789784E-01	-0.08105700E-05	-0.07650199E-08	0.01773956E-11	-0.16734123E+06	-0.05080007E+03



Source: SNLL FIT TO BAC-MP4 DATA

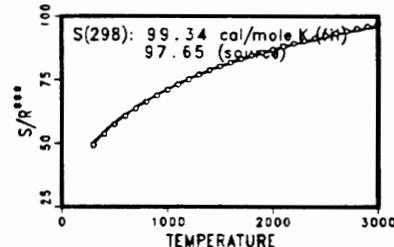
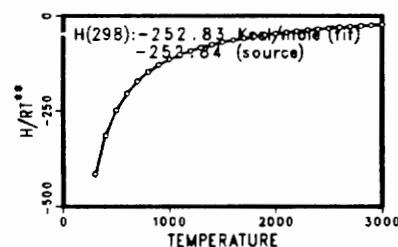
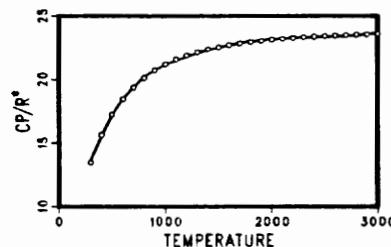
$$\bullet CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

5

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.06404371E+02	0.02601982E+00	-0.02491543E-04	-0.01769542E-06	0.08919883E-10	-0.13025197E+06	0.06002945E+02
1000-3000K	0.15991462E+02	0.06371085E-01	-0.07256823E-05	-0.06292690E-08	0.14951566E-12	-0.13311576E+06	-0.04495265E+03



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet CP/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$** H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$*** S/R = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: SIF4

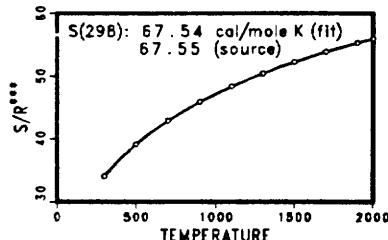
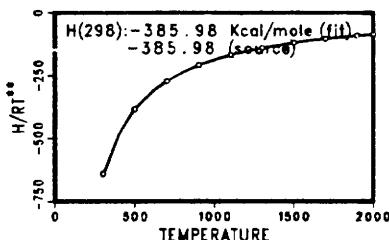
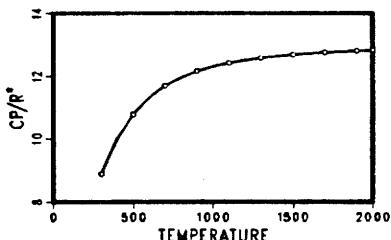
## SILICON TETRAFLUORIDE

GAS

As of: 4/13/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02147416E+02	0.03402219E+00	-0.04756873E-03	0.03252196E-06	-0.08819304E-10	-0.01960449E+07	0.13463150E+02
1000-2000K	0.09985301E+02	0.03532637E-01	-0.11973776E-05	-0.10365486E-09	0.08661585E-12	-0.01977199E+07	-0.02472643E+03



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SIFH3

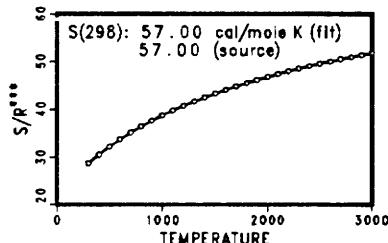
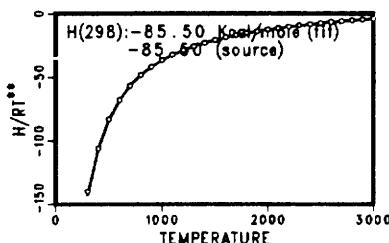
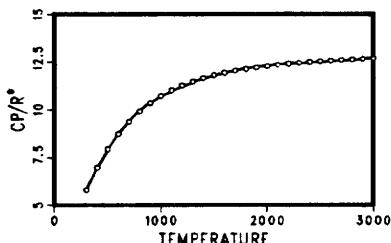
## FLUOROSILANE

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02032189E+02	0.13413632E-01	-0.02806381E-05	-0.07803291E-07	0.03337474E-10	-0.04421627E+06	0.13187677E+02
1000-3000K	0.06799678E+02	0.04747086E-01	-0.04767066E-05	-0.04814665E-08	0.11077613E-12	-0.04577024E+06	-0.12614326E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

