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# **Third Millennium Ideal Gas and Condensed Phase Thermochemical Database for Combustion with Updates from Active Thermochemical Tables**

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September 2005

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# Third Millennium Ideal Gas and Condensed Phase Thermochemical Database for Combustion with Updates from Active Thermochemical Tables

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**Third Millennium Ideal Gas and Condensed Phase  
Thermochemical Database for Combustion**  
with updates from  
**Active Thermochemical Tables**

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and  
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The thermochemical database of species involved in combustion processes is and has been available for free use for over 25 years. It was first published in print in 1984, approximately 8 years after it was first assembled, and contained 215 species at the time. This is the 7<sup>th</sup> printed edition and most likely will be the last one in print in the present format, which involves substantial manual labor. The database currently contains more than 1300 species, specifically organic molecules and radicals, but also inorganic species connected to combustion and air pollution. Since 1991 this database is freely available on the internet, at the Technion-IIT ftp server, and it is continuously expanded and corrected. The database is mirrored daily at an official mirror site, and at random at about a dozen unofficial mirror and “finger” sites.

The present edition contains numerous corrections and many recalculations of data of provisory type by the G3//B3LYP method, a high-accuracy composite *ab initio* calculation. About 300 species are newly calculated and are not yet published elsewhere.

In anticipation of the full coupling, which is under development, the database started incorporating the available (as yet unpublished) values from Active Thermochemical Tables.

The electronic version now also contains an XML file of the main database to allow transfer to other formats and ease finding specific information of interest.

The database is used by scientists, educators, engineers and students at all levels, dealing primarily with combustion and air pollution, jet engines, rocket propulsion, fireworks, but also by researchers involved in upper atmosphere kinetics, astrophysics, abrasion metallurgy, etc.

This introductory article contains explanations of the database and the means to use it, its sources, ways of calculation, and assessments of the accuracy of data.

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Portions of this research are also related to the effort of a Task Group of the International Union of Pure and Applied Chemistry (IUPAC Project 2003-024-1-100)

The XML converter code was developed by Dr. Reinhardt Pinzon (ANL) and Mr. Eitan Burcat.

## IN MEMORIAM

This publication and database is dedicated to the memories of:

- Prof. William C. Gardiner (1933-2000), professor of chemistry at the University of Texas at Austin; initiator and first publisher of this database
- Sanford Gordon (1920-2001) of NASA Lewis in Cleveland, who investigated and designed the NASA polynomials
- Bonnie J. McBride (1934-2005) of NASA Lewis who wrote the CEA and PAC programs and Compiled and maintained the NASA thermochemical database for 45 years

May they rest in peace.

This database is available in electronic form at:

<ftp://ftp.technion.ac.il/pub/supported/aetdd/thermodynamics>

and at the mirror site at

<http://garfield.chem.elte.hu/Burcat/burcat.html>

## Introduction

Thermochemistry started, as generally mentioned by different thermodynamicists, with the articles of Mallard and Le-Chatellier (1883) in which the first sentence is the statement: "All combustion is accompanied by the release of heat that increases the temperature of the burned bodies." In 1897 Marcelin Berthelot published his two volume monograph entitled *Thermochimie* in which he summed up 40 years of calorimetric experimentation.

The first textbook to clearly explain the thermochemical properties was Lewis and Randall (1923).

Thermochemical data, actually heats of formation, were gathered, evaluated and published for the first time in the *International Critical Tables* printed in seven volumes between 1926 and 1930 (and the additional Index in 1933). The editor was E.W. Washburn.

In 1932 appears the *ACS Monograph 60* by Parks and Huffman entitled *The Free Energy of some Organic Compounds*.

In 1936 F.R. Bichowsky and F.D. Rossini published *The Thermochemistry of the Chemical Substances*, in which the authors attempted to standardize the available data and publish them at a common temperature of 18 °C (291 K) and pressure of one atmosphere.

In 1940, Mayer and Mayer published their monograph *Mechanical Statistics*, in which the method of calculating thermochemical properties from spectroscopic data is explained in detail.

In 1947 Rossini published *Selected Values of Properties of Hydrocarbons*, *NBS Circular 461*, (American Petroleum Institute Research Project 44). This was followed by the

famous *NBS Circular 500* (1952), which concentrates on the thermochemistry of organic species, and gives not only enthalpies of formation but also heat capacities ( $C_p$ ), enthalpies ( $H_T-H_0$ ), entropies ( $S$ ) and equilibrium constants ( $K_c$ ) as a function of temperature.

During the 1950's, the loose leaf compendium of the Thermodynamic Research Center (TRC) at A&M University in Texas appeared as a continuation of API Project 44. In this compendium, thermochemistry as a function of temperature is only a small part of their data that include melting and boiling points, vapor pressures, IR spectra, etc. Although their values are technically reliable, a very serious drawback is the lack of documentation on the data and the calculation methods.

In 1960, the first loose leaf edition of the *JANAF Tables* appeared, but was restricted solely to U.S. government agencies. This first edition is devoted to chemical species involving all the elements, but it contains only a very limited number of organic species. This publication, which became very famous when published as the second (bound) edition (1972), set the standard temperature reference at 298.15 K and published the enthalpy increments (a.k.a integrated heat capacities) as ( $H_T-H_{298}$ ) instead of ( $H_T-H_0$ ). This edition of the *JANAF Tables*, with Stull as the main editor, for the first time described in detail their methods of calculating thermochemical properties, which were based mainly on the monograph of Mayer and Mayer [1940]. They also set the temperature range of the tables up to 6000 K in order to assist the needs and request of the space research and industry.

Also in 1960, Thiokol Chemical Corporation published the report



*Thermodynamic Data for Combustion Products* by J.S. Gordon, meant for high performance solid rocket propellants.

In 1961 Duff and Bauer published a Los Alamos report, later (1962) summarized in the *Journal of Chemical Physics*, in which for the first time thermochemical properties of organic molecules, i.e., enthalpy and free energy, were published as polynomials.

In 1963 S. Gordon and B. McBride published the *Thermodynamic Properties of Chemical Substances to 6000 K, NASA Report SP-3001*. This publication revealed for the first time to the public world (because the *JANAF Tables* still had a restricted distribution) the methods of calculating thermochemical data for monoatomic, diatomic and polyatomic species, and introduced a thermodynamic value used by engineers but unknown before to chemists: the “absolute enthalpy”, which sets the value of  $H_T = \Delta_f H_{298} + (H_T - H_{298})$ . This publication lists, also for the first time, the thermochemical properties not only in table format but also as 7 coefficient NASA polynomials. The NASA program to calculate thermochemical properties and 7 term polynomials was published by B. McBride and S. Gordon in 1967.

In 1965, NBS started publishing the *Technical Note 270* in a series of booklets where they present heats of formation at 0 K, at 273.16 K and 298.16 K.

In 1969 appeared the book of Stull, Westrum and Sinke, *Thermodynamics of Organic Compounds*, where the thermochemical properties of 741 stable organic molecules were published in the temperature range of 298 K to 1000 K.

In 1962 appeared the first edition of the Glushko-Gurvich *Thermodynamic Properties of Individual Substances*

(TSIV) in Moscow. This monumental compendium became world known as “Gurvich’s Thermochemical Tables” from the further publications in 1978, 1979, 1982, and specifically from the fourth English-translated edition of 1989, which was also followed by further English editions in 1991, 1996, and 1997.

Other thermochemical properties - were published by Barin and Knacke in 1973 and Barin in 1989.

Evaluations of heats of formation for organic molecules and radicals were published by Cox and Wagman (1970), Pedley and Rylance (1977), Domalski and Hearing (1988) and Pedley, Nylor and Kirby (1989).

### Polynomials

Polynomials are mentioned for the first time by Lewis and Randal as a means to present thermochemical properties such as heat capacity ( $C_p$ ), enthalpy, and so on, as a function of temperature. The publication of elaborate tables of properties was very problematic in a world where computers were not even imagined. Polynomials seemed a compact way to publish a lot of numbers and also a good way to smooth out measurement scatter of the data. Despite the advantages, polynomials were not used abundantly before the proliferation of computers starting about 1965.

Government agencies such as NASA and various National Laboratories had computers by the end of the fifties, and therefore started using polynomials in order to get thermochemical properties as a function of temperature. The functions were needed in order to calculate equilibrium compositions of reactions, which were extensively used before kinetic programs were available. That was the reason for the publication of Bauer and Duff’s paper which included

extensive equilibrium calculations. These authors found out that the full temperature range of 298.15 K to 6000 K cannot be represented by a single polynomial, so they were the first to publish two branch polynomials. There were two sets (each with two branches): one set for heat capacity ( $C_p$ ) and a second set for the free energy function ( $F$ ). The two branches of the set were not coinciding at any temperature and their use in the 1000 K region included a non-continuity jump.

The thermodynamic group at the NASA Lewis Center in Cleveland, led by Sanford Gordon, undertook a long study in order to investigate the problem of chemical equilibrium [Huff, Gordon and Morrell, 1951; Zeleznik and Gordon, 1960; 1961; 1962]. As a result, a close scrutiny of the polynomialization of the thermodynamic data was also undertaken, and they proposed a solution with two important features: a single set of coefficients could be used for as many properties as possible for a single compound, and the same polynomial form should fit all thermodynamic data for gases, liquids, and solids for all possible chemical compounds. Frank Zeleznik and Sanford Gordon (1961) invented the method of simultaneous regression of the thermochemical properties so that more than one property can be approximated by a single polynomial. These works ended up with the famous NASA 7 term polynomials first published by Zeleznik and Gordon (1962) and McBride *et al.* (1963)

In their first form, the polynomials were fit for two temperature ranges. The first polynomial was fit for the temperature region important for combustion, i.e., 1000-6000 K. The second polynomial was fit for the low temperature region, i.e., 300-1000 K. The

two polynomials were “pinned” at 1000 K. They were constrained to reproduce exactly the 1000 K value, thus assuring that both branches will match at 1000 K without discontinuity. The consequence of this method was that the values at the standard reference temperature of 298.15 K, which were not used to create any constraints, were always reproduced with some small error, depending on the polynomial fit. Later, in 1982, following user’s requests, the fitting of the polynomials was slightly changed: the lower branch was extended to 200 K, and the pinning of the polynomials was transferred to the 298.15 K values, while the two branches were still constrained to have the same value at 1000 K.

Because of the need of NASA to calculate properties beyond the 6000 K limit for shuttle orbital reentry problems, the research into the polynomials was extended, and in 1987 a new set of NASA 9 term polynomials were adopted. The foremost quality of these polynomials is that new branches can be added above and below the original range; in addition, their error of reproducing the fitted data was improved between 1 and 2 orders of magnitude. The maximum error at peak temperature of the 7 term polynomials is typically in the range of a tenth of one percent to one percent, while the typical fitting error of the new 9 term polynomials is in the range of one thousandth of a percent and one hundredth of a percent.

The program to calculate thermochemical properties (called PAC for Properties and Coefficients) and the corresponding 7 term polynomials were published by McBride and Gordon in 1967, and a new version that calculates the 9 term polynomials was published in 1992.

Other types of polynomials were

also proposed. For example, the Wilhoit (1975) polynomials were intended to allow the extrapolation of the TRC thermochemical properties beyond the 1000 or 1500 K temperature range. These polynomials are used internally for extrapolation by the PAC program as well as the THERM program (see below). The NIST WebBook site prefers the Shomate polynomials. The Gurvich polynomial for the partition function is seldom used in the west. Various series of negative powers of the temperature were also proposed in the past, and very recently [Lanzafame and Messina 2001-2] a series of logarithmic powers of the temperature was proposed. However, none of them got the wide acceptance and extensive use of the 7 term NASA polynomials, mainly due to the existence of big free databases of polynomials such as the one presented here.

The thermochemical properties can be calculated in general with confidence in the fourth and fifth digit in the range of 150-3000 K. But since many engineering problems require the knowledge of data above and below this range, they are provided in the form of 7 term polynomials to 6000 K and as 9 term polynomials from 50 to 6000 K.

The 7-coefficient NASA polynomials can be used to calculate the following functions:

$$\begin{aligned} \frac{C_p^\circ}{R} &= a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \quad (1) \\ \frac{H_T^\circ}{RT} &= a_1 + \frac{a_2T}{2} + \frac{a_3T^2}{3} + \frac{a_4T^3}{4} + \frac{a_5T^4}{5} + \frac{a_6}{T} \quad (2) \\ \frac{S_T^\circ}{R} &= a_1 \ln T + a_2T + \frac{a_3T^2}{2} + \frac{a_4T^3}{3} + \frac{a_5T^4}{4} + a_7 \quad (3) \end{aligned}$$

$$\frac{G_T^\circ}{RT} = \frac{H_T^\circ}{RT} - \frac{S_T^\circ}{R} = a_1(1 - \ln T) - \frac{a_2T}{2} - \frac{a_3T^2}{6} - \frac{a_4T^3}{12} - \frac{a_5T^4}{20} + \frac{a_6}{T} - a_7 \quad (4)$$

It should be noted that the value  $H_T^\circ$  obtained from the polynomials is the "engineering enthalpy" defined as

$$H_T^\circ = \Delta_f H_{298}^\circ + \int_{298}^T C_p^\circ dT \quad (5)$$

Similarly, the  $G^\circ/RT$  functions of the molecules in a reaction can be used directly to compute the reaction's equilibrium constant in terms of concentrations through

$$K_c = (RT)^{-\Delta\nu} \exp \left( \frac{\Delta a_1 (\ln T - 1) + \frac{\Delta a_2 T}{2} + \frac{\Delta a_3 T^2}{6} + \frac{\Delta a_4 T^3}{12} + \frac{\Delta a_5 T^4}{20} + \frac{\Delta a_6}{T} + \Delta a_7}{1} \right) \quad (6)$$

where the change in mole number is  $\Delta\nu = \sum \nu_j$  and the coefficient changes are  $\Delta a_1 = \sum \nu_j a_{1j}$ . The summations are over all the reactant and product species  $j$  with the stoichiometric coefficients  $\nu_j$  being positive for products and negative for reactants.

The 7 term polynomials actually include 15 constants. The first set of 7 constants belongs to the 1000-6000 K polynomial, the second set of 7 constants belongs to the 200-1000 K polynomial, and the fifteenth constant is  $H_{298}/R \equiv \Delta_f H_{298}/R$ . The latter value (and the corresponding position within the polynomial format) is not used by most other programs, such as CHEMKIN, and therefore does not interfere with their calculations.

The 9-constants polynomials can be used to calculate the following functions:

$$\frac{C_p^\circ}{R} = a_1 T^{-2} + a_2 T^{-1} + a_3 + a_4 T + a_5 T^2 + a_6 T^3 + a_7 T^4 \quad (7)$$

$$\frac{H_T^\circ}{RT} = -a_1 T^{-2} + \frac{a_2 \ln T}{T} + a_3 + \frac{a_4 T}{2} + \frac{a_5 T^2}{3} + \frac{a_6 T^3}{4} + \frac{a_7 T^4}{5} + \frac{a_8}{T} \quad (8)$$

$$\frac{S_T^\circ}{R} = -\frac{a_1 T^{-2}}{2} - a_2 T^{-1} + a_3 \ln T + a_4 T + \frac{a_5 T^2}{2} + \frac{a_6 T^3}{3} + \frac{a_7 T^4}{4} + a_9 \quad (9)$$

$$\frac{G_T^\circ}{RT} = \frac{H_T^\circ}{RT} - \frac{S_T^\circ}{R} = -\frac{a_1 T^{-2}}{2} + \frac{2a_2(1 - \ln T)}{T} + a_3(1 - \ln T) - \quad (10)$$

$$\frac{a_4 T}{2} - \frac{a_5 T^2}{6} - \frac{a_6 T^3}{12} - \frac{a_7 T^4}{20} + \frac{a_8}{T} - a_9$$

and also  $K_c$ , following a similar philosophy as given above for the 7 term polynomial.

### Thermodynamic Calculations

All calculations of thermodynamic quantities related to the partition function (such as heat capacity, entropy, enthalpy increment, etc.) and polynomialization in this database were performed using the McBride and Gordon PAC program. (Gordon and McBride 1967, 1992). For gas-phase species with molecular information the rigid-rotor-harmonic-oscillator (RRHO) method was used, and, if anharmonic information was available, non-rigid-rotor-anharmonic-oscillator (NRRHO) was used. In a very few cases both RRHO and NRRHO are given. For species where the direct tables from another source were used the READIN method was utilized.

Over the years, the PAC program has been changed and extended and new documentation published (McBride and Gordon 1992). At least 4 versions of this

program were used to produce the polynomials listed. Those prepared before 1984 were produced with the PAC3 version in which internal rotations were not calculated simultaneously and the corresponding contributions had to be added separately. PAC4, released in 1984, included the possibility to compute the contributions of internal rotations automatically.

If a set of data is fitted by two polynomials valid over different temperature ranges, the polynomials could in principle meet at different temperatures for different species (Burcat 1984). Ritter's program (Ritter 1990) optimizes this temperature and pins the two polynomials at the given value. However, most programs that use the thermodynamic polynomials prefer a constant pinning value. In the PAC programs, the temperature at which the polynomial branches switch was arbitrarily set to 1000 K. Before PAC4 the polynomials were pinned to the tabular value of 1000 K and therefore reproduced it exactly. In that case, the values at 298 K obtained from the polynomial are not the original tabular values, but slightly different (depending on the local error of the polynomial coefficients). This fact is mentioned in the directory table (Table 6) with an asterisk (\*). In the latest versions, PAC90 PAC97 and PAC99 the lower range polynomial is pinned at 298.15 K to the tabular values and at 1000 K the two polynomials are pinned to each other (thus having the same "hanging" value, which is not necessarily the tabular value). These versions also include Wilhoit type extrapolations, as discussed by Burcat (1984), and optional use of estimated additivity group properties as described by Stein (1985).

## Sources of Data

A large number of sources were used for the present compilation. Where more than one source was available for a species, the value that appeared to be the most reliable (at least at the date of calculation of the polynomial coefficients) was selected. If no thermodynamic data were available in known tabulations or in the archival literature, the literature was searched for experimentally or quantum mechanically calculated vibrational frequencies and moments of inertia. If such data were not available, then approximation methods were used in order to estimate the molecular constants.

Some estimations were made using the parent molecule method, in which vibrational frequencies of radicals were estimated from the vibrations of the parent molecule by deleting relevant vibrations.

Other methods of estimation included the Benson (1976) group additivity method, as used by Stein (1985) in both PAC97 and the NIST 1991 *Structure and Database Estimation Program* (Stein *et al.*, 1991; Stein 1994) and Ritter and Bozzelli's (1990) method in the *Therm* program (Ritter 1990) which also uses additivity groups but in a slightly different manner. In France, a third program exists, *Thergas*, by Muller *et al.*, (1995). This program uses Benson's additivity method and is based on the *CHETAH* program (Furip *et al.*, 1989).

The difference between the Ritter and Bozzelli method and Stein's method is that the first uses discrete point values for each "group" value, adds the separate values for each temperature and then fits a polynomial for the final results using one of three possible extrapolation methods, Wilhoit's method among them. Stein's (1985) method is not fully described. It apparently produces a

polynomial for each of the additivity group fragments, and adds the different polynomials for the estimated final species.

In the last decade semi empirical programs such as the *MOPAC* [Stewart 1989, 1990, 1993] package became widely available, followed by more accurate *ab initio* DFT and wavefunction methods that can be performed with *Gaussian*, *MOLPRO*, *GAMESS* and other electronic structure computation program packages.

Among the methods that calculate the species electronic structure, the density functional theory (DFT) methods have gained an important position, specifically the Becke (1993) exchange functionals coupled with the Lee-Yang-Parr (1988) function widely known as B3LYP. The composite *ab initio* G3 theory (Curtiss *et al.*, 1998) and its variant G3B3 (Baboul *et al.*, 1999) are able to achieve very high accuracy (with a 95% confidence limit that is generally around  $\pm 2$  kcal/mol or better), without requiring (at least for small and medium-sized species) an exorbitant computational effort. These methods are geared up to calculate the enthalpy of formation of the species through the atomization energy, producing also the other needed molecular properties such as geometry and vibrations.

The *ab initio* G3B3 method optimizes the geometry and calculates the molecular frequencies using the DFT B3LYP method. These compare very well with experimental IR and Raman measurements. The enthalpies of formation are then calculated using a composite approach that performs a sequence of calculations at various levels and with various basis sets, effectively estimating the energies at the QCISD(T) level using a large basis set (G3Large).

Thus, the method can calculate the spectroscopic and thermodynamic properties of radicals, which are otherwise very hard to measure experimentally. Using commodity computers (such as PCs), the practical limitation is of the order of 10 “heavy” atoms (i.e., all elements other than hydrogen) due to limitations in memory and computation time. Other *ab initio* methods such as W2 are even more restricted.

In the present database, a substantial effort was undertaken to replace as many as possible of the old version estimates based on additivity methods with new and significantly more accurate G3B3 values. However, many of the species in the database exceed the 10 heavy atom limit. For these bigger species, semi empirical methods (usually PM3 and sometimes AM1) were used to calculate vibrations and moments of inertia, and the enthalpies of formation had to be estimated by the additivity approach, as in earlier versions.

The present edition also started incorporating some of the values that are now available from Active Thermochemical Tables (*vide infra*).

### ***Ab initio* and other Calculations**

The G3//B3LYP (a.k.a. G3B3) calculations were performed using *Gaussian 03* package. The input to this program is prepared using Chem3D to initially construct and equilibrate the species, using sequentially the minimum energy conformation as obtained via Molecular Mechanics and MOPAC 2000 packages.

