The NASA thermo data file format was documented in:

Sanford Gordon and Bonnie J. McBride, "Computer Program for Calculation of Complex Chemical Equilibrium Compositions and Applications: I. Analysis", NASA Reference Publication 1311, October 1994.

Bonnie J. McBride and Sanford Gordon, "Computer Program for Calculation of Complex Chemical Equilibrium Compositions and Applications: II. Users Manual and Program Description", NASA Reference Publication 1311, June 1996.

The equations below for nondimensional specific heat, enthalpy, and entropy, are given in Sanford and Bonnie (1994). Eqs. 4.6-4.8 are the "old" NASA format, and Eqs. 4.9-4.11 are the "new" NASA format as discussed in this file.

Eq. 4.6: Cp0/R = a1 + a2*T + a3*T^2 + a4*T^3 + a5*T^4
Eq. 4.7: H0/RT = a1 + a2/2*T + a3/3*T^2 + a4/4*T^3 + a5/5*T^4 + a6/T
Eq. 4.8: S0/R = a1*ln(T) + a2*T + a3/2*T^2 + a4/3*T^3 + a5/4*T^4 + a7

Eq. 4.9: Cp0/R = a1*T^-2 + a2*T^-1 + a3 + a4*T + a5*T^2 + a6*T^3 + a7*T^4
Eq. 4.10: H0/RT = -a1*T^-2 + a2*T^-1*ln(T) + a3 + a4*T/2 + a5*T^2/3 + a6*T^3/4 + a7*T^4/5 + b1/T
Eq. 4.11: S0/R = -a1*T^-2/2 - a2*T^-1 + a3*ln(T) + a4*T + a5*T^2/2 + a6*T^3/6 + a7*T^4/4 + b2

The following information is quoted directly from McBride and Gordon (1996):

"Appendix A: Format for Thermodynamic Data

The library of thermodynamic data contains data for both reaction products and reactants. All reaction products and some reactants are in the nine-constant functional form discussed in section 4.2 of Gordon and McBride (1994). The format for these data is given here. Thermodynamic data are provided with the program on a separate file, thermo.inp. Sections 2.8 and 5.24 discuss the processing of the thermo.inp data and the storing of the processed data in thermo.lib for subsequent use in the CEA program. Names of species contained in thermo.inp are listed in Appendix B.

The general format is given in table A1. This format is applicable for all gaseous species and for those condensed species whose data extend over a temperature range. For those condensed species with data given at only one temperature, the format is somewhat different. On record 2, instead of the last number being a heat of formation, it is an assigned enthalpy. (Note that if the temperature is 298.15 K, the heat of formation and the assigned enthalpy are equivalent.) The first number in record 2 (number of temperature intervals) is always zero. On record 3, only one number is given, the temperature of the assigned enthalpy on record 2. Two examples are given. Example A1, for chlorine gas, illustrates the general format. Example A2, for liquid acetylene, illustrates the format for a condensed species with data given at only one temperature. The general equations for dimensionless heat capacity, enthalpy, and entropy (eqs. (4.6) to (4.8) <sic> from Gordon and McBride, 1994) are repeated for convenience.

Record	Constants	Format	Column
1	Species name or formula	A24	1 to 24
	Comments (data source)	A56	25-80
2	Number of T intervals	I2	2
	Optional identification code	A6	4-9
	Chemical formulas, symbols, and numbers	5(A2,F6.2)	11-50
	Zero for gas and nonzero for condensed phases	I1	52
	Molecular weight	F13.5	53-65
	Heat of formation at 298.15 K, J/mol	F13.5	66-80
3	Temperature range	2F10.3	2-21
	Number of coefficients for Cp0/R	I1	23
	T exponents in empirical equation for Cp0/R	8F5.1	24-63
	{H0(298.15)-H0(0)}, J/mol	F15.3	66-80
4	First five coefficients for Cp0/R	5D16.8	1-80

```
5      Last three coefficients for Cp0/R               3D16.8      1-48
       Integration constants b1 and b2                 2D16.8      49-80
...    Repeat 3, 4, and 5 for each interval
```

Example A.1:

```
CL2           Chlorine gas. TPIS 1989, v1, pt2, p88.
 2 tpis89 CL  2.00    0.00    0.00    0.00    0.00 0     70.90540          0.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9181.110
  3.46281724D+04 -5.54712949D+02  6.20759103D+00 -2.98963673D-03  3.17303416D-06
 -1.79363467D-09  4.26005863D-13  0.00000000D+00  1.53407075D+03 -9.43835303D+00
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9181.110
  6.09256675D+06 -1.94962688D+04  2.85453491D+01 -1.44996828D-02  4.46388943D-06
 -6.35852403D-10  3.32735931D-14  0.00000000D+00  1.21211722D+05 -1.69077832D+02
```

Empirical equations for example A.1:

```
Heat capacity: Cp0/R = a1*T^-2 + a2*T^-1 + a3 + a4*T + a5*T^2 + a6*T^3 + a7*T^4
Enthalpy: H0(T)/(RT) = -a1*T^-2 + a2*T^-1*ln(T) + a3 + a4*T/2 + a5*T^2/3 +
    a6*T^3/4 + a7*T^4/5 + b1/T
Entropy: S0(T)/R = -a1*T^-2/2 - a2*T^-1 + a3*ln(T) + a4*T + a5*T^2/2 +
    at*T^3/3 + a7*T^4/4 + b2
```

Example A.2:

```
C2H2(L),acetyle  Acetylene. JANAF Prop.Ser.E,1/67. TRC a-3000,10/86.
 0 1 3/95 C   2.00H  2.00    0.00    0.00    0.00 1     26.03788      207599.000
    192.35"
```

Notes:

1. Besides a very different file layout, the most significant change between the older (1971) NASA thermo data and the 1996 data is the generalization to any number of temperature intervals.
2. The preceding discussion only mentions the format of individual species data blocks. In addition, the thermo input file included with the NASA CEA program contains:
   a. Comments at the top of the file marked by exclamation (!) points in the first column
   b. Two lines at the beginning of the species data:
      i. One line containing only "thermo"
      ii. One line with 4 temperatures and a date
   c. A line containing only "END PRODUCTS" separating product species from reactants, and a line at the end of the file containing only "END REACTANTS".
3. There are some differences between the format actually used by CEA and the format described in McBride and Gordon (1996), and some undocumented features:
   a. In the CEA code, the actual read and format statements differ from the documentation by:
      i. The species name on the first line of a block is 15 characters long, not 24. The rest of the line is comments.
      ii. The heat of formation at the end of line 2 is read with f15.3, not f13.5
      iii. The temperature range at the beginning of line 3 is read as 2F11.3, not 2F10.3.
      iv. Line 5 is formatted as 2D16.8,16x,2D16.8 rather than 3D16.8,2D16.8. The 16x acknowledges that the third field is not actually used. The first two fields are the 6th and 7th polynomial coefficients, and the last two fields are the 8th and 9th (integration constants).
   b. Although the number of polynomial coefficients is included in the data, this number is almost always 7 (plus 2 integration constants). In the current NASA database, there are only 3 species that use less than 7 coefficients (P4O10(cr), P4O10(cr), and P4O10(L)). Apparently if less than 7 are used, they are the lowest numbered (a1, a2, a3, ...).
4. In the preceding excerpt from McBride and Gordon (1996), reference is made to eqs. (4.6) to (4.8). These should be eqs. (4.9) to (4.11).