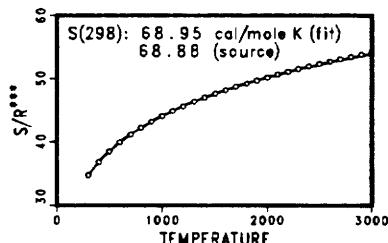
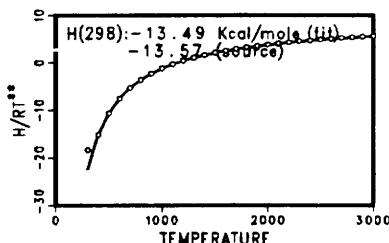
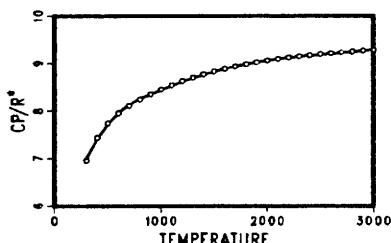
Species: SIFNH

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.05390691E+02	0.06071319E-01	-0.13594903E-05	-0.04267435E-07	0.02603153E-10	-0.08644237E+05	0.02272064E+02
1000-3000K	0.07163298E+02	0.15213245E-02	-0.15363371E-06	-0.11959331E-09	0.02684099E-12	-0.09065496E+05	-0.06764144E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

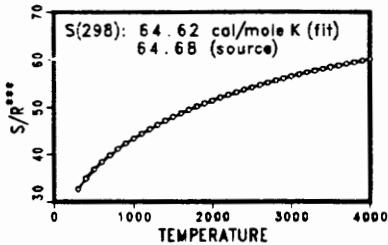
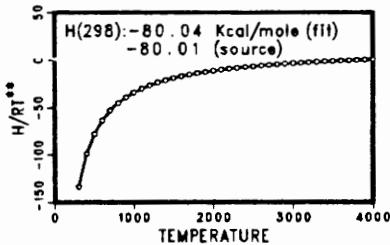
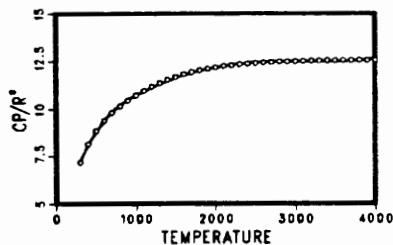
$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SIFNH<sub>2</sub> AMINOFLUOROSILYLENE GAS As of: 2/27/90

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.04214050E+02	0.11054231E-01	-0.10147254E-05	-0.07143728E-07	0.03634922E-10	-0.04200629E+06	0.05318889E+02
1000-4000K	0.08017582E+02	0.03209103E-01	-0.03361364E-05	-0.01796536E-08	0.03385552E-12	-0.04313426E+06	-0.14870236E+02



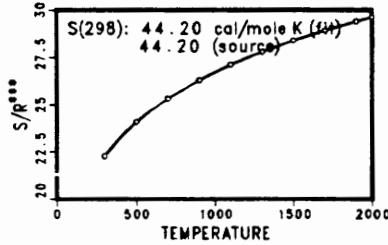
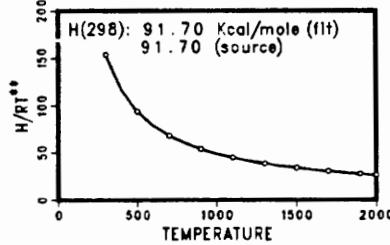
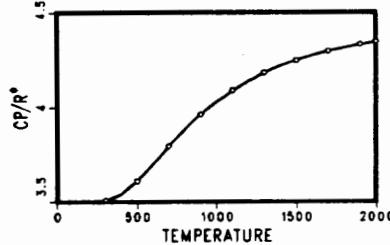
Source: SNL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: SIH SILICON MONOHYDRIDE GAS As of: 12/19/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03836009E+02	-0.02702656E-01	0.06849070E-04	-0.05424184E-07	0.14721313E-11	0.04507593E+06	0.09350778E+01
1000-2000K	0.03110430E+02	0.10949460E-02	0.02898628E-06	-0.02745104E-08	0.07051799E-12	0.04516897E+06	0.04193487E+02



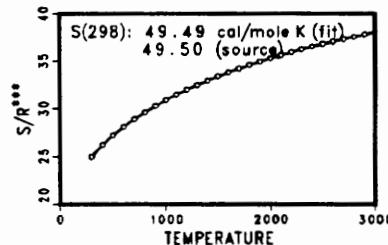
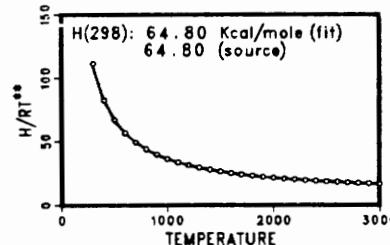
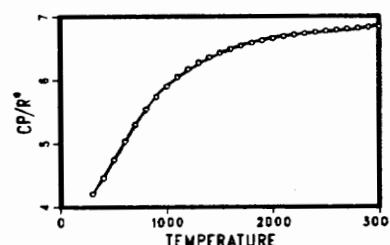
Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: SIH<sub>2</sub> SILYLENE GAS As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03475092E+02	0.02139338E-01	0.07672305E-05	0.05217668E-08	-0.09898824E-11	0.03147397E+06	0.04436585E+02
1000-3000K	0.04142390E+02	0.02150191E-01	-0.02190730E-05	-0.02073725E-08	0.04741018E-12	0.03110483E+06	0.02930745E+01