The G3B3 calculations were performed by explicit sequencing following the procedure of Baboul *et al.* (1999). Thus, the geometry of the species was optimized and its frequencies were calculated at B3LYP/6-31G(*d*) level. The

optimized geometry was subsequently used to perform single point computations at the QCISD(T)/6-31G(*d*), MP4/6-31+G(*d*), MP4/6-31G(2*df,p*), and MP2(full)/G3Large levels (with externally specified basis set in the latter step). The Gaussian output was harvested using a script that extracted the needed values, performed the prescribed arithmetic on the various components of the electronic energy, applied the appropriate higher-level corrections for molecular species and (separately) higher-level corrections and spin-orbit corrections for atoms, computed the zero-point energies from B3LYP frequencies scaled by 0.96, etc. The end-product of the script was a compact listing giving all the relevant components of the electronic energy and spectroscopic constants, as well as atomization energies at 0 K and enthalpies of formation at 0 K and 298.15 K. The atomization energy and enthalpies of formation was computed using standard enthalpies of formation of atoms and enthalpy increments for the elements in reference states (Cox *et al.*, JANAF, Gurvich *et al.*). The procedure was extensively tested beforehand by using it to reproduce a large sample of the values given by Baboul *et al.* (1999).

### **The Internal Rotation Problem**

Ideal gas values for the heat capacity, enthalpy increment, and entropy can be computed from the partition function if sufficient spectroscopic data (rotational constants, frequencies, and low-lying excited electronic states) are available. The rotational constants (i.e. geometry) and frequencies can be obtained with reasonable accuracy from various *ab initio* computations. However, unless the barrier happens to be available from experimental measurements, the contribution of hindered rotors is the one

that is the most difficult to obtain, unless one carries out additional computations along the internal rotor coordinate. Please note that the hindered rotor barrier is not explicitly obtained from G3B3 (and similar) type of computations of the lowest energy conformer. In order to, for example, convert the 0 K enthalpy of formation to the 298 K value, such methods use implicitly the pseudo-vibration approach for the internal rotor.

Aside from the pseudo-vibration approach, the most popular method for calculation of the rotation energy levels and wavefunctions of the internal rotation is by representing the hindered rotor potential via the expansion introduced by Lanne [Lewis *et al.* 1972], who used the six-term summation:

$$V = \frac{1}{2} \sum_{n=1}^6 V_n (1 - \cos n\phi) \quad (11)$$

Often the six terms can however be approximated by one term only (e.g.,  $V_3$  for a methyl rotor) even when the symmetry of the species would require more terms. The value of the single term is typically estimated by comparison to similar species for which such term is either known or already estimated by prior considerations. This shortcut is followed by many thermodynamicists due to the relatively small contribution of the internal rotation to the whole entropy value. This is however a potential point of error (having a tendency to affect the computed entropy somewhat more visibly than the corresponding enthalpy increment or heat capacity), and the user is warned about this simplification.

### Standard Enthalpies of Formation

Standard enthalpies ("heats") of formation of all species can be divided into three categories:

a) those that were experimentally measured either by combustion calori-

metry or by determining the enthalpy of a reaction involving the target (and other) species;

b) those estimated on the basis of experimental values of other (similar or related) compounds;

c) those estimated on the basis of other estimated compounds or structural groups. Standard enthalpies of formation are quoted and re-quoted by different authors, making it sometimes challenging to find out to which of the three categories the quoted  $\Delta_f H^\circ_{298}$  value belongs. When the measured values of individual compounds change with time due to better experimental systems or to errors found in previous measurements, it causes a need to change the  $\Delta_f H^\circ_{298}$  values whose determination or estimation was based on those values. However, there were no convenient means to perform these corrections other than tedious and continuous manual examination of each individual  $\Delta_f H^\circ_{298}$  value. The differences in the auxiliary values used to extract the enthalpy of formation of the species from the measured quantity are frequently at the core of disputes between groups of researchers claiming a different heat of formation for an important species. In this compilation, many decisions as to which value to adopt had to be done in the past arbitrarily for lack of established criteria.

These types of problems, together with other disadvantages connected to the traditional sequential approach to evolving enthalpies of formation, are being currently successfully addressed by the *Active Thermochemical Tables (ATcT)* approach [Ruscic, 2004, and Ruscic *et al.*, 2004], into which this database is now being integrated.

### Active Thermochemical Tables

Active Thermochemical Tables (ATcT) are a new paradigm that catapults

thermochemistry into the 21st century. As opposed to traditional sequential thermochemistry, ATcT provides reliable, accurate, and internally consistent thermochemistry by utilizing the Thermochemical Network (TN) approach.

The traditional approach is geared up to determine the enthalpies of formation of the target species using a sequential procedure. In this procedure, one and only one species is examined during each step. The available measurements (and/or computations) that link the target species to those (and only to those) determined in previous steps are examined. From these, the “best” determination (or, occasionally, the average of a few determinations that appear to be of similar quality) is selected and used to obtain the enthalpy of formation of the target species at one temperature. The spectroscopic data is then used to compute the temperature dependence of the enthalpy and the remaining complement of thermochemical functions pertinent to the target species. At that point the thermochemical properties of the target species are “frozen” and the procedure moves on to the next step, focusing on a new target species.

The primary disadvantage is that the resulting tabulation of enthalpies of formation stores for any species only the final value for the enthalpy, which is in reality connected to other enthalpies across the table via a maze of hidden progenitor-progeny relationships, making it next to impossible to update the resulting data with new information. Namely, even if, for example, a newly-measured bond dissociation energy is used to revise the enthalpy of formation of some species, there are generally other species in the table that are pegged to the old value and would also need to be

revised. Which those are is not clear without investing a very laborious manual effort that examines each and every species in the tabulation.

In addition, the uncertainties obtained in the traditional approach typically do not properly reflect the complete knowledge that was available at the time the tabulation was created. For example, some of the existing knowledge is simply ignored (or taken only as a secondary check) because it did not make it into the subset of “best” determinations. Since there is no feedback to values obtained in the previous steps, the relevant dependencies that are used in later steps in the procedure (and involve directly or indirectly the species that were determined in previous steps) do not contribute to the quantification of the uncertainties in earlier steps nor do they help improve the reliability of values that are already frozen. In short, available knowledge is used only partially.

As opposed to the sequential approach, ATcT are using the Thermochemical Network (TN) approach. The TN does not store enthalpies of formation of various species as such; rather, it stores the various relationships between the enthalpies as given by the actual measurements and/or computations, creating a network of thermochemical interdependencies. In order to obtain the desired enthalpies of formation, the TN is solved simultaneously for all the species it describes, producing a complete set of thermochemical values that are entirely mutually consistent. Furthermore, the dependencies stored in the TN are not based on the selected “best” subset of determinations. Rather, *all* available determinations from the literature are stored in the network. Since those are not necessarily self-consistent (because some of the quoted uncertainties are “optimis-



tic”, i.e., some determinations are not as correct as the uncertainty might imply, or, are, even in fact “wrong”), the TN solution is preceded by a statistical analysis and evaluation of the determinations that span and define the TN. The statistical evaluation of the determinations in the TN is made possible by redundancies in the TN, such as competing measurements of the same enthalpy of reaction, and/or alternate network pathways that interrelate the participating chemical species. The statistical analysis produces a self-consistent TN, from which the optimal thermochemical values are obtained by simultaneous solution in error-weighted space, thus allowing the best possible use of all knowledge present in the TN. This results in significantly better values than the traditional sequential approach, since it uses efficiently *all* the available knowledge and also relies on a statistical analysis. The significantly increased reliability and accuracy of the values obtained from the TN approach manifests itself through uncertainties (which are given as 95% confidence limits, as customary in thermochemistry) that are typically several times smaller than the equivalent sequential values that could be obtained by the traditional sequential approach.

On top of the dramatically improved reliability, accuracy, and consistency of the resulting thermo-chemical values, ATcT offer a number of features that are neither present nor possible in the traditional sequential approach. With ATcT, new knowledge can be painlessly propagated through all affected thermochemical values. Namely, a new measurement can be simply added to the TN, followed by the automatic analysis and solution of the TN, producing a new (revised) complement of thermochemical values for all the species present in the

network, thus fully propagating the consequences of the new measurement through all the affected values.

ATcT also allow hypothesis testing and evaluation, as well as discovery of weak links in the TN. The latter provides pointers to new experimental or theoretical determinations that will most efficiently improve the underlying thermochemical body of knowledge.

The knowledge base of ATcT is organized in a series of “Libraries”. The Main Library contains the Core (Argonne) Thermochemical Network that is currently being developed. At the moment (ver. 1.048), this TN contains fully networked data on > 600 species through > 3500 relevant determinations and is growing on a daily basis. Most of the initial species included in this TN are relatively small and play the role of “hubs” in the network (significantly overlapping with the notion of “key” CODATA species), but as the network grows, larger species are being introduced. Besides the TN, the Main Library also contains the relevant spectroscopic data for gas-phase species and tabular data for condensed-phase species that is needed to compute the heat capacity, enthalpy, increment, entropy, the temperature dependence of the enthalpy/Gibbs energy of formation, etc. As new data is introduced in the TN in the Main Library, a new set of solutions of the TN is periodically computed, producing a new version and storing the prior version into the archives (following an elaborate archival system).

Auxiliary libraries (e.g. CODATA Library, Gurvich Library, JANAF Library, etc.) are more static in nature and contain non-networked data needed to reproduce the values in various historical tabulations for ready-reference purposes.

We are currently undertaking the effort of assimilating the present database as one of the auxiliary ATcT Libraries. Though not containing networked data *per se*, the special feature of this Library will be the ability of getting an automatic update whenever new and/or better information is available through ATcT. Specifically, each time a new solution is obtained from the networked data in the Main Library, the relevant species in this database will be also updated.

At the current stage of its development, the Core (Argonne) Thermochemical Network of ATcT is still concentrating on defining as accurately as possible various “key” (typically small) species and their ions. Consequently, the overlap with the present database is modest. This will, however, gradually change as the ATcT TN grows.

In anticipation of the full merger with automatic update capabilities, some of the values in this database have been manually replaced by the new ATcT values using the ATcT kernel ver. 1.25 and the Core (Argonne) Thermochemical Network ver. 1.048. Whenever the difference between the ATcT and the prior value of the enthalpy of formation was larger than ~1 kJ/mol (or if it was a new species that was not contained in the previous edition of this database), a new polynomial was calculated. In view of the laborious effort involved in manually updating the polynomials, and in anticipation of the development of fully automatic updates, when the difference was smaller than ~1 kJ/mol, the ATcT value was simply added to the comments preceding the polynomial, but the existing polynomial was kept unchanged.

#### Accuracy of Enthalpies of Formation

Though barely at its beginning, ATcT has already produced for a number of “key”

species significantly more accurate thermochemical values, thus considerably increasing the number of species known to very high accuracy. Nevertheless, in general, only a small minority of species of interest in combustion can be assigned standard enthalpies of formation with uncertainty limits so narrow that for combustion modeling purposes they may be taken to be exact (Cox *et al.*, 1989; Cox and Pilcher 1970; Cohen 1996). The most accurately known of all (aside from, of course, the elements in their reference states, for which the value 0 is defined to be exact) are those based on carefully recorded molecular electronic spectra supplemented by quantum-mechanical analysis. Among those the hydrogen atom stands out, and a few diatomic and triatomic species whose electronic spectra have been successfully analyzed to accurately establish the dissociation limit also belong in the exact category. An overview of the uncertainties of the standard enthalpies of formation of the key combustion-relevant atomic to

Table 1. Standard enthalpies of formation in kJ/mol at 298.15 K for small gas-phase species of interest in combustion. (All species from Active Thermochemical Tables v 1.25 using C(A)TN v. 1.048, except the sulfur species which are from the NASA database.)

Species	$\Delta_f H_{298}$
C(g)	717.065 ± 0.146
H(g)	217.997 ± 0.0001
O(g)	249.229 ± 0.002
N(g)	472.459 ± 0.044
S(g)	277.17 ± 0.25
Cl(g)	121.302 ± 0.001
NO(g)	91.097 ± 0.084
CO(g)	-110.538 ± 0.026
H <sub>2</sub> O(g)	-241.815 ± 0.031
CO <sub>2</sub> (g)	-393.472 ± 0.014
SO <sub>2</sub> (g)	-296.84 ± 0.21
NO <sub>2</sub> (g)	34.025 ± 0.085

triatomic species that have been exhaustively studied by calorimetric and spectroscopic methods is given in Table 1. One sees that the accuracy benchmark set by this group of species (in effect setting a standard of what can be achieved in measuring or computing standard enthalpies of reaction) is in the vicinity of 0.1 to 0.2 kJ/mol.

It should be noted that the new ATcT values are expected to bring about significant overall improvements in the accuracy and reliability of the available thermochemistry. However, keeping in mind the present extent of the Core (Argonne) Thermochemical Network that is currently under development, the majority of species currently covered in this database are not (as yet) available through the TN approach, and their values come from traditional sources. Here we would like to make a few cautionary comments on the state of affairs with respect to traditional sources.

Overall, the number of species important in combustion for which experimental values of standard enthalpies of formation can be assigned is comparably small. All are based on chemical reactions to which enthalpy changes of reaction can be assigned with high accuracy either calorimetrically or from the temperature dependence of equilibrium constants. As far as stable molecules of the elements carbon, hydrogen, oxygen and nitrogen are concerned, it is fortunate that combustion reactions themselves serve for this purpose, as the standard enthalpies of formation of the combustion products. Carbon dioxide and water have been painstakingly evaluated and reactions can usually be arranged to occur with accurately measured stoichiometry (Cox and Pilcher, 1970).

Even in the most favorable cases, however, the error bounds that have to be

accepted are larger than one would wish. This is illustrated in Table 2, adapted from Cohen and Benson (1992), who give references to the archival literature. Here one sees that the “best available” standard enthalpy of formation values for the small hydrocarbons come with error ranges that imply significant uncertainty in equilibrium constants. (A  $\pm 1$  kJ/mol uncertainty in the enthalpy or Gibbs energy change of a reaction at 1000 K implies an uncertainty of  $\pm 12$  % in its equilibrium constant.)

Table 2. Standard enthalpies of formation in kJ/mol at 298.15 K for small hydrocarbons (After Cohen and Benson, 1992).

Species	Bomb Calorimeter	Flame Calorimeter
CH <sub>4</sub>	-74.85 $\pm$ 0.29	-74.48 $\pm$ 0.42
C <sub>2</sub> H <sub>6</sub>	-84.68 $\pm$ 0.50	-83.85 $\pm$ 0.29
C <sub>3</sub> H <sub>8</sub>	-103.89 $\pm$ 0.59	-104.68 $\pm$ 0.50
n-C <sub>4</sub> H <sub>10</sub>	-127.03 $\pm$ 0.67	-125.65 $\pm$ 0.67
i-C <sub>4</sub> H <sub>10</sub>	-135.60 $\pm$ 0.54	-134.18 $\pm$ 0.63

Not only are the uncertainty ranges asserted by the evaluators larger than one would wish, the differences between the values obtained with the two most trustworthy calorimetric techniques are seen on close inspection to differ from one another by more than the sum of the stated uncertainty ranges for three of the five cases. Aside from these discrepancies (which can now be successfully treated and resolved via the TN analysis of ATcT), the asserted uncertainty ranges are about twice as large as for the values listed in Table 1. The values are less well known for most of the other stable species of interest in combustion, and still less well known for unstable ones. Among the unstable species, the thermochemistry of free radicals has attracted particular interest in

combustion modeling because of their roles as chain centers.

An overview of current knowledge of the standard enthalpies of formation of some of the common ones is given in Table 3. In contrast to the stable hydrocarbons, where the standard enthalpy of formation is based on one or another of the direct calorimetric methods, values for radicals come from all sorts of very difficult measurements ranging from photoionization mass spectroscopy to reaction rates. It is no surprise that the results are more contentious and less accurate. In Table 3, the uncertainty ranges can be seen to be typically an order of magnitude greater than for stable hydrocarbon values except where the Active Table can help.

For hydrocarbons and their various derivatives containing oxygen and nitrogen atoms, a long history of thermochemical investigation has left a legacy of experimental standard enthalpy of formation values. (Some 3000 have been compiled by Pedley *et al.*, 1986).

The uncertainty level of this legacy varies considerably because of the fluctuating care given to the (mostly) calorimetric measurements and problems of reagent purity and reaction stoichiometry. From early on there have been successful efforts to systematize the database in terms of molecular structure (Reviewed in detail by Cox and Pilcher, 1970). As a result, one can compute a standard enthalpy of formation value for "ordinary" compounds that have not been studied experimentally with almost the same confidence that one can place in the experimental values themselves. A large number of entries in the present tabulation have been derived by the NIST or THERM group additivity programs that offer current embodiments of this idea. The capabilities and limitations of

Table 3. Standard enthalpies of formation in kJ/mol at 298.15 K for common radicals. Values accepted by the IUPAC Task Force for Thermochemistry of Radicals of Relevance in Combustion and Atmospheric Chemistry, 2005.

Species	$\Delta_f H_{298}$
OH(g)	37.34 $\pm$ 0.04
CH(g)	596.30 $\pm$ 0.25
CN(g)	438.81 $\pm$ 0.52
NH(g)	358.76 $\pm$ 0.37
SH(g)	141.87 $\pm$ 0.52
CH <sub>2</sub> OH(g)	-17.18 $\pm$ 0.37
CH <sub>3</sub> O(g)	20.257 $\pm$ 0.42
HO <sub>2</sub> (g)	12.296 $\pm$ 0.25
CHO(g)	42.296 $\pm$ 0.3
CH <sub>2</sub> (g)	391.465 $\pm$ 0.27
CH <sub>3</sub> (g)	146.582 $\pm$ 0.1
C <sub>2</sub> O(g)	291.04 $\pm$ 63
C <sub>2</sub> H(g)	568.06 $\pm$ 0.31
C <sub>2</sub> H <sub>3</sub> (g)	296.61 $\pm$ 0.92
C <sub>2</sub> H <sub>5</sub> (g)	118.66 $\pm$ 2
C <sub>3</sub> H <sub>3</sub> (g)	339 $\pm$ 4
C <sub>3</sub> H <sub>5</sub> (g)	171 $\pm$ 3
<i>n</i> -C <sub>3</sub> H <sub>7</sub> (g)	101.32 $\pm$ 1
<i>i</i> -C <sub>3</sub> H <sub>7</sub> (g)	90.19 $\pm$ 2
C <sub>6</sub> H <sub>5</sub> (g)	339.7 $\pm$ 2.5

group additivity methods for stable organic molecules have been reviewed by Pedley *et al.*, (1986) and Cohen (1996); discussions of the issues involved in making group additivity estimates for radicals are given by Muller *et al.*, (1995) and Lay *et al.*, (1995).

Unfortunately, many of the most interesting molecules and radicals used in combustion modeling are not ordinary at all, but have highly strained rings or electronic structures that are not well represented in the experimental database used for setting group additivity parameters. For such molecules and radicals we recommend to abstain from use of the group additivity methods anyway, and to prefer instead *ab initio*

calculations or, if that appears infeasible, as in case of big species, semi-empirical or semi-theoretical molecular electronic structure calculations.

Since the enthalpies of formation seem to be the most problematic of all the thermochemical values, Table 6 is dedicated to this quantity, where we stress the errors if available. In Table 4 we mention additional values for some species in curled parenthesis.

### **Accuracy of Partition-Function Related Thermochemical Values**

As in all thermochemical compilations, the species properties were calculated with varying degrees of accuracy. Some of the species, such as the element  $N_2$  or the molecule HD, were calculated using very high accuracy methods, while others were calculated using approximation methods.

The rigid-rotor-harmonic-oscillator (RRHO) approximation method was accepted as the standard for polyatomic species, and widely adopted by JANAF, TSIV, Thermodynamic Research Center, Stull, Westrum and Sinke (1969) compilations, and many others. Where applicable, this method was augmented by supplementary internal rotation or other contributions as used by various authors. These calculations are considered here as "accurate" values.

The extrapolation methods used, either Wilhoit or Ritter and Bozzelli, were found to give generally good results, and their maximum deviation from standard RRHO calculations for  $C_p(T)$  is usually below 0.5%. The errors, however, are greater for estimated species. It is assumed that the parent molecule method used for estimation of radical species by the authors (Burcat 1982, Burcat *et al.*, 1979, 1983, 1985) has a maximum error of  $\pm 3\%$  for  $C_p(T)$  while Benson's group

property method used by Stein and Ritter and Bozzelli gives a maximum error for unknown species which is in the  $\pm 8\%$  range for  $\Delta_f H_{300}$ . These are maximum values, and for most cases the errors are by far lower (see Reid, Prausnitz and Poling, 1988, p. 196).

The G3B3 method was assigned a standard error value of  $\pm 8$  kJ/mol which is twice the value of the mean absolute deviation (MAD) for this method, quoted as slightly less than 1 kcal/mol by Baboul *et al.*, (1999).

It should be emphasized that the accuracy of the fit given by the coefficients tabulated on the Internet varies considerably from one species to the next. For essentially all purposes in combustion modeling, however, the accuracy of the polynomials with these coefficients is much better than the uncertainties of the modeling introduced by other sources.

The accuracy by which the given polynomials represent the original calculated tabular values is given, where pertinent, in the header preceding the polynomial. This accuracy value is given in terms of the maximal error among the three fitted properties,  $C_p$ , entropy and absolute enthalpy.  $C_p$  has in most cases the maximal error, and the temperature at which this error was found is given. A large fitting error usually indicates that the underlying tabulated values were not smooth.

Because of different machine round-offs, word lengths, and values of constants used, it is only seldom that the exact original values calculated by the authors are reproduced by a different user. Accuracy in the reproduction of the original values from polynomials can be improved if double precision computation is used (on other than 64 bit word machines), and if the polynomial is

calculated in the recursive form such as:

$$CP = (((A5 * T + A4) * T + A3) * T + A2) * T + A1 \quad (12)$$

### Critical Evaluation of the Polynomials

The thermodynamic data represented by the polynomials were critically evaluated according to their quality aside from the value of the standard enthalpy of formation  $\Delta_f H^\circ_{298}$  that was assigned to the species, which must be evaluated separately as explained above. Five groups were identified and marked **A** to **F**.

**A** designates the most accurate calculations and is reserved for the 'direct summation' method, for diatomic molecules and non-rigid-rotor-anharmonic-oscillator (NRRAO) approximations for which anharmonicity corrections were included.

**B** denotes regular RRHO approximation calculations, including internal rotations where pertinent and/or other electronic excitations. The 'parent' method for the approximation of radicals is included in this category.

**C** includes species whose thermodynamic properties were calculated by the RRHO method but some shortcuts were taken. RRHO calculations with estimated vibrational frequencies are included in this category, as are cases where the internal rotor was neglected and a free rotor was used instead. Some of the data originating with TRC/API tables are considered in this category, since the way they were calculated is not clear.

**D** and **E** categories were reserved for data estimated from group contributions. The normal estimated species were included in the **E** group, while if additional experimental information was used, then the **D** label was assigned.

The **F** category is reserved for

very rough approximations using Benson's additivity groups or other types of estimations with very large error limits.

### Ion Conventions

Unfortunately, there are two different conventions for expressing the enthalpies of formation of ions. One is the "thermal electron" convention, the other the "stationary electron" convention. In the "thermal electron" convention, the enthalpy increment  $H_T - H_0$  of the "electron gas" is equal to  $2.5 RT$ , while in the "stationary electron" convention the enthalpy increment is zero at all temperatures. This choice affects the enthalpies of formation and the Gibbs energies of formation of all ions, but not the other quantities, such as entropies.

For historical reasons, this database adheres to the "thermal electron" convention, which is also the convention adopted by the JANAF Tables, the NBS Tables, and the Gurvich Tables.

Please note that most ion chemists use the "stationary electron" convention, as does the compilation of ion thermochemistry of Lias *et al.* (and hence also the NIST WebBook, which implicitly uses the values for ions from Lias *et al.*, though they are seldom given explicitly). Please also note that commingling values from the two conventions results in serious errors. Hence, it is essential to have the values for all charged species expressed within the same convention. As long as all values that are combined to compute the thermochemistry of a chemical reaction are within the same convention, the resulting enthalpies of reactions, Gibbs energies of reactions, equilibrium constants, etc. are the same in both conventions, except when the "electron gas" (which is treated differently in the two conventions) is explicitly involved as one of the reactants

or products. (Parenthetically, ATcT can work under either convention, though the default is the “stationary convention” preferred by ion chemists.)

The conversion of enthalpies of formation from one convention to the other is quite trivial. At 0 K, the enthalpies of formation are identical in both conventions. At any other temperature, the value for the enthalpy of formation belonging to the “stationary electron” convention can be converted to the value belonging to the “thermal electron” convention by adding the quantity  $q \times 2.5RT$  ( $= q \times 6.197$  kJ/mol at 298.15 K), where  $q$  is the charge of the ion:

$$\Delta_f H_T^{\text{thermal.conv.}}(\text{ABC}^{+q}) = \Delta_f H_T^{\text{station.conv.}}(\text{ABC}^{+q}) + q 2.5 RT \quad (13)$$

$$\Delta_f H_T^{\text{thermal.conv.}}(\text{ABC}^{-q}) = \Delta_f H_T^{\text{station.conv.}}(\text{ABC}^{-q}) - q 2.5 RT$$

For example,  $\Delta_f H_{298}(\text{H}^+) = 1530.047$  kJ/mol under the “stationary electron” convention. Adding 6.197 kJ/mol produces 1536.244 kJ/mol, which is the correct 298.15 K value under the “thermal electron” convention, as used in this database. Similarly,  $\Delta_f H_{298}(\text{H}^-) = 145.228$  kJ/mol under the “stationary electron” convention. Subtracting 6.197 kJ/mol (since the charge is -1) produces 139.031 kJ/mol, which is the correct value under the “thermal electron” convention.

### What is New in the Present Edition

The present version of the database has several new features, beside an increased number of species and the replacement of about 200 E and F species (see above) with more accurate and reliable data. Unpublished data from *Active*

*Thermochemical Tables* (ATcT) ver. 1.25 using the Core (Argonne) Thermochemical Network ver. 1.048 have been included where available.

An additional separate database was initiated (Table 5) to contain NASA 9 coefficient polynomials, and to serve as an enlargement of the original NASA database of Bonnie McBride (<http://cea.grc.nasa.gov>). This database contains polynomials with three temperature intervals but unlike the NASA polynomials, these intervals are 50-200 K, 200-1000 K, and 1000-6000 K. Therefore these can serve for low temperature calculations.

In the main database Table 4 (file burcat.thr) the CAS (Chemical Abstracts) species identification number was added to all species where available.

In the index table Table 6 (hf.doc) we have added the value of  $\Delta_f H_0$  besides  $\Delta_f H_{298}$  and also the value of  $H_{298} - H_0$ .

An important addition to the database is a program written by R. Pinzon and E. Burcat in Phyton (2.4 #60), which allows automatic extraction of data from the main file (burcat.thr) including the data in the header of the polynomial species into an XML file. The XML file produced from our database presented in this printed edition is available via the Net.

### Species not Included in this Database

About 1300 species were included in this compilation. Finding species not included in the compilation may be a tough task.

A) If you are looking for a simple hydrocarbon, paraffin, olefin, or a cyclic specie, there are good chances to find it if it has less than 20 carbon atoms in either the TRC (Thermodynamics Research Center) compilation or in the old Stull, Westrum and Sinke (1969) book. Additional sources are the articles

appearing periodically in the Journal of Physical and Chemical Reference Data.

B) If you are looking for a more complex specie or a radical, the available sources are the computerized databases of NIST Structures and Properties Database # 25 ver 2.0 1994, and the WebBook (Afeefy *et al.*), or periodic articles in the literature. There exists a database of molecular properties by Carl Melius that includes 3700 species. Many of these species are transition states. The Melius thermochemical tables are not available to the public, and only limited thermochemical information ( $\Delta_f H_{300}$  and  $\Delta_f G_{300}$ ) was published with his molecular structure data. The published thermochemical values calculated with the 1987 BAC/MP4 method are of low reliability.

C) For a solid or liquid species (not ideal gas) like  $\text{CaSO}_4$  the place to look for is the JANAF compilation or the Barin (1995) compilation or the report of McBride, Gordon and Reno, NASA TM 4513 (1993).

D) Silicon containing species can be found in the CHEMKIN database (Kee *et al.*, (1992)). Sandia has initiated a database by M. Allendorf that includes presently Al, B, Si and Sn species calculated with the BAC/MP4 method. Other organometalic species of Ga and As can be found in an article by Tirtowidjojo and Pollard (1986).

E) Ion of simple bi- and triatomic species can be found in JANAF. The other compilation that mentions  $\Delta_f H_{298}$  for ion species for some of the molecules and radicals included, is the above mentioned NIST S and P #25 computerized database (1994). The information therein was taken from Lias *et al.*, Journal of Physical and Chemical Reference Data, Vol. 17, (1988), Supplement # 1.

## Conversion Factors

The following conversion factors were used in the present compilation:

$$1 \text{ cal} = 4.184 \text{ J}$$

$$R = 8.314472 \text{ J mol}^{-1} \text{ K}^{-1}$$

$$R = 1.987207 \text{ cal mol}^{-1} \text{ K}^{-1}$$

$$1 \text{ eV} = 23.06055 \text{ kcal mol}^{-1}$$

$$1 \text{ eV} = 8065.537 \text{ cm}^{-1}$$

$$1 \text{ kcal/mol} = 349.7547 \text{ cm}^{-1}$$

$$1 \text{ cm}^{-1} = 2.859146 \text{ cal mol}^{-1}$$

$$1 \text{ cm}^{-1} = 29.9792458 \text{ GHz}$$

$$1 \text{ Hartree} = 627.5101 \text{ kcal mol}^{-1}$$

$$1 \text{ Hartree} = 2625.502 \text{ kJ mol}^{-1}$$

$$1 \text{ Bohr} = 0.5291772 \text{ \AA}$$

$$1 \times 10^{-39} \text{ g cm}^2 = 21.50545 \text{ amu Bohr}^2$$

$$1 \times 10^{-39} \text{ g cm}^2 = 6.022137 \text{ amu \AA}^2$$

$$\text{B/cm}^{-1} = 60.19969/[\text{I}_\text{B}/(\text{amu Bohr}^2)]$$

$$\text{B/cm}^{-1} = 16.85763/[\text{I}_\text{B}/(\text{amu \AA}^2)]$$

$$\text{B/cm}^{-1} = 2.799277/[\text{I}_\text{B}/(10^{-39} \text{ g cm}^2)]$$

## Electronic Files

Updated version of the database in ASCII form (BURCAT.THR), is available for free downloading from:

<ftp://ftp.technion.ac.il/pub/supported/aetd/thermodynamics>.

The site is mirrored daily by:

<http://garfield.chem.elte.hu/Burcat/burcat.html>

Transfer the file to your computer using download, or browse through it with your web browser.

Two table generator programs CAP and CAPOLD written by B. McBride are included, to enable generation of thermodynamic properties from the given nine term and seven term polynomials, respectively. The tables generated provide values of  $C_p$ ,  $S$ ,  $H_T - H_{298}$ ,  $-(G_T - H_{298})/T$  and  $H_T$  as a function of  $T$ . Values of  $\Delta_f H_T$  and  $\log K_c$  can be added at any temperature interval within the polynomial's given limit.

A special file called THERM.DAT contains the file burcat.thr stripped of all comments, to be used with



CHEMKIN and similar programs.

Finally an XML version of the main database (Table 4) is included for the researcher's convenience.

The present database is free for use for non-commercial purposes on condition that proper quotation is given to its source. The database cannot be used for commercial purposes without a written agreement from the authors.

### Journal Abbreviations found in the Database Tables

JCP = *J. Chem. Phys.*

JOC = *J. Org. Chem.*

JPC = *J. Phys. Chem.*

JPC A = *J. Phys Chem. A*

JPCRD = *J. Phys. Chem. Ref. Data*

JTC = *J. Theoret. Chem.*

### References

H.Y. Afeefy, J.F. Liebmann, and S.E. Stein, *Neutral Thermochemical Data*, in: *NIST Standard Reference Database Number 69*, Eds. P.J. Linstrom and W.G. Mallard, NIST, Gaithersburg, MD  
<http://webbook.nist.gov/chemistry>

M. Allendorf, *High Temperature Gas Phase Thermochemical Database*, Combustion Research Facility, Sandia National Laboratories, Livermore, CA  
<http://www.ca.sandia.gov/HiTempThermo/index.html>

*API Project 44*: see F.D. Rossini

A.G. Baboul, L.A. Curtis, P.C. Redfern, and K. Raghavachari, *J. Chem Phys.* **110**, 7650 (1999).

I. Barin, *Thermodynamic Data of Pure Substances*, 3<sup>rd</sup> Ed., VCH, Weinheim, Germany (1995).

I. Barin and O. Knacke, *Thermodynamic Properties of Inorganic Substances*, Springer, Berlin (1973).

A.D. Becke, *J. Chem. Phys.* **98**, 5648 (1993).

S.W. Benson, *Thermochemical Kinetics*, Wiley, New York (1976).

S.W. Benson, *Chem. Rev.* **78**, 23 (1978).

J. Berkowitz, G.B. Ellison, and D. Gutman, *J. Phys. Chem.* **98**, 2744 (1994).

M. Berthelot *Thermochimie*, Vols. 1 and 2, Gauthier-Villars, Paris (1897).

F.R. Bichowsky and F.D. Rossini, *The Thermo-chemistry of the Chemical Substances*. Reinhold, New York (1936).

U. Brinkmann and A. Burcat, *A Program for Calculating the Moments of Inertia of a Molecule*. TAE Report No. 382, Technion, Haifa (1979).

A. Burcat and S.A. Kudchadker, *Acta Chimica Hung.* **101**, 249 (1979).

A. Burcat, *Ideal Gas Thermodynamic Functions of Hydrides and Deuterides. Part I*, TAE Report No. 411, Technion, Haifa (1980).

A. Burcat, *Ideal Gas Thermodynamic Properties of C<sub>3</sub> Cyclic Compounds, Part II*, TAE Report No. 476, Technion, Haifa (1982).

A. Burcat, D. Miller, and W.C. Gardiner, *Ideal Gas Thermodynamic Properties of C<sub>2</sub>H<sub>n</sub>O Radicals, Part III*, TAE Report No. 504, Technion, Haifa (1983).

A. Burcat, F.J. Zeleznik, and B. McBride, *Ideal Gas Thermodynamic Properties of Phenyl, Deuterated Phenyl, Phenoxy and o-Biphenyl Radicals*. NASA TM-83800, NASA, Cleveland, OH (1985).

A. Burcat, *Thermochemical Data for Combustion Calculations*, Chapt. 8 in:

*Combustion Chemistry*, W.C. Gardiner, Ed., Springer-Verlag, New York (1984).

A. Burcat, *Ideal Gas Thermodynamic Data for Buckminsterfullerene C<sub>60</sub> and C<sub>70</sub>*, TAE Report No 680, Technion, Haifa (1984).

A. Burcat, *Ideal Gas Thermodynamic Properties of Propellants and Explosive Compounds*, *AIAA J. Propul. and Power* **16**, 105 (2000).

A. Burcat, *Thermodynamic Properties of Ideal Gas Nitro and Nitrate Compounds*, *J. Phys. Chem. Ref. Data* **28**, 63 (1999).

A. Burcat, L. Khachatryan, and B.L. Dellinger, *Thermodynamics of Chlorinated Phenols, Polychlorinated Dibenzo-p-Dioxins, Polychlorinated Dibenzofurans and Intermediate Species*, *J. Phys. Chem Ref. Data* **32**, 443 (2003).

M.W. Chase, C.A. Davies, J.R. Downey, Jr., D.J. Frurip, R.A. McDonald, and A.N. Syverud, *JANAF Thermochemical Tables*, 3<sup>rd</sup> Ed.; *J. Phys. Chem. Ref. Data* **14**, Suppl. 1 (1985)

M.W. Chase, Jr., Ed., *NIST-JANAF Thermochemical Tables*, 4<sup>th</sup> Ed.; *J. Phys. Chem. Ref. Data* **14**, Monogr. 9 (1998)

*Chem3D*, a program suite for molecular modeling and display with semiempirical calculations built, CambridgeSoft Corporation, Cambridge, MA.

*CHEMKIN*, a program originally written in 1982 by R.J. Kee and J.A. Miller at Sandia National Laboratories. Livermore, CA; currently developed, and marketed by Reaction Design, San Diego, CA.

Y. Chen, A. Rauk, and E. Tschuikow-Roux, *J. Chem. Phys.* **93**, 1187 (1990).

N. Cohen, *J. Phys. Chem.* **96**, 9052 (1997).

N. Cohen, *J. Phys. Chem. Ref. Data*, **25** 1411 (1996).

N. Cohen and S.W. Benson, Chap. 6 in: *The Chemistry of Alkanes and Cycloalkanes*, S. Patai and Z. Rappaport, Eds., Wiley, New York (1992)

J.D. Cox and G. Pilcher, *Thermochemistry of Organic and Organometallic Compounds*, Academic Press, London (1970).

J.D. Cox, D.D. Wagman, and V.A. Medvedev, *CODATA Key Values for Thermodynamics*, Hemisphere, New York (1989).

H. Curran, C. Wu, N. Marinov, W.J. Pitz, C. K. Westbrook, and A. Burcat, *The Ideal gas Thermo-dynamics of Diesel Fuel Ingredients. I. Naphthalene Derivatives and their Radicals*. *J. Phys. Chem. Ref. Data* **29**, 463 (2000).

L.A. Curtis, K. Raghavachari, P.C. Redfern, V. Rassolov, and J.A. Pople, *J. Chem Phys.* **109**, 7764 (1998)

L.A. Curtis, P.C. Redfern, K. Raghavachari, V. Rassolov, and J.A. Pople, *J. Chem Phys.* **110**, 4703 (1999).

E. S. Domalski and E. D. Hearing, *Estimation of the Thermodynamic Properties of Hydrocarbons at 298.15 K*, *J. Phys. Chem. Ref. Data* **17**, 1637 (1988).

O.V. Dorofeeva, L.V. Gurvich, and V.S. Jorish, *J. Phys. Chem. Ref. Data* **15**, 437 (1986).

O.V. Dorofeeva and L.V. Gurvich, *Thermodynamic Properties of Polycyclic Aromatic Hydrocarbons Containing 5 Membered Rings*, USSR Academy of Sciences, Institute for High Temperatures, IVTAN Preprint # 1-263 (1989) (in Russian).

O.V. Dorofeeva and L.V. Gurvich, *J. Phys. Chem. Ref. Data* **24**, 1351 (1995).

R.E. Duff and S.H. Bauer, *The Equilibrium Composition of the C/H/ System at Elevated*

*Temperature*, Los Alamos Report 2556 (1961).

R.E. Duff and S.H. Bauer *J. Chem. Phys* **36**, 1754 (1962).

D.J. Frurip, E. Freedman, and G.R. Hertel, *A.S.T.M. CHETAH program for Hazard Evaluation*, version for mainframe and personal Computer, *Plant/Operations Progress* **8**, #2 (1989).

*GAMESS* (General Atomic and Molecular Electronic Structure System), M.W. Schmidt, K.K. Baldridge, J.A. Boatz, S.T. Elbert, M.S. Gordon, J.H. Jensen, S. Koseki, N. Matsunaga, K.A. Nguyen, S. Su, T.L. Windus, M. Dupuis, J.A. Montgomery *J. Comput. Chem.*, **14**, 1347 (1993).

*Gaussian 03*, Rev. B.02,

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Pittsburgh PA, 2003.

S. Gordon, F. Zeleznik, and V.N. Huff, *A general method for automatic computation of Equilibrium Composition and Theoretical*

*Rocket Performance of Propellants*, NASA TN D-132 (1959)

J.S. Gordon, *Thermodynamic Data for Combustion Products*, REP RMD 210-E3, Thiokol Chem. Corp. (1960)

L.V. Gurvich, *Thermodynamic Properties of Individual Substances* (TSIV), 3<sup>rd</sup> Ed., Vols. 1, 2, 3, and 4, Nauka, Moskva (1978, 1979, 1981, 1982) (in Russian)

L.V. Gurvich, I.V. Veyts, and C.B. Alcock, *Thermodynamic Properties of Individual Substances*, 4<sup>th</sup> Ed. Vols. 1 and 2, Hemisphere, New York (1989, 1991), Vol. 3, Begell House, New York (1996).

V.N. Huff, S. Gordon, and V. Morrell, *General Method and Thermodynamic Tables for Computation of Equilibrium Composition and Temperature of Chemical Reactions*, NASA Report 1037 (1951).

E.W. Washburn, Ed., *International Critical Tables*, Vols I-VII, McGraw-Hill, New York (1926-1930).

M.E. Jacox, *Ground State Vibrational Energy Levels of Polyatomic Transient Molecules*, *J. Phys. Chem. Ref. Data* **13**, 945 (1984).

M.E. Jacox, *Electronic Energy Levels of Small Polyatomic Transient Molecules*, *J. Phys. Chem. Ref. Data* **17**, 269 (1988).

M.E. Jacox, *Rotational and Electronic Energy Levels of Polyatomic Transient Molecules, Supplement 1*, *J. Phys. Chem. Ref. Data* **19**, 1387 (1990).

M.E. Jacox, *Vibrational and Electronic Energy Levels of Polyatomic Transient Molecules*, *J. Phys. Chem. Ref. Data*, Monogr. 3 (1994)

M.E. Jacox, *Vibrational and Electronic Energy Levels of Polyatomic Transient Molecules, Supplement A*, *J. Phys. Chem. Ref. Data*, **27**, 115 (1998)

M.E. Jacox, *Vibrational and Electronic Energy Levels of Polyatomic Transient Molecules, Supplement B*, *J. Phys. Chem. Ref. Data*, **32**, 1 (2003)

*JANAF Tables*: see M.W. Chase

M. Karni, I. Oref, and A. Burcat, *Ab-Initio Calculations and Ideal Gas Thermodynamic Functions of Cyclopentadiene and Cyclopentadiene Derivatives*, *J. Phys. Chem. Ref. Data* **20**, 665 (1991).

R.J. Kee, F.M. Rupley, and J.A. Miller, *The Chemkin Thermodynamic Database*, Sandia Report SAND87-8215B UC-4 (1992).

V.P. Kolesov and T.S. Papina, *Russ. Chem. Rev.* **52**, 754 (1983).

R. Lanzfame and M. Messina, *V Order Logarithmic Polynomials for Thermodynamic calculations in IC*, *Progr. SI and Diesel Engine Modeling*, SAE SP-1625 (ISBN: 0-7680-0789-5), SAE paper 2001-01-1912.

T.H. Lay, J.W. Bozzelli, A.M. Dean, and E.R. Ritter, *J. Phys. Chem.* **99**, 14514 (1995).

C. Lee, W. Yang, and R.G. Parr, *Phys. Rev. B* **37**, 785 (1988).

G.N. Lewis and M. Randall, *Thermodynamics*, McGraw-Hill, New York (1923).

J.D. Lewis, T. B. Malloy, Jr., T.H. Chao, and J. Laane *J. Mol. Struct.* **12**, 427 (1972).

S. G. Lias, J. E. Bartmess, J. F. Liebman, J. L. Holmes, R. D. Levin, and W. G. Mallard, *Gas-Phase Ion and Neutral Thermochemistry*, *J. Phys. Chem. Ref. Data* **17**, Suppl. 1 (1988)

M.M. Mallard and H. Le Chatelier, *Ann. Mines* **4**, 274 (1883); *ibid*, **4**, 379 (1883)

J.E. Mayer and M.G. Mayer *Statistical Mechanics*, Wiley, New York (1940).

B. J. McBride, S. Heibel, J. G. Ehlers, and S. Gordon, *Thermodynamic Properties to 6000*

*K for 210 Substances Involving the First 18 Elements*. NASA-SP-3001 (1963).

B.J. McBride and S. Gordon, *FORTAN IV Program for Calculation of Thermodynamic Data*, NASA TN-D 4097 (1967).

B.J. McBride and S. Gordon, *Computer Program for Calculating and Fitting Thermodynamic Functions*, NASA RP 1271 (1992).