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: SiH<sub>2</sub>Cl

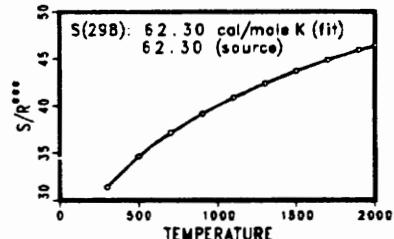
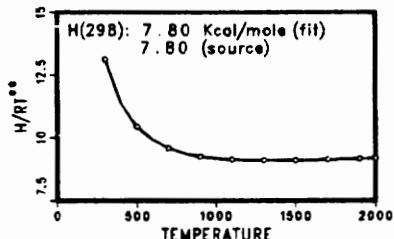
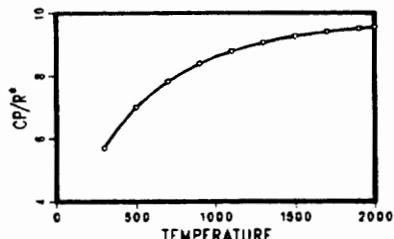
CHLOROSIYL RADICAL

GAS

As of: 12/19/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.01699256E+02	0.01961407E+00	-0.02622973E-03	0.01936416E-06	-0.05846399E-10	0.02743661E+05	0.01683132E+03
1000-2000K	0.05555901E+02	0.04046479E-01	-0.06581751E-05	-0.05027548E-08	0.15991101E-12	0.01912428E+05	-0.01906889E+02



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SiH<sub>2</sub>F

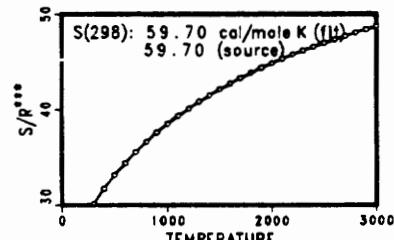
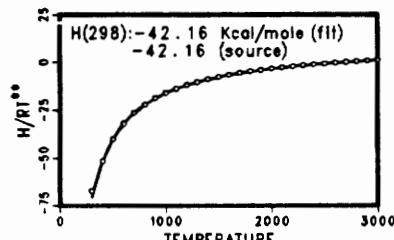
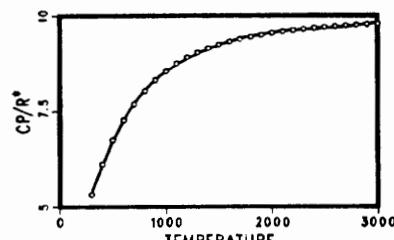
FLUOROSIYL

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02782566E+02	0.09148257E-01	-0.04186787E-05	-0.05388971E-07	0.02412133E-10	-0.02244201E+06	0.11528536E+02
1000-3000K	0.06020398E+02	0.03074039E-01	-0.03248886E-05	-0.03052243E-08	0.07098090E-12	-0.02347670E+06	-0.05919595E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SiH<sub>2</sub>F<sub>2</sub>

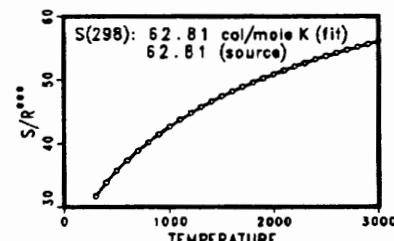
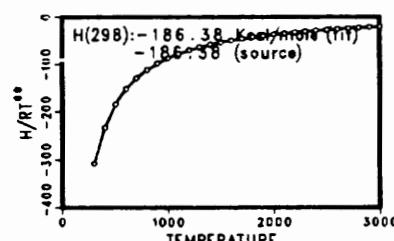
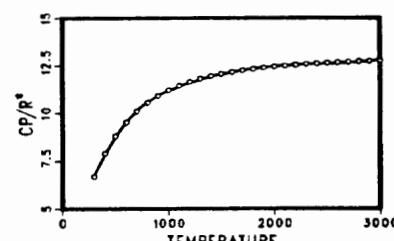
DIFLUOROSILANE

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02701455E+02	0.14565451E-01	-0.11633003E-05	-0.09685830E-07	0.04769590E-10	-0.09522440E+06	0.12006887E+02
1000-3000K	0.07997762E+02	0.03911538E-01	-0.04222679E-05	-0.03913812E-08	0.09171569E-12	-0.09682880E+06	-0.16223999E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet \text{ CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