C. Melius, a database of 3700 species calculated by the BAC/MP4 method, Sandia National Laboratories (1993-1997).  
<http://z.ca.sandia.gov/~melius/index.html>

*MOLPRO* is a package of *ab-initio* programs designed by H.-J. Werner and P. J. Knowles; the authors are H.-J. Werner, P. J. Knowles, M. Schütz, R. Lindh, P. Celani, T. Korona, G. Rauhut, R. D. Amos, A. Bernhardsson, A. Berning, D. L. Cooper, M. J. O. Deegan, A. J. Dobbyn, F. Eckert, C. Hampel, G. Hetzer, A. W. Lloyd, S. J. McNicholas, F. R. Manby, W. Meyer, M. E. Mura, A. Nicklass, P. Palmieri, R. Pitzer, U. Schumann, H. Stoll, A. J. Stone R. Tarroni, and T. Thorsteinsson.

C. Muller, V. Michel, G. Scacchi, and G.M. Come, *THERGAS: a computer program for the evaluation of thermochemical data of molecules and free radicals in the gas phase* *J. Chim. Phys.* **92**, 1154 (1995).

*NBS Tables*: see D.D. Wagman

*NBS TN 270*: see D.D. Wagman

*NBS Circular 500*: see F.D. Rossini

K.M. Pamidimukkala, D. Rogers, and G.B. Skinner, *J. Phys. Chem. Ref. Data* **11**, 83 (1982).

G.S. Parks and H.M. Huffman, *The Free Energies of Some Organic Compounds*, Monograph # 60, Chemical Catalog Co, New York (1932).

J.B. Pedley and J. Rylance, *Computer Analysed Thermochemical Data: Organic and Organometallic Compounds*, University of Sussex, Brighton, England (1977).

J.B. Pedley, R.D. Naylor, and S.P. Kirby, *Thermochemical Data of Organic Compounds*, 2<sup>nd</sup> Ed., Chapman and Hall, London (1986).

*Project 44*: see F.D. Rossini

Python 2.4 (#60, Nov 30 2004, 11:49:19) [MSC v.1310 32 bit (Intel)] on Win32  
<http://www.python.org/>

R.C. Reid, J.M. Prausnitz, and B.E. Poling, *The Properties of Gases and Liquids*, 4<sup>th</sup> Ed., McGraw-Hill, New York (1988).

E.R. Ritter and J.W. Bozzelli, *THERM: Thermodynamic Property Estimation for Gas Phase Radicals and Molecules*, 12<sup>th</sup> Int. CODATA Conf., July 1990.

E.R. Ritter, *THERM User's Manual*, Dept. of Chem. Eng., New Jersey Inst. of Technol., Newark, NJ (1990).

F.D. Rossini, K.S. Pitzer, W.J. Taylor, J.P. Ebert, J.E. Kilpatrick, C.W. Beckett, M.G. Williams, and H.G. Werner *Selected Values of Properties of Hydrocarbons (API Project 44)*, NBS Circular 461 (1947).

F.D. Rossini, D.D. Wagman, W.H. Evans, S. Levine, and I. Jaffe *Selected Values of Chemical Thermodynamic Properties*, NBS Circular 500 (1952).

B. Ruscic, R.E. Pinzon, M.L. Morton, G. von Laszewski, S. Bittner, S.G. Nijsure, K.A. Amin, M. Minkoff, and A.F. Wagner, *Introduction to Active Thermochemical Tables: Several "Key" Enthalpies of Formation Revisited*, *J. Phys. Chem. A* **108**, 9979 (2004).

B. Ruscic, *Active Thermochemical Tables*, in: *2005 Yearbook of Science and Technology*, an annual update to the McGraw-Hill

*Encyclopedia of Science and Technology*, McGraw-Hill, New York (2004).

T. Shimanouchi, *Tables of Molecular Vibrational Frequencies*, NSRDS-NBS-39. (1972); see also: <http://webbook.nist.gov/chemistry>

T. Shimanouchi, *J. Phys. Chem. Ref. Data* **3**, 304 (1974).

S.S. Sidhu, J.H. Kiefer, A. Lifshitz, C. Tamburu, J.A. Walker, and W. Tsang, *Int. J. Chem. Kinet.* **23**, 215 (1991)

S.E. Stein and B.D. Barton, *Thermochim. Acta* **44**, 265 (1981).

S.E. Stein, *J. Phys. Chem.* **89**, 3714 (1985).

S.E. Stein, J.M. Rukkers, and R.L. Brown, *NIST Structures and Properties Database and Estimation Program*, NIST, Gaithersburg, MD (1991).

S.E. Stein, *NIST Structures and Properties Vers. 2.0 Computerized Database 25*, NIST, Gaithersburg, MD (1994).

J.J.P. Stewart, *Optimization of Parameters for Semiempirical Methods. I. Method*, *J. Comput. Chem.* **10**, 209 (1989); II. Applications, *ibid*, **10**, 221 (1989).

J.J.P. Stewart, *Reviews of Computational Chemistry*, K.B. Lipkowitz and D.B. Boyd Eds., VCH, New York (1990), p. 45.

J.J.P. Stewart, *MOPAC 7 Manual* (1993).

D.R. Stull, E.F. Westrum, and G.C. Sinke, *The Chemical Thermodynamics of Organic Compounds*, Wiley, New York (1969).

M. Tirtowidjojo and R. Pollard, *J. Crystal Growth* **77**, 200 (1986).

*TRC Thermodynamic Tables - Hydrocarbons*, formerly API Project 44. (see Rossini); published as loose leaf sheets by

Thermodynamic Research Center, Texas A&M University, College Station, TX; present supplements by NIST-TRC, Boulder, CO

W. Tsang, *J. Am. Chem. Soc.* **107**, 2872 (1985).

W. Tsang, *Heats of Formation of Organic Free Radicals by Kinetic Methods*, Chapt. 2 in: *Energetics of Organic Free Radicals*, J.A.M. Simones, A. Greenberg, and J.F. Liebman, Eds. (SEARCH series) Chapman and Hall, London (1996).

*TSIV*: see L.V. Gurvich

D.D. Wagman, W.H. Evans, I. Holow, V.S. Parker, S.M. Bailey, and R.H. Schumm, *NBS Technical Note 270-1 to 8*, (1965-1981); the final revised version appeared as:

D.D. Wagman, W.H. Evans, V.S. Parker, R.H. Schumm, I. Holow, S.M. Bailey, K L Churney, and R.L. Nuttall, *The NBS Tables of Chemical Thermodynamic Properties. Selected Values for Inorganic and C<sub>1</sub>-C<sub>2</sub>*

*Organic Substances*. *J. Phys. Chem. Ref. Data* **11**, Suppl. 2 (1982).

R.C. Wilhoit, *Ideal Gas Thermodynamic functions*, *TRC Current Data News* **3**, #2 (1975).

C.L. Yu, Y.X. Zhang, and S.H. Bauer, *J. Mol. Struct. THEOCHEM* **432**, 63 (1998).

F.J. Zeleznik and S Gordon, *An Analytical Investigation of Three General methods of Calculating Chemical Equilibrium Compositions*, NASA TN-D 473 (1960)

F.J. Zeleznik and S Gordon, *Simultaneous Least Square Approximation of a Function and its first integrals, with application to Thermodynamic Data*, NASA-TN-D-767 (1961).

F.J. Zeleznik and S Gordon, *A General IBM704 or 7090 Computer program for Computation of Chemical Equilibrium Compositions, Rocket Performance and Chapman-Jouguet Detonations*, NASA TN-D 1454 (1962).



Table 4  
Third Millennium Thermodynamic Database for Combustion and Air-Pollution Use  
with updates from  
Active Thermochemical Tables.

DEDICATED TO THE MEMORY OF WILLIAM (BILL) C. GARDINER (1933-2000), PROFESSOR OF  
CHEMISTRY AT THE UNIVERSITY OF TEXAS, AUSTIN TX. INITIATOR AND FIRST PUBLISHER  
OF THIS DATABASE. MAY HE REST IN PEACE.

Database Authors: Alexander Burcat and Branko Ruscic  
The Database was last updated on September 2005  
Discard Previous Versions

This database is provided free of charge for non commercial use, on condition  
that proper quotation will be included in the pertinent publications.  
IT IS STRICTLY FORBIDDEN TO INCLUDE THIS DATABASE AS IS OR PARTS OF IT IN  
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COMMERCIAL USE WITHOUT WRITTEN PERMISSION FROM THE AUTHORS.

The latest print quotation to be made to this database is:

Alexander Burcat and Branko Ruscic  
"Third Millennium Ideal Gas and Condensed Phase Thermochemical Database for  
Combustion with updates from Active Thermochemical Tables" TAE # 960; ANL-50/20  
Technion-IIT, Aerospace Engineering, and Argonne National Laboratory, Chemistry  
Division, 2005.

or

Alexander Burcat and Branko Ruscic  
Ideal Gas Thermochemical Database with updates from Active Thermochemical Tables  
<<ftp://ftp.technion.ac.il/pub/supported/aetdd/thermodynamics>>;date.  
mirrored at <<http://garfield.chem.elte.hu/Burcat/burcat.html>>;date.

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Geosciences and Biosciences of the Office of Basic Energy Sciences, and by the Mathematical,  
Information, and Computational Science Division of the Office of Advanced Scientific Computing  
Research, under Contract No. W-31-109-ENG-38.  
This work has benefited from the support and effort of the team members of the Collabora-  
tory for Multi-Scale Chemical Science (CMCS), sponsored by the U.S. Department of Energy's Division  
of Mathematical, Information, and Computational Sciences of the Office of Advanced Scientific  
Computing Research. Portions of this research are also related to the effort of a Task Group of the  
International Union of Pure and Applied Chemistry (2003-024-1-100).

CODES APPEARING IN THE "DATE" FIELD and "REF=" fields:

A-ARGONNE NAT.LABS. Argonne IL 60349  
ATcT A- Branko Ruscic, unpublished results from Active Thermochemical Tables  
v.1.25 using the Core (Argonne) Thermochemical Network v. 1.049 (May 2005).  
B-Ihsan Barin database  
CODA- CODATA Tables  
D-Delaware University  
F-THERGAS calculations.  
IU-IUPAC data, calculated by the committee for revising radical thermochemistry.  
J-JANAF tables and date of table.  
G(L)-NASA Glen (former Lewis) Research Center  
P- Thermodynamic Research Center [TRC] (Formerly American Petroleum Institute)  
R-or Rus or TPIS Russian Tables (TSIV/TPIS), Gurvich and date of edition.  
S-Louisiana State University (LSU) Baton-Rouge LA.



Table 4 (continued)

T- Technion-Israel Inst. Technology Haifa 32000, Israel  
 TT-New HF298 adjusted on old polynomial.

THE NUMBER PRECEDING EACH SPECIES IS THE CHEMICAL ABSTRACT (CAS) IDENTIFICATION.

132259-10-0

AIR calculated from ingredients %N2=78.084 %O2=20.9476 %Ar=0.9365 %CO2=0.0319  
 This format is not capable of automatic formula calculation for this species!!!  
 See New NASA Polynomials REF=McBride & Gordon NASA RP-1271 1992 Structure  
 for automatic formula calculation should be:

N	1.560	0.42AR	0.01C	0.00	Max Lst Sq Error Cp @ 2500 K 0.19%	
AIR	L 9/95	WARNING!	O.G	200.000	6000.000	B 28.96518 1
	3.08792717E+00	1.24597184E-03	-4.23718945E-07	6.74774789E-11	-3.97076972E-15	2
	-9.95262755E+02	5.95960930E+00	3.56839620E+00	-6.78729429E-04	1.55371476E-06	3
	-3.29937060E-12	-4.66395387E-13	-1.06234659E+03	3.71582965E+00	-1.50965000E+01	4

7429-90-5

AL(cr)	REF	ELEMEN	CODA89AL	1.	0.	0.	0.S	200.000	933.610	B	26.98154	1
					0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
					0.00000000E+00	0.00000000E+00	1.01040191E+00	1.20769743E-02	-2.62083556E-05			3
					2.64282413E-08	-9.01916513E-12	-6.54454196E+02	-5.00471254E+00	0.00000000E+00			4
AL(L)	REF	ELEMENT	CODA89AL	1.	0.	0.	0.L	933.610	6000.000	B	26.98154	1
					3.81862551E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
					-9.49651808E+01	-1.75229704E+01	3.81862551E+00	0.00000000E+00	0.00000000E+00			3
					0.00000000E+00	0.00000000E+00	-9.49651808E+01	-1.75229704E+01	0.00000000E+00			4

7429-90-5

Al HF298=329.7+/-4.2 KJ REF=JANAF

AL	J 6/83AL	1.	0.	0.	0.G	200.000	6000.000	B	26.98154	1	
						2.53385701E+00	-4.65859492E-05	2.82798048E-08	-8.54362013E-12	1.02207983E-15	2
						3.89045662E+04	5.37984179E+00	3.11112433E+00	-3.59382310E-03	8.14749313E-06	3
						-8.08808966E-09	2.93132463E-12	3.88283390E+04	2.84045730E+00	3.96535695E+04	4

13967-22-1

ALH SIGMA=1 STATWT=1 Be=6.3907 WE=1682.56 WEXE=29.09 ALPHAE=0.1858

HF298=259.4+/-20 KJ REF=JANAF

ALH	J 6/63AL	1.H	1.	0.	0.G	300.000	5000.000	B	27.98948	1	
						3.33668980E+00	1.28778640E-03	-4.98699410E-07	9.22946330E-11	-6.34516940E-15	2
						3.00917610E+04	3.09548828E+00	3.65768570E+00	-1.97446980E-03	6.86633980E-06	3
						-6.20414040E-09	1.86631030E-12	3.01464580E+04	2.08851108E+00	3.11985222E+04	4

14457-64-8

ALO	T0=0	STATWT=2	Be=0.64136	WE=979.23	WEXE=6.97	ALFAE=0.0058
	T0=5282.	STATWT=4	Be=0.5365	WE=728.5	WEXE=4.15	ALFAE=0.0050
	T0=20635.2	STATWT=2	Be=0.60408	WE=870.05	WEXE=3.52	ALFAE=0.00447
	T0=33055.	STATWT=4	Be=0.60	WE=856.	WEXE=6.	ALFAE=0.004
	T0=30200.	STATWT=4	Be=0.565	WE=820.	WEXE=5.0	ALFAE=0.004
	T0=31600.	STATWT=8	Be=0.565	WE=820.	WEXE=5.0	ALFAE=0.004
	T0=33000.	STATWT=4	Be=0.565	WE=820.	WEXE=5.0	ALFAE=0.004
	T0=34700.	STATWT=4	Be=0.565	WE=820.	WEXE=5.0	ALFAE=0.004
	T0=34900.	STATWT=2	Be=0.565	WE=820.	WEXE=5.0	ALFAE=0.004
	T0=40187.	STATWT=2	Be=0.5652	WE=817.5	WEXE=4.8	ALFAE=0.0046

HF298=66.9+/-8 kJ REF=JANAF

ALO	J12/79AL	1.O	1.	0.	0.G	300.000	5000.000	A	42.98094	1	
						3.31390640E+00	1.04524210E-03	2.74855330E-07	-1.79286060E-10	1.99878130E-14	2
						7.09433360E+03	7.20963426E+00	2.81161030E+00	3.95842610E-03	-3.36953040E-06	3
						6.73304970E-10	4.00894550E-13	7.06550370E+03	9.20895756E+00	8.05147516E+03	4

Table 4 (continued)

20768-67-6

ALOH SIGMA=1 STATWT=1 B0=0.538347 cm-1 NU=1600,1000(2),900 HF298=-179.9  
+/- 13 kJ REF=JANAF

ALOH	J12/67AL	1.O	1.H	1.	0.G	300.000	5000.000	C	43.98888	1
	3.68606740E+00	3.36368220E-03	-1.24662440E-06	2.13822050E-10	-1.38983190E-14					2
	-2.30461050E+04	3.69015562E+00	2.61322110E+00	2.77168940E-03	7.41578300E-06					3
	-1.13546020E-08	4.55695590E-12	-2.25867970E+04	1.00753303E+01	-2.16392416E+04					4

11092-32-3

ALO2 ALUMINUM OXIDE SIGMA=2 B0=0.184455cm-1 T0(STATWT)=0(4),15000(4),20000(2)  
NU=930,700,200(2) HF298=-86.19+/-32 KJ REF=JANAF

ALO2	J12/79AL	1.O	2.	0.	0.G	300.000	5000.000	C	58.98034	1
	6.60646410E+00	1.08022520E-03	-5.22293440E-07	1.13242200E-10	-8.52909680E-15					2
	-1.25324320E+04	-8.01717584E+00	3.25451480E+00	1.42758440E-02	-2.11032480E-05					3
	1.50562590E-08	-4.21426140E-12	-1.18125820E+04	8.30255496E+00	-1.03664132E+04					4

24623-77-6

ALO2H ALUMINUM HYDROXIDE OXIDE SIGMA=1 STATWT=1 IA=0.1301 IB=16.9121  
IC=17.0422 NU=3400,1200,1100,700,500,400 HF298=-460+/-63 KJ REF=JANAF

ALO2H	J12/68AL	1.O	2.H	1.	0.G	300.000	5000.000	B	59.98828	1
	6.42643460E+00	3.22303620E-03	-1.21393480E-06	2.10745000E-10	-1.38280000E-14					2
	-5.76261540E+04	-7.45759253E+00	2.48004560E+00	1.61492640E-02	-1.60335240E-05					3
	6.44661660E-09	-4.09947690E-13	-5.66827590E+04	1.23070710E+01	-5.53546581E+04					4

12004-36-3

AL2O ALUMINUM OXIDE SIGMA=2 T0(STATWT)=0(1),23286(1),34331(3),36233(1)  
B0=0.104378 cm-1 NU=994,471,160(2) HF298=-145.2+/-17 KJ REF=JANAF

AL2O	J12/79AL	2.O	1.	0.	0.G	300.000	5000.000	B	69.96248	1
	6.77206270E+00	8.25500920E-04	-3.62910010E-07	6.95313000E-11	-4.73452110E-15					2
	-1.96431970E+04	-8.77233125E+00	4.07326560E+00	1.13076130E-02	-1.65651620E-05					3
	1.17842840E-08	-3.30055030E-12	-1.90542300E+04	4.40834835E+00	-1.74618202E+04					4

12252-63-0

AL2O2 SIGMA=4 STATWT=1 IA=8.6080 IB=14.5167 IC=23.1247 NU=650,600,496,  
400,350,200 HF298=-394.6+/- 32 KJ REF=JANAF

AL2O2	J12/79AL	2.O	2.	0.	0.G	300.000	5000.000	C	85.96188	1
	9.15909760E+00	9.68539270E-04	-4.32585130E-07	8.51788400E-11	-6.16153700E-15					2
	-5.04280590E+04	-1.91564680E+01	2.75964110E+00	2.99975990E-02	-5.21904970E-05					3
	4.22826860E-08	-1.30753600E-11	-4.92260320E+04	1.11007720E+01	-4.74536598E+04					4

1344-28-1

AL2O3 HF298=-1675.7 kJ REF=JANAF

AL2O3(S)	J12/79AL	2.O	3.	0.	0.S	300.000	2327.000	C	101.96128	1
	1.18336660E+01	3.77088780E-03	-1.78631910E-07	-5.60088070E-10	1.40768250E-13					2
	-2.05711310E+05	-6.35998350E+01	-4.91383090E+00	7.93984430E-02	-1.32379180E-04					3
	1.04467500E-07	-3.15663300E-11	-2.02626220E+05	1.54780730E+01	-2.01540284E+05					4
AL2O3(L)	J12/79AL	2.O	3.	0.	0.L	2327.000	6000.000	C	101.96128	1
	2.31482410E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
	-2.11405200E+05	-1.38602050E+02	2.31482410E+01	0.00000000E+00	0.00000000E+00					3
	0.00000000E+00	0.00000000E+00	-2.11405200E+05	-1.38602050E+02	0.00000000E+00					4

Table 4 (continued)

1344-28-1

Al<sub>2</sub>O<sub>3</sub>(G) HF298=-546.9 kJ REF=NASA (Glen) database Original data from Gurvich  
1996. Max Lst Sq Error Cp @ 1200 K 0.19%

Al <sub>2</sub> O <sub>3</sub>	T 1/03AL 2.0 3. 0. 0.G	200.000 6000.000 B 101.96128	1
1.17994008E+01 1.76967069E-03-7.04350190E-07 1.22091430E-10-7.69101328E-15			2
-6.97015909E+04-3.04301080E+01 5.63511151E+00 2.44249707E-02-3.39640439E-05			3
2.31585910E-08-6.27550763E-12-6.82839486E+04 1.39618674E-02-6.57754937E+04			4

7440-37-1

Ar HF298=0. REF=C.E. Moore "Atomic Energy Levels" NSRDS-NBS 35 (1971) p.211

Ar REF ELEMENT	L 6/88AR 1 0 0 0G	200.000 6000.000 A 39.94800	1
0.25000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00			2
-0.74537500E+03 0.43796749E+01 0.25000000E+01 0.00000000E+00 0.00000000E+00			3
0.00000000E+00 0.00000000E+00-0.74537500E+03 0.43796749E+01 0.00000000E+00			4

14791-69-6

Ar+ HF298=1526.778 kJ HF0=1520.572 kJ REF=C.E. Moore "Atomic Energy Levels"  
NSRDS-NBS 35 (1971) {HF298=1526.778+/-9.85E-4 kJ REF=ATcT A} Max Lst Sq Error  
Cp @ 1300 K 0.26%

Ar+	g 1/99AR 1.E -1. 0. 0.G	298.150 6000.000 A 39.94745	1
2.88112242E+00-1.61448253E-04 1.88408792E-08 1.05317052E-12-2.29902592E-16			2
1.82698356E+05 3.47046630E+00 2.58499602E+00-1.27110792E-03 5.12646199E-06			3
-5.84033673E-09 2.13932496E-12 1.82879208E+05 5.48412539E+00 1.83628188E+05			4

7440-42-8

B HF298=560+/-12 kJ REF=JANAF

B	J 6/83B 1. 0. 0. 0.G	200.000 6000.000 B 10.81100	1
2.49860273E+00 1.40267322E-06 1.09458278E-09-1.20006414E-12 2.43121994E-16			2
6.66075914E+04 4.21887979E+00 2.51054099E+00-6.23801328E-05 1.42178099E-07			3
-1.41697796E-10 5.15018749E-14 6.66053894E+04 4.16367209E+00 6.73521350E+04			4

740-42-8

B(S) REF ELEMENT	J 3/79B 1. 0. 0. 0.S	300.000 2350.000 B 10.81000	1
0.12508638E 01 0.34056258E-02-0.24349586E-05 0.87414463E-09-0.10498288E-12			2
-0.60694437E 03-0.75854277E 01-0.17810789E 01 0.16367573E-01-0.23992225E-04			3
0.17285547E-07-0.48891231E-11-0.16242365E 02 0.69007440E 01 0.000000 E 00			4
B(L) REF ELEMENT	J 3/79B 1. 0. 0. 0.L	2350.000 5000.000 B 10.81000	1
0.38245440E 01 0.00000000 0.00000000 0.00000000 0.00000000			2
0.34140016E 04-0.20732328E 02 0.38245440E 01 0.00000000 0.00000000			3
0.00000000 0.00000000 0.34140016E 04-0.20732328E 02 0.00000000			4

20583-55-5

BCL SIGMA=1 STATWT=1 BE=0.6914 WE=843.65 WEXE=5.167 ALFAE=0.00657

HF298=141.4 kJ REF=JANAF

BCL	J12/64B 1.CL 1. 0. 0.G	300.000 5000.000 B 46.26370	1
4.10205710E+00 4.86591930E-04-1.88643260E-07 3.58333420E-11-2.50990690E-15			2
1.56879580E+04 1.95525119E+00 2.83644630E+00 4.43688120E-03-4.38875220E-06			3
1.51610780E-09 3.26461950E-14 1.60013610E+04 8.34533209E+00 1.70084902E+04			4

22395-93-3

BCLF SIGMA=1 STATWT=2 IA=0.7794 IB=14.8586 IC=15.638 NU=1220,929,360

HF298=-314+/-29 kJ REF=JANAF

BCLF	J12/64B 1.CL 1.F 1. 0.G	300.000 5000.000 C 65.26210	1
5.70767570E+00 1.41002030E-03-6.01141370E-07 1.13670440E-10-7.93680630E-15			2
-3.96933270E+04-1.53503845E+00 3.31202340E+00 7.41987630E-03-4.34859490E-06			3
-1.13740570E-09 1.37638900E-12-3.90175480E+04 1.09483562E+01-3.77402953E+04			4

Table 4 (continued)

13842-52-9

BCL2 SIGMA=2 T0 (STATWT)=0 (2), 11000 (2), 28003 (1), 28153 (1), 29455 (1), 29542 (1)

IA=1.4577 IB=24.2203 IC=25.678 NU=725,700,250 HF298=-79.5+/-12.6 kJ

REF=JANAF

BCL2	J 6/72B	1.CL	2.	0.	0.G	300.000	5000.000	C	81.71640	1
6.44598380E+00	5.79279480E-04	-2.60497050E-07	6.35963580E-11	-5.39822150E-15						2
-1.16613040E+04	-4.46086977E+00	3.29747860E+00	1.20825760E-02	-1.61237550E-05						3
9.62658560E-09	-2.05991990E-12	-1.09565370E+04	1.10425333E+01	-9.56076191E+03						4

10294-34-5

BCL3 SIGMA=6 STATWT=1 IA=IB=27.0443 IC=54.0887 NU=986.3 (2), 471.0, 470.6, 243.0

HF298=-403.0+/-2.1 kJ REF=JANAF

BCL3	J12/64B	1.CL	3.	0.	0.G	300.000	5000.000	B	117.16910	1
8.59853800E+00	1.55319230E-03	-6.70006020E-07	1.27891120E-10	-9.00000590E-15						2
-5.13570710E+04	-1.51584297E+01	3.73952650E+00	1.81058130E-02	-2.13404610E-05						3
1.08283350E-08	-1.73259670E-12	-5.02146090E+04	9.05312747E+00	-4.84628831E+04						4

13768-60-0

BF SIGMA=1 STATWT=1 BE=1.5286 WE=1410.3 WEXE=11.98 ALFAE=0.0168

HF298=-115.9+/-13.8 kJ REF=JANAF

BF	J12/64B	1.F	1.	0.	0.G	300.000	5000.000	B	29.80940	1
3.57718880E+00	1.01929080E-03	-4.12515640E-07	7.71964380E-11	-5.34987410E-15						2
-1.51272640E+04	3.26612227E+00	3.46136090E+00	-9.56854680E-04	6.01357440E-06						3
-6.49780570E-09	2.23553490E-12	-1.49698200E+04	4.46077947E+00	-1.39390003E+04						4

13842-55-2

BF2 SIGMA=2 T0 (STATWT)=0 (2), 16000 (2) IA=0.7385 IB=7.3289 IC=8.0674

NU=1213,1080,500 HF298=-589.9+/-13 kJ REF=JANAF

BF2	J 6/72B	1.F	2.	0.	0.G	300.000	5000.000	C	48.80781	1
5.44474570E+00	1.75332110E-03	-7.84444740E-07	1.57198590E-10	-1.13110710E-14						2
-7.28603670E+04	-2.27331909E+00	3.03093030E+00	7.24110210E-03	-2.82509190E-06						3
-2.89204130E-09	2.00461020E-12	-7.21511020E+04	1.04457036E+01	-7.09553140E+04						4

7637-07-2

BF3 SIGMA=6 STATWT=1 IA=IB=8.0838 IC=16.1676 NU=1463.3 (2), 888, 696.7, 480.7 (2)

HF298=-1135.6+/-1.7 kJ REF=JANAF

BF3	J 6/69B	1.F	3.0	0.	0.G	300.000	5000.000	B	67.80621	1
7.02419850E+00	3.22215590E-03	-1.37051540E-06	2.59196710E-10	-1.81223100E-14						2
-1.39180720E+05	-1.11843009E+01	2.44682440E+00	1.52763120E-02	-1.07846170E-05						3
6.89075020E-10	1.48931870E-12	-1.37901350E+05	1.25678211E+01	-1.36586061E+05						4

13766-26-2

BH BORANE STATWT=1 BE=12.036 WE=2368 WEXE=49 ALFAE=0.413

HF298=442.7+/-8.4 kJ REF=JANAF

BH	J12/64B	1.H	1.	0.	0.G	300.000	5000.000	C	11.81894	1
2.89190790E+00	1.58329460E-03	-5.82617290E-07	1.02420680E-10	-6.76695690E-15						2
5.23287140E+04	3.79624329E+00	3.68622060E+00	-1.30554350E-03	2.67421050E-06						3
-9.10737380E-10	-1.55911360E-13	5.21763300E+04	-5.52454012E-02	5.32391023E+04						4

13709-83-6

BHF2 DIFLUOROBORANE SIGMA=2 STATWT=1 IA=1.0402 IB=7.9974 IC=9.0376

NU=2640,1411,1174,1158,928,544 HF298=-733.9+/-3.3 kJ REF=JANAF

BHF2	J12/65B	1.H	1.F	2.	0.G	300.000	5000.000	B	49.81575	1
5.31845270E+00	4.74444660E-03	-1.93378580E-06	3.55083820E-10	-2.42936670E-14						2
-9.03750120E+04	-3.04314020E+00	2.40536020E+00	9.27558440E-03	1.33864610E-06						3
-8.68078950E-09	4.12110150E-12	-8.93884090E+04	1.28880442E+01	-8.82623625E+04						4

Table 4 (continued)

14452-64-3

BH2 SIGMA=2 STATWT=2 B0=5.807235 NU=2650,2430,840 HF298=201+/-63 kJ  
REF=JANAF

BH2	J12/64B	1.H	2.	0.	0.G	300.000	5000.000	C	12.82688	1
	3.36252850E+00	3.90128540E-03	-1.50975510E-06	2.66728050E-10	-1.77130530E-14					2
	2.29190280E+04	1.25928259E+00	2.39582820E+00	7.47762600E-03	-7.20195140E-06					3
	4.58263980E-09	-1.25106800E-12	2.31626500E+04	6.07647039E+00	2.41541598E+04					4

13283-31-3

BH3 SIGMA=6 STATWT=1 IA=IB=0.3378 IC=0.6757 NU=2976(2),2394,1765(2),802  
HF298=106.7+/-10 kJ REF=JANAF

BH3	J12/64B	1.H	3.	0.	0.G	300.000	5000.000	C	13.83482	1
	2.06217260E+00	7.26558950E-03	-2.75103370E-06	4.78037090E-10	-3.13342850E-14					2
	1.19237530E+04	8.84945083E+00	3.94870330E+00	-5.21705430E-04	7.64811640E-06					3
	-4.61486940E-09	5.63186160E-13	1.16188090E+04	-4.55174579E-02	1.28316429E+04					4

12505-77-0

BO SIGMA=1 T0(STATWT)=0(2),23836(2),23959(2),39957(2),43175(2) BE=1.800  
WE=1895.66 WEXE=11.90 ALFAE=0.01676 HF298=0+/-8 kJ REF=JANAF

BO	J 6/68B	1.O	1.	0.	0.G	300.000	5000.000	B	26.81040	1
	3.15649560E+00	1.38165890E-03	-5.50496300E-07	9.91166780E-11	-6.41645460E-15					2
	-1.03034220E+03	6.03748954E+00	3.72972500E+00	-2.08783240E-03	5.73628490E-06					3
	-4.38948280E-09	1.09166320E-12	-1.06188590E+03	3.62554104E+00	-1.45402311E-01					4

23361-55-9

BOCL (OBC1) SIGMA=1 STATWT=1 B0=0.165056 NU=1850,690,400(2)  
HF298=-316.3+/-29 kJ REF=JANAF

BOCL	J12/65B	1.O	1.CL	1.	0.G	300.000	5000.000	C	62.26310	1
	5.71355660E+00	1.86646890E-03	-7.74878980E-07	1.43985720E-10	-9.93177450E-15					2
	-3.99773530E+04	-4.88040355E+00	3.27053210E+00	1.02277500E-02	-1.20701630E-05					3
	7.20255620E-09	-1.69147380E-12	-3.93782080E+04	7.34930225E+00	-3.80417115E+04					4

23361-56-0

BOF (OBF) SIGMA=1 STATWT=1 B0=0.309392 NU=1900,1050,500(2)  
HF298=-602+/-13 kJ REF=JANAF

BOF	J12/65B	1.O	1.F	1.	0.G	200.000	6000.000	C	45.80880	1
	5.39296603E+00	2.07444500E-03	-7.93600586E-07	1.33476571E-10	-8.21779331E-15					2
	-7.43113852E+04	-4.76500545E+00	2.23703738E+00	1.33495496E-02	-1.81530614E-05					3
	1.36093676E-08	-4.24382397E-12	-7.35283735E+04	1.10069410E+01	-7.24035451E+04					4

38150-67-3

BOF2 OBF2 SIGMA=2 T0(STATWT)=0(2),17171(2),22390(2) IA=7.4051 IB=8.4655  
IC=15.8706 NU=1377,1100,856,850,500,491 HF298=-837+/-15 kJ REF=JANAF

BOF2	J12/66B	1.O	1.F	2.	0.G	300.000	5000.000	C	64.80721	1
	7.30772330E+00	2.99036200E-03	-1.30596170E-06	2.53082420E-10	-1.76873330E-14					2
	-1.03345760E+05	-1.11924159E+01	1.74459770E+00	1.86932770E-02	-1.52461640E-05					3
	2.65594700E-09	1.37986060E-12	-1.01867580E+05	1.73531391E+01	-1.00645369E+05					4

13840-88-5

BO2 SIGMA=2 T0(STATWT)=0(2),149(2),18291.6(4),24508(2) B0=0.33036  
NU=1321.7,1056,454 HF298=-285+/-8 kJ REF=JANAF

BO2	J 6/68B	1.O	2.	0.	0.G	300.000	5000.000	B	42.80980	1
	5.81984340E+00	1.86265740E-03	-8.13027970E-07	1.57358210E-10	-1.09442380E-14					2
	-3.62551170E+04	-6.56090797E+00	3.12120480E+00	8.46808830E-03	-4.59722780E-06					3
	-1.64200210E-09	1.66582330E-12	-3.54833070E+04	7.54789163E+00	-3.42194143E+04					4

Table 4 (continued)

14452-61-0  
 B2 SIGMA=2 T0=0(3) BE=1.236121 WE=1061.61 WEXE=9.536 ALFAE=0.01442411  
 T0=1271(5) BE=1.305 WE=1215.81 WEXE=9.995 ALFAE=0.0113  
 T0=14829(3) BE=1.275 WE=1114.83 WEXE=16.318 ALFAE=0.0175  
 T0=30573.4(3) BE=1.183086 WE=946.59 WEXE=2.652 ALFAE=0.1133323  
 HF298=829.7+/-33.5 kJ REF=JANAF  
 B2 J 3/79B 2. 0. 0. 0.G 200.000 6000.000 B 21.62200 1  
 5.23869155E+00-5.23607507E-04 1.69704978E-07-2.06549042E-11 9.41435925E-16 2  
 9.79873828E+04-6.00742217E+00 3.79099744E+00-5.87536359E-03 3.00514162E-05 3  
 -3.91439173E-08 1.60419428E-11 9.87229998E+04 3.43463203E+00 9.97878648E+04 4

12045-60-2  
 B2O SIGMA=2 STATWT=1 IA=0.1624 IB=5.3179 IC=5.4803 NU=1800,1250,600  
 HF298=96+/-105 kJ REF=JANAF  
 B2O J 6/66B 2.0 1. 0. 0.G 300.000 5000.000 C 37.62140 1  
 4.73005380E+00 2.39414860E-03-1.00083240E-06 1.86975100E-10-1.29536720E-14 2  
 9.88533540E+03-6.35851289E-01 3.52947300E+00 3.19938260E-03 3.03292570E-06 3  
 -5.74912550E-09 2.28473490E-12 1.03632010E+04 6.23963143E+00 1.15742290E+04 4

13766-28-4  
 B2O2 (BO)2 SIGMA=2 STATWT=1 B0=0.112313 NU=2065,1910,570,565,285  
 HF298=-456.1+/-8.4 kJ REF=JANAF  
 B2O2 J12/64B 2.0 2. 0. 0.G 300.000 5000.000 B 53.62080 1  
 6.99385740E+00 3.59403930E-03-1.47536110E-06 2.72251240E-10-1.86959960E-14 2  
 -5.72961780E+04-1.21677771E+01 3.68070780E+00 1.53611320E-02-1.86060970E-05 3  
 1.21714510E-08-3.24110180E-12-5.64866470E+04 4.35612734E+00-5.48483506E+04 4

1303-86-2  
 B2O3(L) HF298=-1253.4 kJ REF=JANAF  
 B2O3(L) J 6/71B 2.0 3.0 0.0 0.L 300.000 3000.000 B 69.61820 1  
 0.15600114E 02 0.00000000 0.00000000 0.00000000 0.00000000 2  
 -0.15684455E 06-0.83126444E 02 0.31433274E 02-0.21578039E 00 0.64057986E-03 3  
 -0.70572420E-06 0.26509150E-09-0.15490139E 06-0.12803880E 03-0.15074514E+06 4

1303-86-2  
 B2O3 SIGMA=2 STATWT=1 IA=2.9763 IB=31.0977 IC=34.0740 NU=2073(2),1240,  
 730,521,480,460,457,172 HF298=-836.0+/-4.2 kJ REF=JANAF  
 B2O3 J 6/71B 2.0 3. 0. 0.G 300.000 5000.000 B 69.62020 1  
 8.39941060E+00 4.74363380E-03-1.95523040E-06 3.61877490E-10-2.49072320E-14 2  
 -1.03571580E+05-1.58100009E+01 3.66088370E+00 2.02620760E-02-2.19473380E-05 3  
 1.22530040E-08-2.70384020E-12-1.02365240E+05 8.10622068E+00-1.00544127E+05 4

13703-91-8  
 B3O3Cl3 (BOCl)3 TRICHLOROBOROXIN SIGMA=6 STATWT=1 IA=IB=97.7637 IC=195.5274  
 NU=1300(2),1037,980(2),920(2),807,690,600,400(3),390(2),333,150(2),140,120(2)  
 HF298=-1632+/-8 kJ REF=JANAF  
 B3O3Cl3 J 3/65B 3.0 3.CL 3. 0.G 300.000 5000.000 C 186.78930 1  
 1.92825640E+01 6.31725810E-03-2.72429260E-06 5.20479100E-10-3.66777900E-14 2  
 -2.03208830E+05-6.78851521E+01 4.04449830E+00 5.42605970E-02-5.57507610E-05 3  
 2.22231280E-08-1.41812950E-12-1.99416320E+05 9.05672255E+00-1.96248045E+05 4

Table 4 (continued)

13703-95-2

B3O3F3 (BOF)3 TRIFLUOROBOROXIN SIGMA=6 STATWT=1 IA=IB=45.8345 IC=91.6691  
 NU=1450(2),1381(2),1280,1233,966(2),790,714,630(2),570,440,420(2),220(2),185(2),  
 170 HF298=-2365.2+/-4.2 kJ REF=JANAF

B3O3F3	J 3/65B	3.O	3.F	3.	0.G	300.000	5000.000	C	137.42641	1
1.68586160E+01	8.86857540E-03	-3.78810580E-06	7.18704010E-10	-5.03769170E-14						2
-2.90931040E+05	-5.98587523E+01	3.07988610E+00	4.56365920E-02	-3.30988260E-05						3
2.55388390E-09	4.43587610E-12	-2.87122130E+05	1.14753917E+01	-2.84460743E+05						4

289-56-5

B3O3H3 BOROXIN SIGMA=6 STATWT=1 IA=IB=13.971 IC=27.9421 NU=2620(2),2530,  
 1560,1404(2),1335(2),1115(2),940(2),920,903,735,550,400(2),300,230(2)  
 HF298=-1218+/-42 kJ REF=JANAF

B3O3H3	J 3/65B	3.O	3.H	3.	0.G	200.000	6000.000	C	83.45502	1
1.21201212E+01	1.22811209E-02	-4.60922487E-06	7.65824542E-10	-4.67623793E-14						2
-1.51648629E+05	-3.98918007E+01	2.76989078E+00	2.53425900E-02	1.22486701E-05						3
-3.73057611E-08	1.74556897E-11	-1.48431026E+05	1.15218019E+01	-1.46436050E+05						4

13460-51-0

H3B3O6 BORIC AQCID (HBO2)3 SIGMA=3 STATWT=1 IA=43.6915 IB=45.5585  
 IC=89.2499 NU=3500(3),1300(2),1100,1150,1000(4),950,900(2),750(2),600(3),550,  
 500(2),450(2),350(3),250,200(2) HF298=-2272+/-13 kJ REF=JANAF

H3B3O6	J12/64H	3.B	3.O	6.	0.G	300.000	5000.000	C	131.45322	1
2.01535790E+01	1.30162860E-02	-5.06696190E-06	9.03082530E-10	-6.05324100E-14						2
-2.81040920E+05	-7.96763324E+01	-2.27051160E+00	8.70248940E-02	-9.15877140E-05						3
3.94453920E-08	-3.66660350E-12	-2.75695230E+05	3.25296526E+01	-2.73237150E+05						4

1304-28-5

BaO Calculated by NASA from Gurvich's 1982 compendium. HF298=-117.95 kJ Max  
 Lst Sq Error Cp @ 2700 K \*\*0.94%\*\*

BaO	T 2/03BA	1.O	1.	0.	0.G	200.000	6000.000	B	153.32640	1
3.55502804E+00	1.95444826E-03	-1.45135366E-06	4.38035990E-10	-3.76904801E-14						2
-1.53106549E+04	7.55560778E+00	2.78388903E+00	6.15838284E-03	-9.25760577E-06						3
6.55343820E-09	-1.77963615E-12	-1.52198605E+04	1.09786578E+01	-1.41858029E+04						4

10097-32-2

BR HF298=111.86+/-0.06 REF=JANAF {HF298=111.860+/-0.055 kJ REF=ATcT A}

BR	J 6/82BR	1	0	0	OG	200.000	6000.000	A	79.90400	1
0.20866945E+01	0.71459733E-03	-0.27080691E-06	0.41519029E-10	-0.23016335E-14						2
0.12857696E+05	0.90837335E+01	0.24820782E+01	0.18570465E-03	-0.64313029E-06						3
0.84642045E-09	-0.30137068E-12	0.12709455E+05	0.68740409E+01	0.13453589E+05						4

13863-41-7

BrCL Bromine Monochloride From Gurvich's original 89 Tables. HF298=14.79 kJ  
 HF0=22.23 kJ {HF298=14.76+/-0.08 kJ REF=ATcT A; HF298=14.64 kJ REF=JANAF 65}  
 Max Lst Sq Error Cp @ 2400 K 0.66%.

BrCL	tpis89BR	1.CL	1.	0.	0.G	200.000	6000.000	B	115.35670	1
4.94407451E+00	-9.04227983E-04	5.97460034E-07	-1.22751767E-10	7.57259137E-15						2
2.29402149E+02	6.95986052E-01	2.91316204E+00	8.01066984E-03	-1.63333407E-05						3
1.52022507E-08	-5.27061456E-12	6.70852744E+02	1.04867475E+01	1.77871131E+03						4

Table 4 (continued)

13536-59-9

DBr Deuterium Bromide HF298=-37.036 kJ HF0=-29.16 kJ REF=Gurvich 89 Max Lst Sq Error Cp @ 6000 K 0.37%

DBr	RUS 89D	1.BR	1.	0.	0.G	200.000	6000.000	B	81.91810	1
	3.22932705E+00	1.27632694E-03	-4.73731331E-07	8.51651961E-11	-5.76511714E-15					2
	-5.51301106E+03	5.74862955E+00	3.68870551E+00	-1.77751272E-03	5.00542963E-06					3
	-3.55775119E-09	7.52451506E-13	-5.51277091E+03	3.91436607E+00	-4.45444121E+03					4

13863-59-7

BrF Bromine Monofluoride From Gurvich's 89 original Tables. HF0=-51.2+/-1 kJ HF298=-58.85 kJ Max Lst Sq Error Cp @ 6000 K 0.96%.