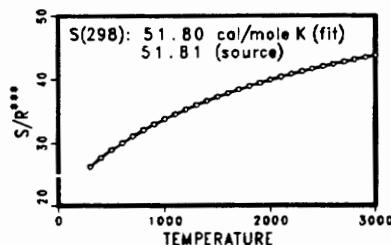
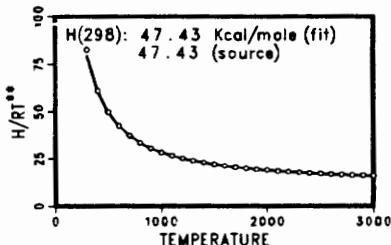
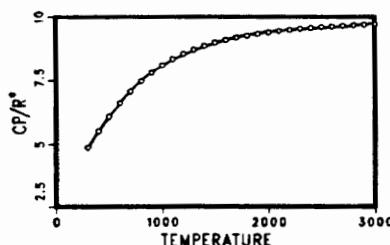
$$\bullet \text{ H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{ S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SiH<sub>3</sub> SİYL RADICAL GAS As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02946733E+02	0.06466763E-01	0.05991653E-05	-0.02218413E-07	0.03052669E-11	0.02270173E+06	0.07347948E+02
1000-3000K	0.05015906E+02	0.03732750E-01	-0.03609053E-05	-0.03729193E-08	0.08468491E-12	0.02190233E+06	-0.04291368E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

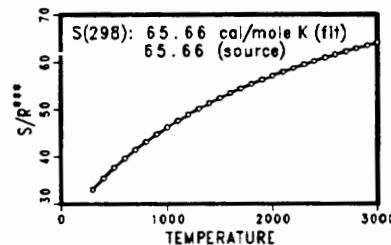
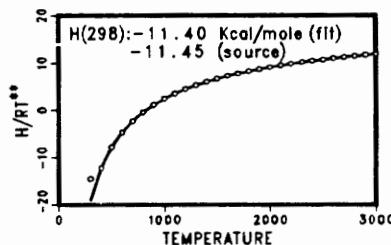
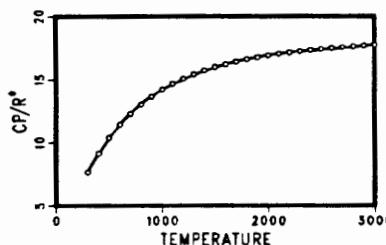
$$\bullet \text{H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: SiH<sub>3</sub>NH<sub>2</sub> SİYLAMINE GAS As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02936348E+02	0.16747041E-01	-0.03232858E-05	-0.09171970E-07	0.03979516E-10	-0.07334716E+05	0.11414373E+02
1000-3000K	0.08109945E+02	0.07215752E-01	-0.06052251E-05	-0.07086088E-08	0.15578638E-12	-0.08999782E+05	-0.16516504E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

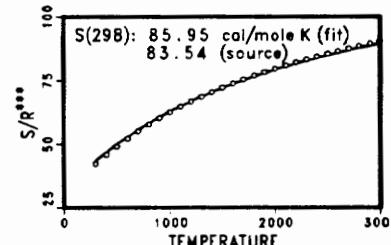
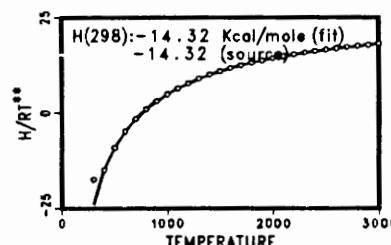
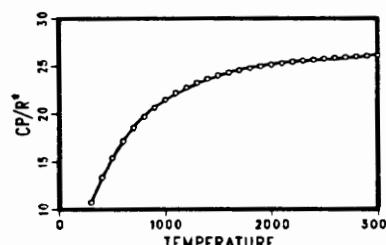
$$\bullet \text{H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: SiH<sub>3</sub>NHSiH<sub>3</sub> DISİYLAMINE GAS As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02468749E+02	0.02940254E+00	-0.06248179E-05	-0.01731461E-06	0.07545261E-10	-0.09209690E+05	0.02059559E+03
1000-3000K	0.12652963E+02	0.10667481E-01	-0.10073358E-05	-0.10812221E-08	0.02452363E-11	-0.12497210E+05	-0.03441428E+03



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bullet \text{H/RT} = a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7$$