BrF	tpis89BR	1.F	1.	0.	0.G	200.000	6000.000	B	98.90240	1
	4.70485660E+00	-4.93114310E-04	3.17567567E-07	-4.74173599E-11	1.33803517E-15					2
	-8.59408850E+03	5.66622956E-01	2.77974859E+00	6.21877572E-03	-9.36181591E-06					3
	6.67211180E-09	-1.82558967E-12	-8.11296109E+03	1.02094886E+01	-7.07816155E+03					4

7787-71-5

BrF3 Bromine Trifluoride SIGMA=2 STATWT=1 IAIBIC=4528. Nu=675,614,552,350,242,238 HF298=-255.6+/-3 kJ HF0=-244.8 kJ REF=Gurvich 89. Max Lst Sq Error Cp @ 700 K 0.22%.

BrF3	tpis89BR	1.F	3.	0.	0.G	200.000	6000.000	B	136.89921	1
	9.20828836E+00	8.30392457E-04	-3.29835256E-07	5.68255169E-11	-3.55627443E-15					2
	-3.37231773E+04	-1.76182105E+01	1.99378648E+00	3.61697802E-02	-6.89696747E-05					3
	6.09279559E-08	-2.03597331E-11	-3.24449700E+04	1.59970023E+01	-3.07414388E+04					4

7789-30-2

BrF5 Bromine Pentafluoride SIGMA=4 STATWT=1 IAIBIC=28900. Nu=684,644(2),584,547,415(2),370,312,277,245(2) HF298=-428.8+/-2 kJ HF0=-413.65 kJ REF=Gurvich 89 Max Lst Sq Error Cp @ 200 K 0.33%.

BrF5	tpis89BR	1.F	5.	0.	0.G	200.000	6000.000	B	174.89602	1
	1.44221600E+01	1.65635753E-03	-6.58250468E-07	1.13445087E-10	-7.10133924E-15					2
	-5.63413631E+04	-4.47395740E+01	-6.78291507E-01	7.69576912E-02	-1.49146145E-04					3
	1.33361285E-07	-4.49679290E-11	-5.37154081E+04	2.53375233E+01	-5.15724919E+04					4

15656-19-6

BrO T0=0 STATWT=2 Be=0.4299 De=0.594E-6 ALPHAE=0.003639 WE=727.05 WEXE=4.932 T0=968 STATWT=2 Be=0.4299 De=0.594E-6 ALPHAE=0.003639 WE=727.05 WEXE=4.932 T0=27871 STATWT=2 Be=0.314 De=0.474E-6 ALPHAE=0.0034 WE=511.3 WEXE=4.83 T0=29321 STATWT=2 Be=0.314 De=0.474E-6 ALPHAE=0.0034 WE=511.3 WEXE=4.8 HF298=125.8+/-2.4 kJ REF=M.W.Chase JPCRD 25 (1996), 1069 Max Lst Sq Error Cp @ 400 K 0.45 %.

BRO	T02/97BR	1.O	1.	0.	0.G	200.000	6000.000	A	95.90340	1
	5.07219100E+00	-4.35812081E-04	1.75747890E-07	-2.82506168E-11	1.92290510E-15					2
	1.35030084E+04	-1.08904614E+00	2.55466821E+00	6.43468019E-03	-2.95159758E-06					3
	-4.90190824E-09	3.64995652E-12	1.41165412E+04	1.17071098E+01	1.51301760E+04					4

67177-47-3

BrO2 Br-O-O SIGMA=1 STATWT=2 IA=1.2011 IB=21.5417 IC=22.7428 NU=1487,250,160 HF298=108.0+/-40. kJ REF=M.W.Chase JPCRD 25 (1996), 1069 Max Lst Sq Error Cp @ 1300 K 0.21 %.

BrO2	Br-O-O	T02/97BR	1.O	2.	0.	0.G	200.000	6000.000	B	111.90280	1
	6.00363127E+00	9.92540840E-04	-3.82278926E-07	6.45667378E-11	-3.98629626E-15					2	
	1.10621232E+04	3.62860950E-02	5.09638120E+00	3.60676575E-03	-4.28370757E-06					3	
	3.72707925E-09	-1.47204500E-12	1.13407206E+04	4.78601414E+00	1.29893403E+04					4	



Table 4 (continued)

21255-83-4

BrO2 O-Br-O SIGMA=2 STATWT=2 IA=3.0275 IB=10.2087 IC=13.2361 NU=800,300,852 HF298=152.0+/-25. kJ REF=M.W.Chase JPCRD 25 (1996), 1069 Max Lst Sq Error Cp @ 400 K 0.18 %.

BrO2 O-Br-O	T02/97BR 1.0	2.	0.	0.G	200.000	6000.000	B 111.90280	1
6.24396373E+00	7.82813558E-04	-3.08534350E-07	5.28853891E-11	-3.29803612E-15				2
1.62066239E+04	-3.61634966E+00	3.07292385E+00	1.13245422E-02	-1.28765411E-05				3
5.90293758E-09	-6.56032315E-13	1.69641688E+04	1.22438586E+01	1.82812938E+04				4

32062-14-9

BrO3 SIGMA=3 STATWT=2 IA=IB=12.2156 IC=14.7352 NU=442,800,320.(2),828.(2) HF298=221.0+/-50. kJ REF=M.W.Chase JPCRD 25 (1996), 1069 Max Lst Sq Error Cp @ 1200 K 0.21 %.

BrO3	T02/97BR 1.0	3.	0.	0.G	200.000	6000.000	C 127.90220	1
8.69236256E+00	1.35841486E-03	-5.36468670E-07	9.20768329E-11	-5.74736730E-15				2
2.36159592E+04	-1.64447310E+01	1.49818242E+00	3.04080397E-02	-4.72006811E-05				3
3.49686979E-08	-1.00736007E-11	2.51344798E+04	1.84248093E+01	2.65800390E+04				4

7726-95-6

Br Liquid REFERENCE ELEMENT REF=B. McBride NASA Glen HF298=0 HF0=0 Max Lst Sq Error Cp @ 300 K 0.009%.

Br2(cr)	g 8/01BR 2.	0.	0.	0.C	200.000	265.900	159.80800	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2
0.00000000E+00	0.00000000E+00	9.12518645E+00	-8.26112489E-02	6.99829476E-04				3
-2.40833656E-06	3.21095684E-09	-3.30407584E+03	-3.01718869E+01	0.00000000E+00				4
Br2(L)	g 8/01BR 2.	0.	0.	0.C	265.900	332.503	159.80800	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2
0.00000000E+00	0.00000000E+00	1.04345553E+01	1.11059257E-01	-1.06796924E-03				3
3.25845464E-06	-3.27383354E-09	-3.50676499E+03	-4.91093408E+01	0.00000000E+00				4

7726-95-6

Br2 GAS HF298=30.91 kJ HF0=45.705 kJ. From Gurvich's tables. {HF298=30.897 +/-0.11 kJ REF=ATcT A} Max Lst Sq Error Cp @ 1300 K 0.60 %.

Br2	tpis89BR 2.	0.	0.	0.G	200.000	6000.000	B 159.80800	1
5.18742349E+00	-1.38674198E-03	9.34858666E-07	-2.07087532E-10	1.41823540E-14				2
2.10700879E+03	7.68476585E-02	3.34350669E+00	6.35013278E-03	-1.36341193E-05				3
1.31622796E-08	-4.67916478E-12	2.53514183E+03	9.07866893E+00	3.71759731E+03				4

68322-97-4

Br2O BrBr-O SIGMA=1 STATWT=3 IA=4.7079 IB=51.8084 IC=56.5163 NU=804,150,236 HF298=168.0+/-20. kJ REF=M.W.Chase JPCRD 25 (1996), 1069 Max Lst Sq Error Cp @ 1200 K 0.13 %

Br2O BrBr-O	T02/97BR 2.0	1.	0.	0.G	200.000	6000.000	B 175.80740	1
6.61241475E+00	4.02586598E-04	-1.58975806E-07	2.72841078E-11	-1.70297367E-15				2
1.81249753E+04	-3.99723764E-01	4.44451500E+00	9.35658684E-03	-1.49756620E-05				3
1.14829127E-08	-3.42674585E-12	1.85758718E+04	1.00676579E+01	2.02056405E+04				4

21308-80-5

Br2O Br-O-Br SIGMA=2 STATWT=1 IA=2.5488 IB=62.1189 IC=64.6677 NU=526.1,180,623.4 HF298=107.6+/-3.5 kJ REF=M.W.Chase JPCRD 25 (1996), 1069 Max Lst Sq Error Cp @ 1200 K 0.094%

Br2O Br-O-Br	T02/97BR 2.0	1.	0.	0.G	200.000	6000.000	B 175.80740	1
6.60036780E+00	4.19198661E-04	-1.66518672E-07	2.86896506E-11	-1.79550923E-15				2
1.08520131E+04	-2.99978832E+00	3.04140956E+00	1.75424857E-02	-3.28632899E-05				3
2.86038685E-08	-9.44453191E-12	1.14930042E+04	1.36453473E+01	1.29412317E+04				4

Table 4 (continued)

10031-22-8

PbBr<sub>2</sub> HF298=-104.39+/-6.3 kJ REF=JANAF 1973 {HF298=-103.9 REF=Gurvich 1991}

PbBr<sub>2</sub> J12/73PB 1.BR 2. 0. 0.G 300.000 5000.000 C 367.00800 1  
 6.94729060E+00 6.01990010E-05-2.65566850E-08 5.15960120E-12-3.68370500E-16 2  
 -1.46454410E+04 1.18015799E+00 6.39020910E+00 2.52890500E-03-4.19037430E-06 3  
 3.13675230E-09-8.79767450E-13-1.45417920E+04 3.81752929E+00-1.25553875E+04 4

7782-42-5

C Carbon Solid Graphite Reference Element

C(GR) REF ELEMENT P 4/83C 1 0 0 0C 200.000 5000.000 B 12.01100 1  
 0.14556924E+01 0.17170638E-02-0.69758410E-06 0.13528316E-09-0.96764905E-14 2  
 -0.69512804E+03-0.85256842E+01-0.31087207E+00 0.44035369E-02 0.19039412E-05 3  
 -0.63854697E-08 0.29896425E-11-0.10865079E+03 0.11138295E+01 0.00000000E+00 4

7440-44-0

C Amorphous Carbon, Acetylene black, Lamp black HF298=716.68+/-0.45 kJ  
REF=C.E. Moore "Selected Tables of Atomic Spectra" NSRDS-NBS Sec 3 (1970)

p A6 I. {HF298=717.065+/-0.146 kJ REF=ATcT A}

C L 7/88C 1 0 0 0G 200.000 6000.000 A 12.01100 1  
 0.26055830E+01-0.19593434E-03 0.10673722E-06-0.16423940E-10 0.81870580E-15 2  
 0.85411742E+05 0.41923868E+01 0.25542395E+01-0.32153772E-03 0.73379223E-06 3  
 -0.73223487E-09 0.26652144E-12 0.85442681E+05 0.45313085E+01 0.86195097E+05 4

14067-05-1

C+ HF298=1809.444 kJ HF0=1797.651 kJ REF=C.E. Moore "Selected Tables of Atomic Spectra" NSRDS-NBS Sec 3 (1970) p A6 I. {HF298=1809.828+/-0.146 kJ REF=ATcT A}  
 Max Lst Sq Error Cp @ 400 K 0.008%

C+ g 6/98C 1.E -1. 0. 0.G 298.150 6000.000 A 12.01015 1  
 2.50827618E+00-1.04354146E-05 5.16160809E-09-1.14187475E-12 9.43539946E-17 2  
 2.16879645E+05 4.31885990E+00 2.61332254E+00-5.40148065E-04 1.03037233E-06 3  
 -8.90092552E-10 2.88500586E-13 2.16862274E+05 3.83454790E+00 2.17624909E+05 4

3889-77-8

CBr BROMOMETHYLIDENE RADICAL SIGMA=1 STATWT=2 IB=5.8035

WE=725.39HF298=495.85 kJ HF0=500.1 kJ REF=Martin & Burcat JPC A 108, (2004),  
 7752 Max Lst Sq Error Cp @ 400 K 0.13%

CBR T 4/04C 1.BR 1. 0. 0.G 200.000 6000.000 C 91.91470 1  
 4.22276728E+00 2.88156903E-04-1.13837110E-07 1.95419868E-11-1.21993861E-15 2  
 5.82936956E+04 3.45831381E+00 2.86960998E+00 4.95324292E-03-5.93796515E-06 3  
 2.93797020E-09-4.07448826E-13 5.86073246E+04 1.01813191E+01 5.96362071E+04 4

353-59-3

CBrClF<sub>2</sub> HALON 1211 FC-12B1 STATWT=1 SIGMA=1 IAIBIC=6.3E-113 NU=1102,872,  
 648,440,337,220,1150,425,290 HF298=-435+/-15 KJ REF=Gurvich 91 Max Lst Sq  
 Error Cp @ 1200 K 0.28%

CF2CLBr tpis91C 1.F 2.CL 1.BR 1.G 200.000 6000.000 B 165.36421 1  
 1.07966238E+01 2.26676279E-03-8.90038695E-07 1.52198147E-10-9.47616870E-15 2  
 -5.60746593E+04-2.48667347E+01 2.10552027E+00 3.56772138E-02-5.28319040E-05 3  
 3.84797478E-08-1.11145080E-11-5.41357072E+04 1.77301712E+01-5.23181763E+04 4

Table 4 (continued)

75-63-8

CBrF3 Freon 1301 STATWT=1 SIGMA=3 IAIBIC=2.36E-113 NU=1084,761.4,351,1209(2),  
548(2),302.7(2) HF298=-650.59+/-1.97 kJ REF=ATcT A {HF298=-648.8+/-2.3 kJ  
REF=Gurvich 91} Max Lst Sq Error Cp @ 1300 K 0.33%.

CF3Br Freon 1301 ATcT/AC 1.F 3.BR 1. 0.G 200.000 6000.000 B 148.90991	1
1.02441971E+01 2.82088779E-03-1.10430609E-06 1.88474696E-10-1.17193712E-14	2
-8.19308539E+04-2.45567155E+01 1.92067214E+00 3.10919159E-02-3.85950853E-05	3
2.31847352E-08-5.46470390E-12-7.99043849E+04 1.71123451E+01-7.82475456E+04	4

4371-77-1

CBr2 DIBROMOMETHYLENE RADICAL SIGMA=2 STATWT=1 IA=2.1936 IB=63.5591  
IC=65.7527 Nu=196,598,641 T0=10000. SIGMA=2 STATWT=3 T0=14964. SIGMA=2  
STATWT=1 REF=JACOX and Gurvich 1979. HF298=82.10 kcal HF0=356.89 kJ

REF=Martin & Burcat JPC 108 (2004),7752 Max Lst Sq Error Cp @ 1300 K 0.5%

CBr2 RADICAL T 4/04C 1.BR 2. 0. 0.G 200.000 5000.000 B 171.81870	1
7.24933213E+00-8.58902960E-04 5.63433533E-07-9.47618492E-11 4.79033481E-15	2
3.89684139E+04-6.85243356E+00 2.95655957E+00 1.69562062E-02-3.03146341E-05	3
2.54004972E-08-8.13473762E-12 3.99004119E+04 1.39613758E+01 4.13140883E+04	4

75-61-6

CBr2F2 Halon 1202 FC-12B2 SIGMA=2 IAIBIC=1693.E-115 NU=1090,623,340,  
165,282,1153,367,831,330 HF298=-380+/-15 KJ REF=Gurvich 91 Max Lst Sq Error  
Cp @ 1200 K .26%

CF2Br2 RUS 91C 1.F 2.BR 2. 0.G 200.000 6000.000 B 209.81551	1
1.09382687E+01 2.12037940E-03-8.32403094E-07 1.42324890E-10-8.86069092E-15	2
-4.94636952E+04-2.47517671E+01 2.86773869E+00 3.32789929E-02-4.96372935E-05	3
3.65111014E-08-1.06608303E-11-4.76659753E+04 1.47813777E+01-4.57032345E+04	4

4471-18-5

CBr3 TRIBROMOMETHYL RADICAL SIGMA=3 STATWT=2 IA=IB=67.8823 IC=135.3705  
Nu=773(2),325.2,241,157.4(2) REF=JACOX HF298=63.68 kcal REF=Martin & Burcat  
JPC 108 (2004),7752 Max Lst Sq Error Cp @ 1200 K 0.14%

CBr3 T 2/04C 1.BR 3. 0. 0.G 200.000 6000.000 B 251.72270	1
9.23234074E+00 7.99416503E-04-3.16167102E-07 5.43171582E-11-3.39266689E-15	2
2.90724613E+04-1.27165464E+01 4.24874806E+00 2.27424021E-02-3.91200366E-05	3
3.19712338E-08-1.00758327E-11 3.00544432E+04 1.10469792E+01 3.20448373E+04	4

558-13-4

CBr4 TetraBromoMethane SIGMA=12 STATWT=1 IA=IB=IC=133.1264 NU=122(2),  
182(3),267,672(3) HF298=28.49+/-1.5 kcal HF0=148.90 kJ REF=Martin & Burcat  
JPC 108 (2004),7752 + Shimanouchi {HF298=28.68+/-3.6 kJ Gurvich 1991}

Max Lst Sq Error Cp @ 1200 K 0.14%.

CBr4 T04/04C 1.BR 4. 0. 0.G 200.000 6000.000 B 331.62670	1
1.21245741E+01 9.15750324E-04-3.63156485E-07 6.25001719E-11-3.90854515E-15	2
1.04626368E+04-2.67954406E+01 5.10358598E+00 3.39593343E-02-6.24045027E-05	3
5.36483603E-08-1.75710183E-11 1.17592386E+04 6.21074038E+00 1.43366428E+04	4

3889-76-7

CCl CHLOROMETHYLIDENE REF=Gurvich 1991 POLYNOMIALS FROM ORIGINAL TABLE.  
HF0=428.86 kJ REF=Kumaran et al JPC A 101,(1997),8653 HF298=432.61 kJ

Max Lst Sq Error Cp @ 400 K 0.33%

CCL g 8/99C 1.CL 1. 0. 0.G 200.000 6000.000 B 47.46340	1
4.17004432E+00 3.81512193E-04-1.31550106E-07 2.76232662E-11-2.22142338E-15	2
5.06890146E+04 2.94940729E+00 3.76699432E+00-1.49297520E-03 9.61147378E-06	3
-1.27137798E-08 5.27369513E-12 5.09118011E+04 5.66470872E+00 5.20308543E+04	4

Table 4 (continued)

1691-88-9

CClF RADICAL SIGMA=1 STATWT=1 A0=2.349 B0=0.214 C0=0.196 NU=1156,449,759  
 T0=25277.8 SIGMA=1 STATWT=1 A0=2.349 B0=0.214 C0=0.196 NU=1274,392,722  
 REF=Jacox 94 HF298=25.876+/-30. KJ REF=Gurvich 91 Max Lst Sq Error Cp @  
 1300 K 0.20%.

CFCL	g 9/99C	1.F	1.CL	1.	0.G	200.000	6000.000	B	66.46180	1
	5.94292685E+00	1.09262734E-03	-4.31688315E-07	7.39218712E-11	-4.51750496E-15					2
	1.08570002E+03	-3.48119469E+00	2.95153844E+00	9.82190319E-03	-8.63478127E-06					3
	1.86445560E-09	6.70154274E-13	1.86424703E+03	1.17893425E+01	3.10851439E+03					4

353-49-1

COClF CARBONIC CHLORIDE FLUORIDE SIGMA=1 STATWT=1 IA=7.480 IB=16.008  
 IC=23.31 NU=1868,1095,776,667,501,415 HF298=-426.8+/-33 KJ REF=JANAF

COCLF	J 6/61C	1.O	1.CL	1.F	1.G	300.000	5000.000	B	82.46150	1
	7.08810810E+00	3.18164790E-03	-1.37633160E-06	2.65440050E-10	-1.89289690E-14					2
	-5.38837810E+04	-8.68499361E+00	1.70666610E+00	2.27225650E-02	-3.01156390E-05					3
	2.04835660E-08	-5.65722280E-12	-5.26199020E+04	1.79876256E+01	-5.13293738E+04					4

1691-89-0

CClF2 RADICAL STATWT=2 IAIBIC=3700.E-117 NU=1148,1208,761,599,400,350  
 REF=TSIV 91 HF298=-275.+/-25 KJ Max Lst Sq Error Cp @ 1300 K 0.29%

CF2CL	tpis91C	1.F	2.CL	1.	0.G	200.000	6000.000	B	85.46021	1
	8.02826537E+00	2.01883629E-03	-7.90446242E-07	1.34920166E-10	-8.38987185E-15					2
	-3.59242877E+04	-1.26213146E+01	2.23327502E+00	2.07400983E-02	-2.34004409E-05					3
	1.18983365E-08	-2.08808316E-12	-3.44781789E+04	1.65915805E+01	-3.30747092E+04					4

75-72-9

CClF3 CHLOROTRIFLUOROMETHANE FC-13 SIGMA=3 IAIBIC=9450.

NU=1216(2),1108,782,562(2),475,347(2) HF298=-710.02+/-2.19 kJ REF=ATcT A  
 {HF298=-704.2 kJ REF=Gurvich 91; HF298=-707.93+/-3.3 KJ REF=JANAF} Max Lst  
 Sq Error Cp @ 1300 K 0.34%.