Species: SIH<sub>3</sub>NSIH<sub>3</sub>

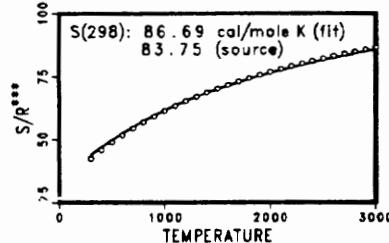
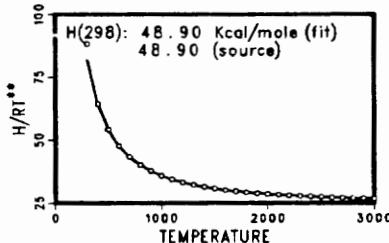
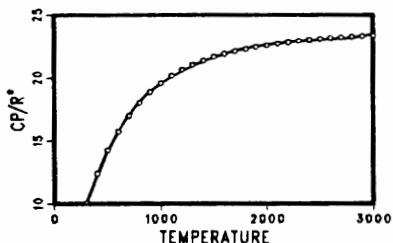
DISILYLAMIDOGEN

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02827574E+02	0.02580646E+00	-0.04200477E-05	-0.15038588E-07	0.06388324E-10	0.02265351E+06	0.01997012E+03
1000-3000K	0.12014620E+02	0.09187517E-01	-0.09159516E-05	-0.09380967E-08	0.02156435E-11	0.01965065E+06	-0.02978185E+03



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: SIH<sub>4</sub>

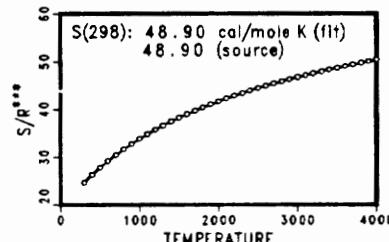
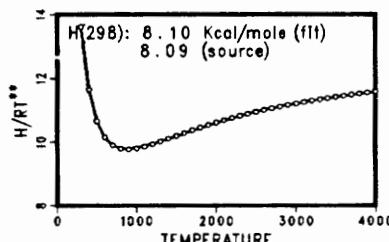
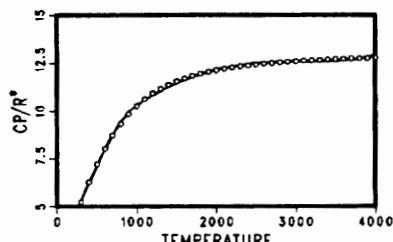
SILANE

GAS

As of: 12/13/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02475166E+02	0.09003721E-01	0.02185394E-04	-0.02681423E-07	-0.06621080E-11	0.02925488E+05	0.07751014E+02
1000-4000K	0.06893873E+02	0.04030500E-01	-0.04183314E-05	-0.02291394E-08	0.04384766E-12	0.11070374E+04	-0.01749116E+03



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: SIHCl<sub>2</sub>

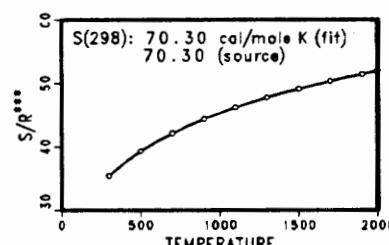
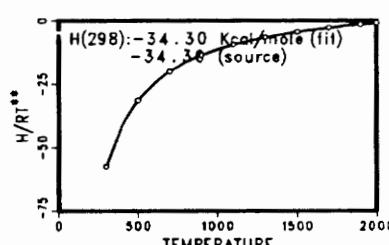
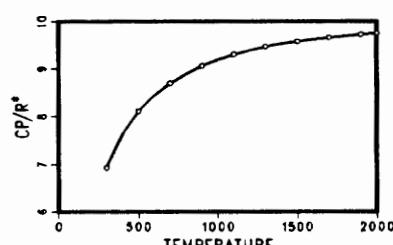
DICHLOROSILYL RADICAL

GAS

As of: 12/19/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02368353E+02	0.02401088E+00	-0.03717219E-03	0.02851997E-06	-0.08530494E-10	-0.01875884E+06	0.16145866E+02
1000-2000K	0.07229734E+02	0.02869205E-01	-0.08849876E-05	-0.07495865E-09	0.05752338E-12	-0.01971399E+06	-0.07052663E+02



Source: SNLL FIT TO DATA GENERATED USING VIBRATIONAL FREQUENCIES

$$\begin{aligned} * \text{CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ ** \text{H/RT} &= a_1 + a_2 T / 2 + a_3 T^2 / 3 + a_4 T^3 / 4 + a_5 T^4 / 5 + a_6 / T \\ *** \text{S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2 / 2 + a_4 T^3 / 3 + a_5 T^4 / 4 + a_7 \end{aligned}$$

Species: SIHF

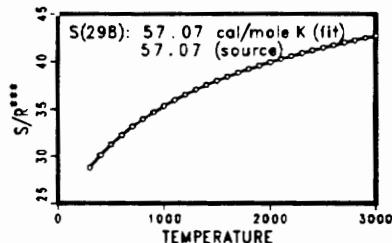
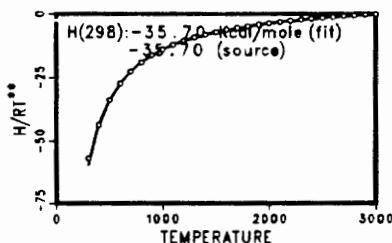
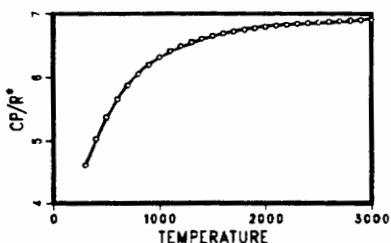
## FLUOROSILYLENE