CF3CL	FC-13	ATcT/AC	1.F	3.CL	1.	0.G	200.000	6000.000	B	104.45861	1
	1.00910272E+01	2.97814049E-03	-1.16598694E-06	1.99015814E-10	-1.23754356E-14					2	
	-8.90715215E+04	-2.52797602E+01	1.20856943E+00	3.31175441E-02	-4.09170603E-05					3	
	2.42831659E-08	-5.60239796E-12	-8.69114408E+04	1.91836730E+01	-8.53952909E+04					4	

506-77-4

ClCN CYANOGEN CHLORIDE SIGMA=1 B0=0.19817 D0=5.503E-8 NU=2215.5,714.52,  
 378.3 x11=-4 x22=-0.65 x33=-7 x12=-6.8 x23=-7.236 x13=-2.8 g22=0.95  
 ALPHA1=8.25E-4 ALPHA2=-5.46E-4 ALPHA3=1.06E-3 HF298=137.95 kJ REF=JANAF

CLCN	J 6/66CL	1.C	1.N	1.	0.G	300.000	5000.000	A	61.47044	1
	5.49200210E+00	2.09872480E-03	-7.74159140E-07	1.38238820E-10	-9.23348640E-15					2
	1.47491610E+04	-3.73046245E+00	3.33908540E+00	1.03974680E-02	-1.37046500E-05					3
	9.50619620E-09	-2.59252600E-12	1.52375390E+04	6.83103255E+00	1.65917045E+04					4

2602-42-8

COCl CARBONYL CHLORIDE SIGMA=1 STATWT=2 IA=0.7159 IB=13.0005 IC=13.7165  
 NU=1880,570,281 HF298=-62.8+/-42 KJ REF=JANAF

COCL	J12/65C	1.O	1.CL	1.	0.G	300.000	5000.000	B	63.46310	1
	5.42912360E+00	1.61215350E-03	-6.60062800E-07	1.21271140E-10	-8.28586010E-15					2
	-9.33050070E+03	3.82874056E-01	4.28637920E+00	5.08689800E-03	-5.07294110E-06					3
	2.96479830E-09	-7.70934530E-13	-9.01252120E+03	6.25118670E+00	-7.54776465E+03					4

Table 4 (continued)

1605-72-7

CCl2 DICHLOROMETHYLENE SIGMA=2 TO (STATWT)=0 (1), 1000 (3) IA=1.6707  
 IB=22.7097 IC=24.4070 NU=730,757.9,335.2 HF298=238.1+/-1.7 HF0=230.5 kJ  
 REF=IUPAC 2003 Ruscic et al JPCRD

CCl2	IU3/03C	1.CL	2.	0.	0.G	200.000	6000.000	A	82.91670	1

1691-90-3

CCl2F RADICAL STATWT=2 IAIBIC=12000.E-117 NU=747,919,1143,300,400,350  
 REF= TSIV 91 HF298=-105.+/-20 KJ Max Lst Sq Error Cp @ 1300 K 0.24%

CFCL2	RUS	91C	1.F	1.CL	2.	0.G	200.000	6000.000	C	101.91450	1

75-71-8

CCl2F2 DICLORODIFLUOROMETHANE FREON-12 SIGMA=2 STATWT=1 IAIBIC=24900. NU=1098,  
 667,454.2,261.5,322,922,437,1169,442 REF=Gurvich 91 HF298=-490.8 kJ.  
 REF=TRC-6/89 Max Lst Sq ErrorCp @ 1200 K 0.29%.

CF2CL2	FREON-12	g	7/99C	1.F	2.CL	2.	0.G	200.000	6000.000	B	120.91291	1

75-44-5

CCL2O PHOSGEN HF298=-52.46 Kcal REF=Gurvich 91 {HF298=-219.077+/-0.28 kJ  
 REF=ATct A}

COCL2	RUS	91C	1.O	1.CL	2.	0.G	200.000	6000.000	B	98.91580	1

3170-80-7

CCl3 TRICHLOROMETHYL RADICAL SIGMA=6 STATWT=2 IA=IB=26.7361 IC=53.4723  
 NU=898 (2), 460, 450, 240 REF=JANAF HF298=17.0+/-0.6 Kcal REF= Hudgens et al  
 JPC 95, (1991), 4400 Max Lst Sq Error Cp @ 1200 K 0.20%.

CCl3 Radicals	S09/01C	1.CL	3.	0.	0.G	200.000	6000.000	B	118.36910	1

75-69-4

CCl3F TRICHLOROFLUOROMETHANE FC-11 SIGMA=3 STATWT=1 IAIBIC=58200. Nu=1081,  
 536,350,846 (2), 395 (2), 243 (2) REF=Gurvich 91 HF298=-283.7 kJ REF=TRC 6/89  
 Max Lst Sq Error Cp @ 1200 K 0.25%.

CFCL3	FC-11	g	7/99C	1.F	1.CL	3.	0.G	200.000	6000.000	B	137.36720	1

Table 4 (continued)

109026-11-1

CCL3O\* Trichloromethoxy Radical SIGMA=3 IA=33.36892 IB=34.98685 IC=51.86822  
 STATWT=2 NU=175,727,541,453,356,354,313,223,194 REF=Bozzelli, JPC,105,(2001),  
 4504 HF298=-4.4 kcal REF=NIST 2001 Max Lst Sq Error Cp @ 400 and 1200 K 0.23%  
 CCL3O\* Radical T12/01C 1.CL 3.0 1. 0.G 200.000 6000.000 B 134.36850 1  
 1.14909797E+01 1.56122123E-03-6.15126171E-07 1.05428446E-10-6.57464465E-15 2  
 -6.01860947E+03-2.78463259E+01 2.24693874E+00 4.50634603E-02-8.33966388E-05 3  
 7.30353534E-08-2.44131851E-11-4.28300968E+03 1.56894415E+01-2.21415333E+03 4

3170-80-7

CCl4 CARBONTETRACHLORIDE SIGMA=12 IAIBIC=118000.E-117 NU=797(3),460,315(3),  
 220(2) HF298=-95.6+/-2.5 kJ REF=Gurvich 1991/Manion JPCRD 31(2002),123.  
 {HF208=-95.367+/-0.55 kJ REF=ATcT A} HF298(liq)=-127.792+/-0.55 kJ REF=ATcT A  
 CCL4 L12/81C 1.CL 4. 0. 0.G 298.150 5000.000 B 153.82300 1  
 1.17390960E+01 1.28375530E-03-4.96502590E-07 8.35250200E-11-5.11072240E-15 2  
 -1.54190900E+04-3.07909700E+01 5.79662990E+00 1.79774390E-02-1.09565460E-05 3  
 -6.66818070E-09 6.45548980E-12-1.39409650E+04-5.70110920E-01-1.15237980E+04 4

13776-70-0

CD METHYLIDENE-D RAD SIGMA=1. T0=0(2)=18(2) WE=2101 WEXE=34.7 BE=7.808  
 ALFAE=.212 T0=23182(4) WE=2144.5 WEXE=48.7 BE=8.032 ALFAE=.26 T0=25993(2)  
 WE=1808 WEXE=201.5 BE=7.171 ALFAE=.528 T0=31828(2) WE=2073.4 WEXE=5.7  
 BE=7.880 ALFAE=0.282 RHO=1.0E-5 HF298=593.3 kJ REF=BURCAT (1980) MAX LST SQ  
 ERROR CP @ 5000K 0.52 %  
 CD T 2/80C 1D 1 0 0G 300.000 5000.000 B 14.0251 1  
 0.26841459E+01 0.18855776E-02-0.48628311E-06 0.38441708E-10 0.64605384E-15 2  
 0.70531750E+05 0.70322804E+01 0.35427971E+01-0.47720969E-03 0.10656331E-05 3  
 0.73458772E-09-0.74328873E-12 0.70311938E+05 0.26416878E+01 0.71355979E+05 4

676-49-3

CDH3 METHANE-D STATWT=1. SIGMA=3. A0=C0=5.25 B0=3.878 NU=2945,2200,1300,  
 3017(2),1471(2),1155(2) HF298=-78.45 kJ REF=BURCAT (1980) MAX LST SQ ERROR CP @  
 1300K 0.94% .  
 CDH3 T05/79C 1D 1H 3 0G 300.000 5000.000 B 17.0489 1  
 0.29389458E+01 0.84684640E-02-0.28219238E-05 0.41319725E-09-0.21738508E-13 2  
 -0.10964586E+05 0.42781033E+01 0.26380539E+01 0.41823313E-02 0.72133871E-05 3  
 -0.58564389E-08 0.79961938E-12-0.10462590E+05 0.75096125E+01-0.94354328E+04 4

24286-05-3

CDO FORMYL-D RAD STATWT=2. SIGMA=1 A0=14.8803888 B0=1.28210559 C0=1.1733573  
 NU=858,1814,1910 Calculated from original tables of direct summation HF0=40.52  
 kJ REF=Marenich & Boggs JCP 107 (2003),2343 MAX LST SQ ERROR CP @ 1500 K 0.66%  
 CDO IU5/03C 1.D 1.0 1. 0.G 200.000 6000.000 A 30.02420 1  
 3.94049716E+00 3.05762633E-03-9.52036760E-07 1.60149611E-10-1.09618875E-14 2  
 3.47656882E+03 3.86074826E+00 3.95151630E+00-9.48107671E-04 1.00805008E-05 3  
 -1.02322511E-08 3.34361621E-12 3.71808874E+03 4.89958505E+00 4.92451113E+03 4

14863-68-4

CD2 METHYLENE-D2 RAD SIGMA=2. T0=0(3)=30300(1) IA=.0744 IB=.60878 IC=.6831  
 NU=2115,767,2345 T0=2600(1) IA=.24223 IB=.50049 IC=.74272 NU=2209,926,2273  
 T0=9700(1) IA=.06458 IB=.6511 IC=.71567 NU=2093,545,2338 REF=Burcat 1980  
 HF298=382.59 KJ MAX LST SQ ERROR CP @ 1300K 0.72% .  
 CD2 T05/80C 1D 2 0 0G 300.000 5000.000 B 16.0392 1  
 0.36602430E+01 0.33572798E-02-0.12381643E-05 0.20197106E-09-0.12083819E-13 2  
 0.44684898E+05 0.25685925E+01 0.38409843E+01 0.12651016E-02 0.18910869E-05 3  
 -0.77415541E-09-0.25377709E-12 0.44799531E+05 0.22334236E+01 0.46014570E+05 4

Table 4 (continued)

1664-98-8

CD2O METHANAL-D2 (FORMALDEHIDE-D2) STATWT=1. SIGMA=2 IA=.59244 IB=2.5995  
 IC=3.2048 NU=2056,1700,1106,2160,990,938 HF298=-27.46 kcal. REF=CHAO,WILHOIT &  
 HALL MAX LST SQ ERROR CP @ 1300 K 0.8 % .

CD2O	T 8/81C	1D	20	1	OG	300.000	5000.000	B	32.0386	1
	0.46622076E+01	0.50203055E-02	-0.18413848E-05	0.29739944E-09	-0.17558905E-13					2
	-0.15805738E+05	-0.17688099E+01	0.25921259E+01	0.59901401E-02	0.39293818E-05					3
	-0.62653172E-08	0.18746567E-11	-0.14881922E+05	0.10390113E+02	-0.13818716E+05					4

2122-44-3

CD3 METHYL-D3-RAD STATWT=1. SIGMA=6. IA=IB=.596 IC=1.191 T0=0(2),46200(2)  
 NU=2153,463,2381(2),1026(2) HF298=138.69 kJ REF=BURCAT(1980) MAX LST SQ ERROR  
 Cp @ 1300K 0.71%

CD3	T11/79C	1D	3	0	OG	300.000	5000.000	B	18.0533	1
	0.44567032E+01	0.49626939E-02	-0.17476059E-05	0.27139846E-09	-0.15351469E-13					2
	0.14782500E+05	-0.23810688E+01	0.34687710E+01	0.49496330E-02	0.19827057E-05					3
	-0.36768906E-08	0.12036257E-11	0.15276805E+05	0.36025786E+01	0.16680117E+05					4

13031-32-8

CD3NO2 Nitro-Methane D3 STATWT=1 SYMNO=3 IA = 6.96802 IB = 10.1365 IC = 15.945  
 IRED=0.88227 V(2)=0.16 kcal/mole ROSYM=2 NU = 435,542,631,885,942,1038,1046,  
 1075,1404,1548,898,2147,2283,2317 HF(298)= -14.768 kcal/mole REF = A. Burcat  
 TAE Report 824a May 1999 Max Lst Sq Error Cp @ 1300 K 0.61%

CD3NO2	T01/00C	1.D	3.N	1.O	2.G	200.000	6000.000	B	64.05885	1
	8.82522748E+00	9.35166732E-03	-3.53835387E-06	5.90989862E-10	-3.62227246E-14					2
	-1.13067808E+04	-2.08804860E+01	2.37203218E+00	1.42408389E-02	2.16286890E-05					3
	-4.09339693E-08	1.78857173E-11	-8.89033378E+03	1.55850830E+01	-7.43151250E+03					4

558-20-3

CD4 METHANE-D4 STATWT=1. SIGMA=12. A0=B0=C0=2.634 NU=2109,1092(2),2259(3),  
 996(3) REF=BURCAT (1980) MAX LST SQ ERROR CP @ 1300K 0.94% . HF298=-89.01 kJ

CD4	RRHO	T05/79C	1D	4	0	OG	300.000	5000.000	B	20.0674	1
	0.47153826E+01	0.75838268E-02	-0.27129208E-05	0.42667048E-09	-0.24420637E-13					2	
	-0.12937410E+05	-0.61998917E+01	0.19176292E+01	0.91806799E-02	0.47843714E-05					3	
	-0.88772119E-08	0.29830964E-11	-0.11712711E+05	0.10130220E+02	-0.10705742E+05					4	

558-20-3

CD4 METHANE-D4 ANHARMONIC. DATA AS FOR RRHO. X11=-13.6 X12=-1.54 X13=-40.6  
 X14=-2.2 X22=-.2 X23=-4.8 X24=-10.9 X33=-9.6 X34=-12.7 X44=-6.4 ALFA1=.07  
 ALFA2=-.06 ALFA3=.03 ALFA4=.05 REF=TSIV(CH4) MAX LST SQ ERROR CP @ 1300K .9%

CD4 * ANHARMONIC	T06/81C	1D	4	0	OG	300.000	5000.000	A	20.0674	1
	0.44482183E+01	0.81195608E-02	-0.27020378E-05	0.43419712E-09	-0.24605867E-13					2
	-0.12860102E+05	-0.47861973E+01	0.19425707E+01	0.89269280E-02	0.54267666E-05					3
	-0.89088488E-08	0.28879408E-11	-0.11714484E+05	0.10036650E+02	-0.10705742E+05					4

811-98-3

CD4O (CD3OD) Methanol-d4 STATWT=1 SIGMA=1 IA=1.32750 IB=4.37622 IC=4.60714  
 IR=0.0993 ROSYM=3 V(3)=373.2 cal. NU=2274,2260,2080,1024,1135,1060,776,983,  
 2228,1080,892 REF=Shimanouchi, NIST Webbook 2001. HF0=-207.07 kJ based on  
 HF0(CH3OH)=-190.114 kJ Max Lst Sq Error Cp @ 200 K 0.73%.

CD3OD	T06/02C	1.D	4.O	1.	O.G	200.000	6000.000	B	36.06681	1
	6.04917775E+00	8.89558611E-03	-3.31066729E-06	5.46963308E-10	-3.32659293E-14					2
	-2.89654851E+04	-8.37255929E+00	3.88645048E+00	-2.67005954E-03	4.85836046E-05					3
	-6.24068205E-08	2.47546189E-11	-2.75371566E+04	6.97316454E+00	-2.61794946E+04					4

Table 4 (continued)

3889-75-6

CF FLUOROMETHYLIDENE SIGMA=1 Be=1.4172 cm<sup>-1</sup> WE=1308.1 WEXE=11.10  
 ALPHAE=0.0184 T0 (STATWT)=0 (2), 77.11 (2), 25000 (4), 42705 (2), 49452 (2)  
 HF298=255.2+/-8 KJ REF=JANAF Calculated from Original TRC 6/88 tables  
 HF298=246.932+/-0.7 kJ REF=ATcT A {HF298=255.23+/-8 kJ REF=Gurvich 91;  
 HF298=242.3 kJ REF=TRC 6/88} Max Lst Sq Error Cp @ 700 K 0.20%  
 CF ATcT/AC 1.F 1. 0. 0.G 200.000 6000.000 B 31.00910 1  
 3.74644062E+00 8.01632001E-04-2.95064248E-07 5.03803598E-11-3.08738254E-15 2  
 2.84554882E+04 3.84191679E+00 3.99598712E+00-4.62546013E-03 1.58270762E-05 3  
 -1.73528410E-08 6.45553921E-12 2.86045210E+04 3.67054970E+00 2.96989239E+04 4

33412-11-2

CF+ Fluoromethylidene Ion SIGMA=1 STATWT=1 We=1380 WeXe=11.6 Be=1.4361  
 ALFAE=0.193 T0=35000. STATWT=6. REF=JANAF 70 HF298=1131.29+/-0.92 kJ  
 REF=ATcT A {HF0=1327.6+/-0.96 kJ REF=JANAF 70} Max Lst Sq Error Cp @ 1300 K  
 0.26%.  
 CF+ ATcT/AC 1.F 1.E -1. 0.G 298.150 6000.000 B 31.00855 1  
 3.67563573E+00 8.53237936E-04-3.05718490E-07 4.97729598E-11-2.84072768E-15 2  
 1.34839163E+05 2.84780658E+00 3.58302425E+00-1.86525968E-03 8.53751431E-06 3  
 -9.32468003E-09 3.33948856E-12 1.35018426E+05 4.07366057E+00 1.36062378E+05 4

1495-50-7

FCN CYANOGEN FLUORIDE STATWT=1 SIGMA=1 B0=0.353106 cm<sup>-1</sup> NU=2290,1077,420 (2)  
 HF298=35.98+/-16.7 kJ REF=JANAF  
 FCN J 6/69F 1.C 1.N 1. 0.G 300.000 5000.000 C 45.01614 1  
 5.08985570E+00 2.41706840E-03-9.76827660E-07 1.78134420E-10-1.21185670E-14 2  
 2.57807810E+03-2.87278107E+00 3.25169410E+00 8.30731440E-03-8.36663580E-06 3  
 4.41256440E-09-9.08824230E-13 3.05511980E+03 6.44214763E+00 4.32821878E+03 4

1871-24-5

COF CARBONYLFLUORIDE SIGMA=1 STATWT=2 IA=0.3399 IB=7.8768 IC=8.2167  
 NU=1855,1018,626 HF298=-171.5+/-63 KJ REF=JANAF  
 COF J12/65C 1.O 1.F 1. 0.G 300.000 5000.000 B 47.00880 1  
 4.89082140E+00 2.21797030E-03-9.25507250E-07 1.72701200E-10-1.19553430E-14 2  
 -2.23579840E+04 9.92783959E-01 3.20197270E+00 5.58377700E-03-1.49054810E-06 3  
 -2.31260690E-09 1.36143530E-12-2.18170430E+04 1.00607391E+01-2.06312897E+04 4

2154-59-8

CF2 DIFLUOROMETHYLENE SIGMA=2 STATWT=1 A0=2.947 B0=0.417 C0=0.365 NU=1225,  
 1114,666 T0=19828 SIGMA=2 STATWT=3 A0=4.577 B0=0.334 C0=0.311 Nu=1180,1011,  
 517 T0=37226 SIGMA=2 STATWT=1 A0=4.577 B0=0.334 C0=0.311 Nu=1180,1011,  
 496 REF=Gurvich 91 HF298=-191.26+/-1.36 kJ REF=ATcT A {HF298=-182.00+/-6.3 kJ  
 REF=JANAF 6/70; HF298=-186.6 kJ REF=TRC 6/88} Max Lst Sq Error Cp @ 400 K 0.34%  
 CF2 ATcT/AC 1.F 2. 0. 0.G 200.000 6000.000 B 50.00751 1  
 5.35787718E+00 1.80622418E-03-7.80465045E-07 1.47642691E-10-9.44754424E-15 2  
 -2.49202461E+04-2.63410779E+00 3.56435487E+00 1.23021056E-03 1.39909866E-05 3  
 -2.13708286E-08 9.10710807E-12-2.42062274E+04 7.83907808E+00-2.30031595E+04 4

54250-40-7

CF2+ DiFluoroMethylene Ion SIGMA=2 STATWT=2 IA=0.7415 IB=7.9066 IC=8.6481  
 Nu=1588,1100,650 T0=40180 STATWT=2 REF=Jacox 94 JANAF HF298=917.23+/-1.6 kJ  
 REF=ATcT A {HF0=337.4+/-0.9 kcal REF=JANAF 12/70} Max Lst Sq Error Cp @ 1300 K  
 0.37%.  
 CF2+ ATcT/AC 1.F 2.E -1. 0.G 298.150 6000.000 50.00696 1  
 5.16266064E+00 1.83946474E-03-7.10161849E-07 1.20015997E-10-7.40239685E-15 2  
 1.08446811E+05-7.83454761E-01 3.14394077E+00 5.16389849E-03 7.51371704E-07 3  
 -5.04934253E-09 2.39470869E-12 1.09128054E+05 1.02287592E+01 1.10292729E+05 4



Table 4 (continued)

353-50-4

CF2O SIGMA=2 STATWT=1 A0=0,3940571 B0=.3920397 C0=0.1961657 Nu=1944,1242, 962,774,619,582 HF298=-640+/-5 kJ REF= Gurvich 1991 {HF298=-640.1+/-1.1 kJ REF=ATcT A} Max Lst Sq Error Cp @ 1300 K 0.40%.

COF2	RUS 91C	1.0	1.F	2.	0.G	200.000	6000.000	B	66.00721	1
6.81631730E+00	3.16473282E-03	-1.21776269E-06	2.05582261E-10	-1.26893125E-14						2
-7.95482716E+04	-9.52864566E+00	2.12979489E+00	1.41019723E-02	-5.94381359E-06						3
-5.30544790E-09	3.97367469E-12	-7.81745339E+04	1.51109093E+01	-7.69738686E+04						4

2264-21-3

CF3 TRIFLUOROMETHYL SIGMA=3 STATWT=2 A0=0.364 B0=0.364 C0=0.189 NU=1089, 701,1260(2),509(2) HF298=-467.4+/-1.97 kJ REF=ATcT A {HF298=467.4 kJ REF=TRC 6/88; HF298=-470.28+/-4.2 KJ REF=JANAF} Max Lst Sq Error Cp @ 1300 K 0.36%.

CF3	ATcT/AC	1.F	3.	0.	0.G	200.000	6000.000	B	69.00591	1
7.42981696E+00	2.61728694E-03	-1.02141596E-06	1.73975666E-10	-1.08028191E-14						2
-5.89817716E+04	-1.22816891E+01	2.38179059E+00	1.37269527E-02	-3.47674937E-06						3
-9.01697393E-09	5.57384083E-12	-5.74893250E+04	1.43743316E+01	-5.62149784E+04						4

18851-76-8

CF3+ TriFluoroMethyl Ion SIGMA=6 STATWT=1 IA=IB=8.3708 IC=16.7416 Nu=888, 791,1662(2),480 REF=Jacox 98 and JANAF 12/71 HF298=411.627+/-1.96 kJ REF=ATcT A {HF0=412.07 kJ REF=JANAF 71} Max Lst Sq Error Cp @ 1300 K 0.44%.