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03223727E+02	0.04981220E-01	-0.03173051E-05	-0.02822231E-07	0.12478316E-11	-0.01914167E+06	0.08906423E+02
1000-3000K	0.05073508E+02	0.15332789E-02	-0.01840658E-05	-0.14400376E-09	0.03452517E-12	-0.01973879E+06	-0.10795069E+01



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: SIHF2

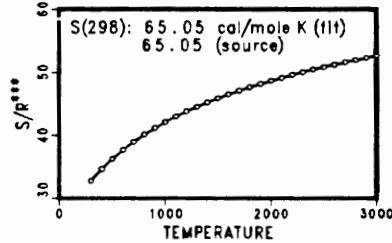
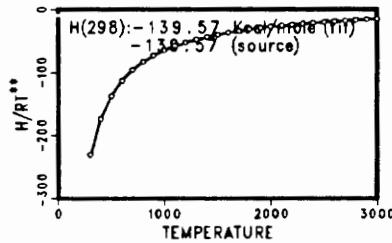
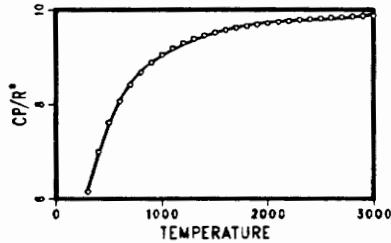
## DIFLUOROSILYL

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03377237E+02	0.10366072E-01	-0.12390823E-05	-0.07267981E-07	0.03794989E-10	-0.07168358E+06	0.10521894E+02
1000-3000K	0.07216536E+02	0.02253240E-01	-0.02737472E-05	-0.02173460E-08	0.05255331E-12	-0.07280241E+06	-0.09783487E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: SIHF3

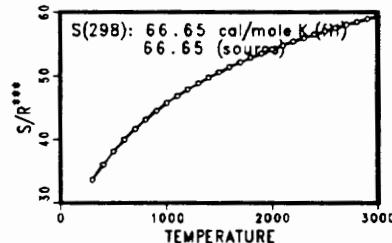
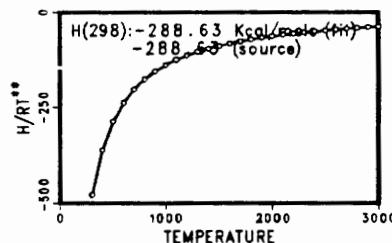
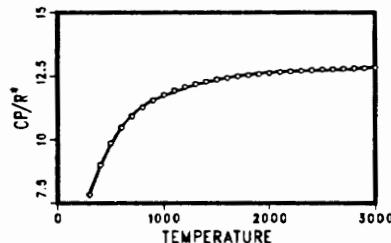
## TRIFLUOROSILANE

GAS

As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03918053E+02	0.14639172E-01	-0.01856069E-04	-0.10582003E-07	0.05617543E-10	-0.14704386E+06	0.07024261E+02
1000-3000K	0.09363567E+02	0.02947555E-01	-0.03577633E-05	-0.02858224E-08	0.06915728E-12	-0.14860736E+06	-0.02169452E+03



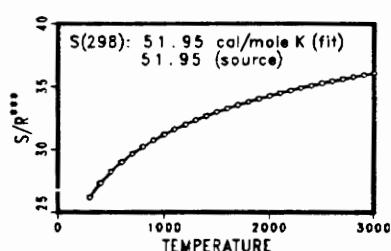
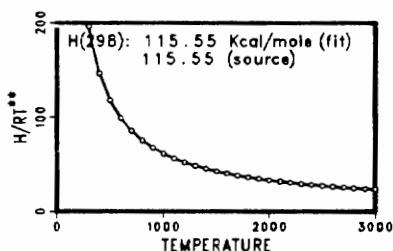
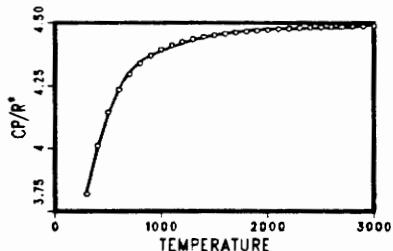
Source: SNLL FIT TO BAC-MP4 DATA

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: SIN SILICON NITRIDE GAS As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03149181E+02	0.02584376E-01	-0.05804624E-05	-0.01805626E-07	0.10410949E-11	0.05710563E+06	0.07474389E+02
1000-3000K	0.04122909E+02	0.03521457E-02	-0.07161080E-06	-0.02154956E-09	0.06667570E-13	0.05683927E+06	0.02389837E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

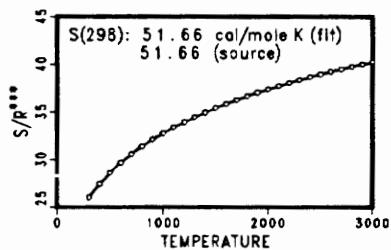
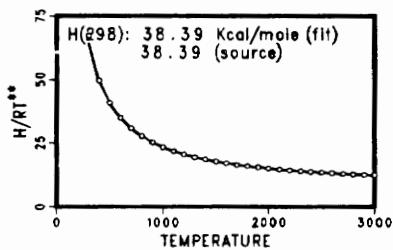
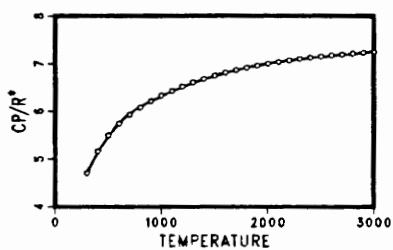
$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SINH GAS As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03166974E+02	0.05805822E-01	-0.09524443E-05	-0.03991892E-07	0.02283188E-10	0.01813560E+06	0.06298439E+02
1000-3000K	0.04928800E+02	0.16286244E-02	-0.13671971E-06	-0.13904604E-09	0.02998968E-12	0.01767789E+06	-0.02823472E+02



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

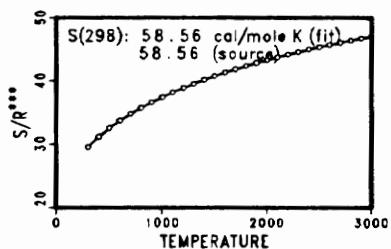
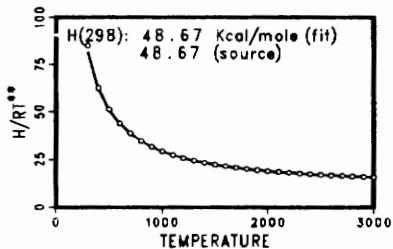
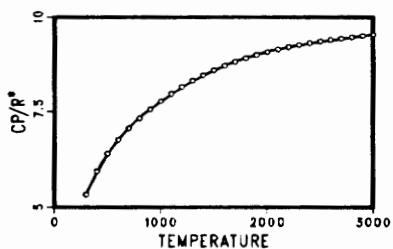
$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SINH2 AMINOSILYLIDYNE GAS As of: 4/24/89

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03362769E+02	0.07261175E-01	-0.08721233E-05	-0.04400014E-07	0.02419532E-10	0.02318445E+06	0.08223867E+02
1000-3000K	0.05186435E+02	0.03016656E-01	-0.02165476E-05	-0.02722658E-08	0.05706182E-12	0.02270507E+06	-0.12421399E+01



Source: SNLL FIT TO BAC-MP4 DATA

$$\bullet \text{CP/R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

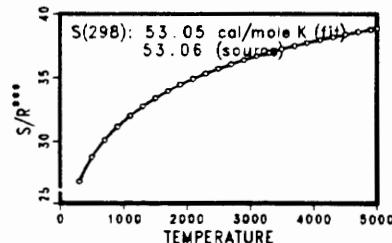
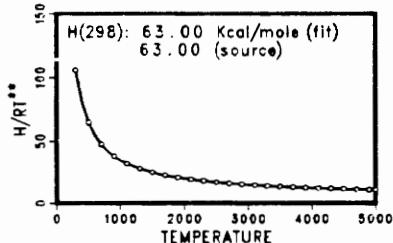
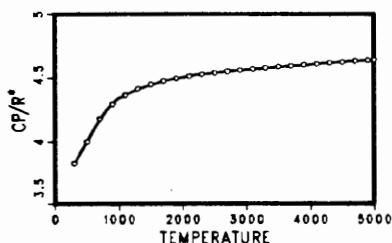
$$\bullet \text{H/RT} = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$

$$\bullet \text{S/R} = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

Species: SN SULFUR NITRIDE GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03407345E+02	0.01797887E-01	-0.02018969E-04	0.02107857E-07	-0.09527593E-11	0.03062373E+06	0.06821481E+02
1000-5000K	0.03888286E+02	0.06778427E-02	-0.02725308E-05	0.05135927E-09	-0.03593836E-13	0.03044496E+06	0.04194291E+02



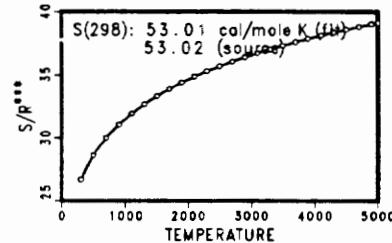
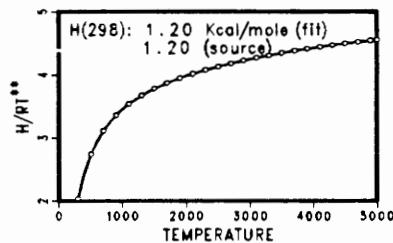
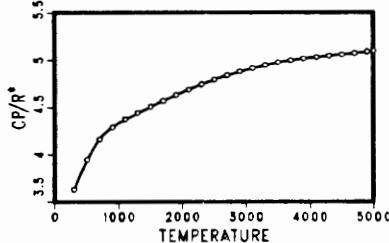
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: SO SULFUR MONOXIDE GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.03080401E+02	0.01803105E-01	0.06705022E-05	-0.02069005E-07	0.08514657E-11	-0.03986163E+04	0.08581028E+02
1000-5000K	0.04021077E+02	0.02584856E-02	0.08948142E-06	-0.03580144E-09	0.03228430E-13	-0.07119620E+04	0.03452522E+02



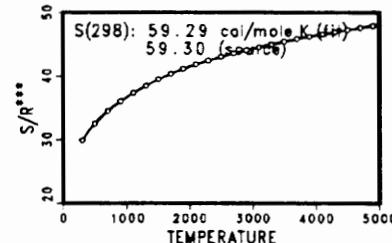
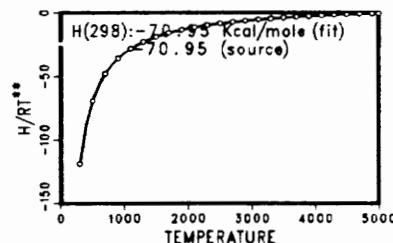
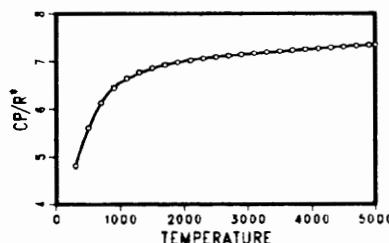
Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: S02 SULFUR DIOXIDE GAS As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02911438E+02	0.08103022E-01	-0.06906710E-04	0.03329015E-07	-0.08777121E-11	-0.03687881E+06	0.11117403E+02
1000-5000K	0.05254498E+02	0.01978545E-01	-0.08204226E-05	0.15763830E-09	-0.11204512E-13	-0.03756885E+06	-0.11460563E+01



Source: SNLL FIT TO JANAF TABLES

$$\begin{aligned} \bullet \text{ CP/R} &= a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \\ \bullet \text{ H/RT} &= a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T \\ \bullet \text{ S/R} &= a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7 \end{aligned}$$

Species: S03

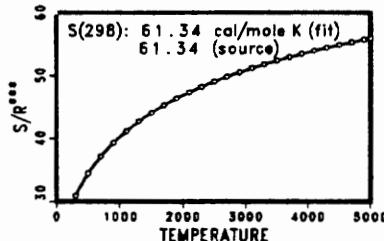
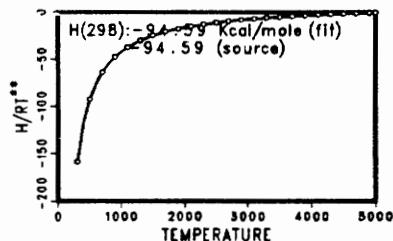
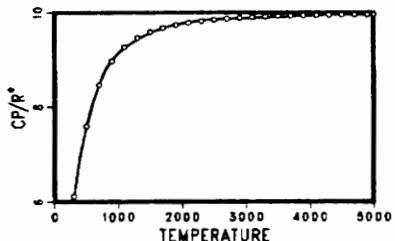
SULFUR TRIOXIDE

GAS

As of: 12/12/86

Fit

Coefficients	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
0300-1000K	0.02575282E+02	0.15150916E-01	-0.12298717E-04	0.04240257E-07	-0.05266812E-11	-0.04894410E+06	0.12195116E+02
1000-5000K	0.07050668E+02	0.03246560E-01	-0.14088974E-05	0.02721535E-08	-0.01942364E-12	-0.05020667E+06	-0.11064426E+02



Source: SNLL FIT TO JANAF TABLES

$$\bullet \text{ CP}/R = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$
$$\bullet\bullet H/RT = a_1 + a_2 T/2 + a_3 T^2/3 + a_4 T^3/4 + a_5 T^4/5 + a_6/T$$
$$\bullet\bullet\bullet S/R = a_1 \ln(T) + a_2 T + a_3 T^2/2 + a_4 T^3/3 + a_5 T^4/4 + a_7$$

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