CF3+	ATcT/AC	1.F	3.E	-1.	0.G	298.150	6000.000		69.00536	1
6.82085071E+00	3.16762437E-03	-1.22042222E-06	2.06188834E-10	-1.27330282E-14						2
4.69690028E+04	-9.99626735E+00	2.31882353E+00	1.60922297E-02	-1.53695233E-05						3
7.35412967E-09	-1.43415092E-12	4.82223927E+04	1.32252874E+01	4.95070666E+04						4

2314-97-8

CF3I TRIFLUOROIODOMETHANE SIGMA=3 IA=14.7097 IB=IC=54.7578 NU=1185(2),1074, 742,539(2),284,260(2) HF298=-589.11+/-3.3 KJ REF=JANAF {HF298=588.89+/-1.96 REF=ATcT A}

CF3I	J 6/69C	1F	3I	1	0G	200.000	6000.000	B	195.91068	1
0.10375057E+02	0.26880979E-02	-0.10525827E-05	0.17967408E-09	-0.11173263E-13						2
-0.74551179E+05	-0.24024941E+02	0.25628907E+01	0.28507572E-01	-0.33699705E-04						3
0.18730304E-07	-0.39219886E-11	-0.72621870E+05	0.15237838E+02	-0.70853243E+05						4

21811-29-0

CF3O Radical SIGMA=3 STATWT=2 IA=13.9573 IB=14.4617 IC=15.2254 NU=1289, 1250,1188,897,609,587,566,395,242.4 HF298=-150.74 kcal HF0=-149.60 kcal REF=Burcat G3B3 calc Max Lst Sq Error Cp @ 1300 K 0.34%

CF3O Radical	T07/04C	1.F	3.O	1.	0.G	200.000	6000.000	B	85.00531	1
9.76423201E+00	3.30092424E-03	-1.28961521E-06	2.19815579E-10	-1.36560199E-14						2
-7.94771282E+04	-2.37694198E+01	1.82041152E+00	2.65327204E-02	-2.45066904E-05						3
7.86171828E-09	2.73540764E-13	-7.73780958E+04	1.68621895E+01	-7.58568931E+04						4

17167-98-5

CF3O2 CF3O\* RADICAL SIGMA=1 STATWT=2 IA=14.4736 IB=24.9063 IC=25.19106 IR(OO)=2.0124 ROT BARRIER V(3)=1217.14 cm-1 ROSYM=3 NU=1341,1288,1251,1124, 878.6,686.6,593.2,570.8,442,420,278.8 HF298=-149.95 kcal REF=Melius database F42D private communication (HF298=-173.5 kcal REF=Bozzelli's Therm) Max Lst Sq Error Cp @ 1300 K 0.33%.

CF3O2 RADICAL	T10/97C	1.F	3.O	2.	0.G	200.000	6000.000	B	101.00501	1
1.22037091E+01	3.39739140E-03	-1.33527750E-06	2.28468036E-10	-1.42307780E-14						2
-7.99109047E+04	-3.41946453E+01	1.55041706E+00	3.73972544E-02	-4.08839888E-05						3
1.89635072E-08	-2.54712965E-12	-7.72518205E+04	1.95583929E+01	-7.54523069E+04						4

Table 4 (continued)

75-73-0

CF4 TETRAFLUOROMETHANE FC-14 SIGMA=12 IAIBIC=3180. Nu=909,435(2),632(3),  
1283(3) REF=Gurvich 91 HF298=-933.12 kJ REF=TRC 94 {HF298=-933.0 kJ  
REF=Zachariah, Westmoreland, Burgess, Tsang& Melius JPC 100,(1996),8737;  
HF298=-933.2 kJ REF=Gurvich 91; HF298=-933.399+/-0.53 kJ REF=ATcT A} Max Lst  
Sq Error Cp @ 1300 K 0.40%

CF4	FC-14	g	7/99C	1.F	4.	0.	0.G	200.000	6000.000	B	88.00431	1
9.47336526E+00	3.59407743E-03	-1.40334012E-06	2.39113889E-10	-1.48513407E-14								2
-1.15816621E+05	-2.49736848E+01	1.05119594E+00	2.78318369E-02	-2.46683439E-05								3
6.75882532E-09	9.14850873E-13	-1.13574198E+05	1.81936795E+01	-1.12227900E+05								4

3315-37-5

CH METHYLLIDYNE RADICAL CALCULATED FROM Gurvich's Tables IB=01973 We=2732.46  
HF298=595.8+/-0.6 kJ HF0=592.5+/-0.6 kJ REF= Ruscic et al JPCRD 2005  
{HF298=596.30+/-0.25 kJ REF=ATcT A}

CH	IU3/03 C	1.H	1.	0.	0.G	200.000	6000.000	A	13.01864	1
0.25209369E+01	0.17653639E-02	-0.46147660E-06	0.59289675E-10	-0.33474501E-14						2
0.70946769E+05	0.74051829E+01	0.34897583E+01	0.32432160E-03	-0.16899751E-05						3
0.31628420E-08	-0.14061803E-11	0.70612646E+05	0.20842841E+01	0.71658188E+05						4

17141-28-5

CHBr BROMOMETHYLENE SIGMA=1 STATWT=2 IA=0.1804 IB=6.6096 IC=6.7900  
NU=2905,1156,683 T0=910. T0=11937 HF298=377.86+/-2 kJ REF=Martin & Burcat  
JPC 108 (2004),7752 Max Lst Sq Error Cp @ 1300 K 0.10%

CHBR	T 2/04C	1.H	1.BR	1.	0.G	200.000	6000.000	C	92.92264	1
5.28977462E+00	1.41064245E-03	-4.82019526E-07	7.96049279E-11	-4.95428931E-15						2
4.36578258E+04	-4.88685664E-01	2.94301638E+00	6.74163923E-03	3.17779159E-07						3
-8.95038102E-09	5.24099443E-12	4.42807928E+04	1.16897579E+01	4.54454923E+04						4

593-98-6

CHBrClF BromoChloroFluoroMethane SIGMA=1 STATWT=1 IAIBIC=28600. Nu=3026,  
1311,1206,1079,788,664,426,314.5,225 HF298=-230+/-15 kJ REF=Gurvich 91  
{HF298=-229.95+/-8 kJ REF=Ruscic G3B3 calc} Max Lst Sq Error Cp @ 1300 K 0.33%

CHFCLBr	A 6/05	***WARNING***	G	200.000	6000.000	B	147.37374	1
8.52418597E+00	4.15098908E-03	-1.53297038E-06	2.52169636E-10	-1.52968772E-14				2
-3.07897222E+04	-1.40266403E+01	2.84647307E+00	2.04936069E-02	-1.70058829E-05				3
4.11372351E-09	9.31156800E-13	-2.92803600E+04	1.50636514E+01	-2.76624840E+04				4

1511-62-2

CHBrF2 (HBFC-22B1) STATWT=1 SIGMA=1 IAIBIC=8790. NU=3031,1280,1136,  
717,577,240,1344,1108,323 REF=Gurvich 91 HF298=-425.46+/-1.07 kJ REF=ATcT A  
{HF298=-422+/-2 kJ REF=TSIV 91} Max Lst Sq Error Cp @ 1300 K 0.38%.

CHBRF2	HBFC-22B1	ATcT/AC	1.H	1.F	2.BR	1.G	200.000	6000.000	B	130.91945	1
7.99574233E+00	4.68075570E-03	-1.73758062E-06	2.86772954E-10	-1.74346268E-14							2
-5.42115449E+04	-1.24352101E+01	3.31738394E+00	1.31438938E-02	1.77618966E-06							3
-1.45480682E-08	7.51885656E-12	-5.27345603E+04	1.27225958E+01	-5.11707846E+04							4

14362-13-1

CHBr2 BromoMethyl Radical SIGMA=2 STATWT=2 IA=2.1915 IB=68.71279  
IC=70.84395 NU=3202,1165,778,633,424.5,185 REF=JACOX HF298=47.44 kcal  
REF=Martin & Burcat JPC 108 (2004),7752 {HF298=54.3 REF=McMillen Golden 1982}  
Max Lst Sq Error Cp @ 6000 K 0.22%

CHBR2	T 2/04C	1.H	1.BR	2.	0.G	200.000	6000.000	B	172.82664	1
6.98912016E+00	2.60344199E-03	-9.18425207E-07	1.46505921E-10	-8.69891195E-15						2
2.14931363E+04	-5.09358817E+00	2.78930563E+00	1.91599709E-02	-2.64119986E-05						3
1.80644053E-08	-4.78973925E-12	2.23892774E+04	1.53305876E+01	2.38725986E+04						4

Table 4 (continued)

75-25-2

CHBr3 BROMOFORM SIGMA=3 STATWT=1 IA=68.7854 IB=68.7854 IC=135.4688  
 Nu=3050,1146(2),669(2),541,222,155(2) HF298=54.27 kJ REF=Martin & Burcat JPC  
 108 (2004),7752 Max Lst Sq Error Cp @ 6000 K 0.25%  
 CHBR3 BROMOFORM T 2/04C 1.H 1.BR 3. 0.G 200.000 6000.000 B 252.73064 1  
 9.33702350E+00 3.32595225E-03-1.21194327E-06 1.97616744E-10-1.19155492E-14 2  
 3.29366728E+03-1.50773866E+01 3.64744682E+00 2.37778637E-02-2.97514832E-05 3  
 1.82750488E-08-4.31214235E-12 4.61115559E+03 1.30919213E+01 6.52672016E+03 4

2108-20-5

CHCL RADICAL SIGMA=1 STATWT=1 NU=3000,1201,815 A0=15.759 B0=0.605 C0=0.581  
 T0=1470. SIGMA=1 STATWT=3 A0=15.759 B0=0.605 C0=0.581 Nu=3000,1201,850  
 T0=12280 SIGMA=1 STATWT=1 A0=15.759 B0=0.605 C0=0.581 Nu=3000,987,873  
 REF=TSIV 91 + Jacox HF298=297.1 REF=TRC 12/93 {HF298=308.28 kJ REF=TSIV 91}  
 MAX LST SQ ERROR CP @ 700 K 0.47%  
 CHCL g 9/99C 1.H 1.CL 1. 0.G 200.000 6000.000 48.47134 1  
 6.65408153E+00 1.74570320E-04-4.37504887E-08 8.56396359E-12-6.70548082E-16 2  
 3.32813768E+04-1.07631238E+01 4.62343477E+00-1.03131685E-02 5.00558316E-05 3  
 -6.21788813E-08 2.46055782E-11 3.44816438E+04 3.27962111E+00 3.57327131E+04 4

33272-71-8

CHClF CHLOROFLUOROMETHYL RADICAL SIGMA=1 STATWT=2 IAIBIC=370E-117 NU=3000,  
 1150,760,1300,1200,380 REF=TSIV HF298=-83.14 KJ  
 CHCLF L 4/86C 1.H 1.CL 1.F 1.G 298.150 5000.000 C 67.47030 1  
 0.65730400E 01 0.29733933E-02-0.10222593E-05 0.15512820E-09-0.85432759E-14 2  
 -0.12409480E 05-0.51201038E 01 0.33409529E 01 0.10670263E-01-0.39450997E-05 3  
 -0.48872693E-08 0.34919463E-11-0.11491043E 05 0.11776594E 02-0.10064453E 05 4

75-45-6

CHClF2 CLORODIFLUOROMETHANE (HCFC-22) SIGMA=1 STATWT=1 IA=8.2004  
 IB=17.3858 IC=24.0489 NU=3026,1312,1178,806,598,419,1343,1115,369 REF=Chen  
 JPCRD 5, (1976),571 HF298=-490.72+/-2.28 kJ REF=ATcT A {HF298=-475.+/-15. KJ  
 REF=TSIV 79} Max Lst Sq Error Cp @ 1300 K 0.41%  
 CHF2CL HCFC-22 ATcT/AC 1.H 1.F 2.CL 1.G 200.000 6000.000 B 86.46815 1  
 7.76128170E+00 4.91347187E-03-1.82716472E-06 3.01909107E-10-1.83696720E-14 2  
 -6.20359067E+04-1.29719847E+01 2.58815578E+00 1.48447979E-02 1.50136954E-07 3  
 -1.39370626E-08 7.48510026E-12-6.04284954E+04 1.47131828E+01-5.90197137E+04 4

3474-12-2

CHCL2 RADICAL SIGMA=2 STATWT=2 NU=757,902,3000,300,1226,360 IAIBIC=15100E-  
 117 REF=TSIV Calculated from original TRC tables to 3000. K and extrapolated  
 using Wilhoit polynomials HF298=95.8 kJ REF=TRC 12/93 {HF298=73.9 kJ  
 REF=Gurvich 79} MAX LST SQ ERROR CP @ 1300 K 0.21%.  
 CHCL2 g12/93C 1.H 1.CL 2. 0.G 200.000 6000.000 C 83.92404 1  
 6.80210912E+00 2.86000875E-03-1.03664482E-06 1.68416656E-10-1.01027167E-14 2  
 9.16929806E+03-5.70765415E+00 3.41194137E+00 1.40168850E-02-1.42771614E-05 3  
 6.24721839E-09-6.15096358E-13 9.99583151E+03 1.12991582E+01 1.15220260E+04 4

75-43-4

CHCl2F DICHLOROFLUOROMETHANE FC-21 TRC DATA EXTRAPOLATED TO 5000 K USING  
 WILHOIT'S POLYNOMIALS. HF298=-68.1 Kcal  
 CHCL2F FC-21 P12/75C 1.H 1.CL 2.F 1.G 298.150 5000.000 C 102.92330 1  
 0.85083923E 01 0.40345713E-02-0.14268226E-05 0.22247303E-09-0.12630173E-13 2  
 -0.37427910E 05-0.15411654E 02 0.31107159E 01 0.16295891E-01-0.47331187E-05 3  
 -0.94798160E-08 0.61323750E-11-0.35862211E 05 0.12963858E 02-0.34269462E 05 4

Table 4 (continued)

345234-24-4

\*CCl2OH Dichloromethanol Radical STATWT=2 IA=11.2982579 IB=26.2798183  
 IC=37.05366 IR=0.13684 ROSYM=2 V(2)=734.5 kcal REF+ Bozzelli et al JPC 105,  
 (2001, 4504 HF298=-22.7 kcal REF=NIST 2001 MAX LST SQ ERROR Cp @ 400 & 1200 K  
 0.19%.

CCL2OH RADICAL	T12/01C	1.CL	2.O	1.H	1.G	200.000	6000.000	B	99.92374	1	
						9.04056721E+00	2.87032241E-03	-9.87387267E-07	1.55039889E-10	-9.11112809E-15	2
						-1.44761757E+04	-1.59551709E+01	2.11156612E+00	3.46879806E-02	-5.98032879E-05	3
						5.05956283E-08	-1.65224560E-11	-1.31581816E+04	1.68137718E+01	-1.14230183E+04	4

67-66-3

CHCl3 (CHLOROFORM) TRICHLOROMETHANE TRC DATA EXTRAPOLATED TO 5000 K USING  
 WILHOIT'S POLYNOMIALS. HF298=-102.928 kJ {HF298=-103.259+/-0.77 kJ REF=ATcT A}  
 HF298(liq)=-133.784+/-0.72 kJ REF=ATcT A

CHCL3	P	6/81C	1.H	1.CL	3.	0.G	298.150	5000.000	C	119.37790	1			
						0.89938030E	01	0.35652192E-02	-0.12537648E-05	0.19479131E-09	-0.11032021E-13	2		
						-0.15609000E	05	-0.17631689E	02	0.36819801E	01	0.16611021E-01	-0.66180801E-05	3
						-0.81291560E-08	0.59433135E-11	-0.14141844E	05	0.99835104E	01	-0.12379277E	05	4

35911-92-3

CCl3OH TrichloroMethanol SIGMA=1 IA=34.984273 IB=35.31263 IC=50.644705  
 IR=0.13695 ROSYM=3 V(3)=629.6 cm-1 NU=3604,1311,1113,784(2),522,417,392,344,  
 333,247 HF298=-65.960+/-0.76 kcal REF=Bozzelli et al. JPC 105 (2001),4504.  
 Max Lst Sq Error Cp @ 1200 K 0.23%

CCl3OH Bozzelli	T12/01C	1.CL	3.O	1.H	1.G	200.000	6000.000	B	135.37644	1	
						1.15617652E+01	3.40353310E-03	-1.20404095E-06	1.92737569E-10	-1.14815680E-14	2
						-3.71195773E+04	-2.87400802E+01	1.93683294E+00	4.74652448E-02	-8.26081967E-05	3
						7.00496001E-08	-2.29009678E-11	-3.52771007E+04	1.68237134E+01	-3.31921713E+04	4

23171-70-2

CHD2NO2 Nitro-Methane D2 STATWT = 1 SIGMA = 1 IA = 6.76188 IB = 9.55869  
 IC = 15.2841 I(red) = 0.754032 V(2) = 0.125 kcal/mole NU= 443,577,643,896,  
 923,977,1060,1285,1285,1405,1554,2187,2313,3000 REF=McKean & Watt J. Molec.  
 Struct. 61, (1976), 164. HF298= -13.795 kcal/mole REF = A. BURCAT TAE  
 Report # 824a, 1998 Max Lst Sq Error Cp @ 1300 K 0.58%

\*\*\* WARNING \*\*\* THIS COMPOUND CONTAINS 5 ELEMENTS BUT THE FORMULA LINE NO 1 CAN  
 ACCOMODATE ONLY FOUR. See 9-THERM POLYNOMIALS\*\*\*\*

NITRO-METHANE D2	T04/98	WARNING!	G	200.000	6000.000	B	63.05268	1	
				8.08961148E+00	9.83765066E-03	-3.67240992E-06	6.08123340E-10	-3.70523025E-14	2
				-1.05585014E+04	-1.58799705E+01	2.86575841E+00	9.70884039E-03	2.98575468E-05	3
				-4.74818909E-08	1.98756686E-11	-8.40693607E+03	1.46207846E+01	-6.94164250E+03	4

676-80-2

CHD3 METHANE-D3 STATWT=1. SIGMA=3. AE=CE=2.62 BE=3.27 NU=2993,2142,1003,  
 2263(2),1291(2),1036(2) HF298=-85.29 kJ. REF=BURCAT MAX LST SQ ERROR CP @  
 1300K 0.94% .

CHD3	T05/79C	1H	1D	3	0G	300.000	5000.000	B	19.0612	1	
						0.40764599E+01	0.79434291E-02	-0.27834194E-05	0.42990389E-09	-0.24151396E-13	2
						-0.12245391E+05	-0.13486305E+01	0.21469107E+01	0.74287578E-02	0.56749586E-05	3
						-0.77548528E-08	0.21464679E-11	-0.11265895E+05	0.10451311E+02	-0.10257971E+05	4

Table 4 (continued)

13453-52-6

CHF RADICAL STATWT=2 SIGMA=1 IA=0.172 IB=2.240 IC=2.412 NU=1189,1404,2733  
 HF298=39.0 kcal REF=Zachariah,Westmoreland,Burgess,Tsang&Melius JPC,100,(1996),  
 8737-8747 Max Lst Sq. Error Cp @ 6000 K 0.51%

CHF RADICAL	T 8/99C	1.H	1.F	1.	0.G	200.000	6000.000	B	32.01734	1
		3.81407171E+00	2.91531169E-03	-1.06577623E-06	1.74013614E-10	-1.04973609E-14				2
		1.82312890E+04	4.65785213E+00	4.41475567E+00	-5.51349381E-03	2.18470808E-05				3
		-2.34089450E-08	8.48772577E-12	1.84034839E+04	3.21728174E+00	1.96254500E+04				4

2670-13-5

CHF2 RADICAL STATWT=2 IAIBIC=92.E 117 NU=1165,1175,3000,600,1316,500  
 REF=TSIV 1979 HF298=-254. KJ Max Lst Sq Error Cp @ 6000 K 0.38%

CHF2	RUS 79C	1H	1F	2	0G	200.000	6000.000	C	51.01575	1
		0.58958702E+01	0.37705626E-02	-0.13837102E-05	0.22663348E-09	-0.13705690E-13				2
		-0.32778360E+05	-0.42892918E+01	0.30342605E+01	0.75276516E-02	0.55750157E-05				3
		-0.14409464E-07	0.67681867E-11	-0.31812224E+05	0.11424782E+02	-0.30549004E+05				4

75-46-7

CHF3 (FLUOROFORM) TRIFLUOROMETHANE (HFC-23) SIGMA=3 IA=IB=7.898 IC=14.403  
 NU=507(2),700,1117,1152(2),1372(2),3036 REF=Zachariah, Westmoreland, Burgess,  
 Tsang & Melius JPC 100,(1996),8737-8747 HF298=-165.7 Kcal REF=TRC/81  
 {HF298=-695.28+/-1.96 kJ REF=ATcT A} Max Lst Sq Error Cp @ 1300 K 0.45%.

CHF3 FLUOROFORM	T 9/99C	1.H	1.F	3.	0.G	200.000	6000.000	B	70.01385	1
		7.24609031E+00	5.42386441E-03	-2.02314394E-06	3.34946402E-10	-2.04067524E-14				2
		-8.63258026E+04	-1.28982398E+01	2.73539203E+00	8.72478957E-03	1.74821510E-05				3
		-3.21504750E-08	1.41694928E-11	-8.46839564E+04	1.24879863E+01	-8.33830015E+04				4

75-47-8

CHI3 (IODOFORM) TriIodoMethane SIGMA=3 IA=IB=132.8005 IC=263.4337 NU=2974,  
 427,153,1065(2),573(2),111(2) HF298=210.874 +/-4.2 kJ HF0=218.8 kJ  
 REF=Kudchadker & Kudchadker JPCRD 4,(1975),457 {HF298(solid)=181.1+/-1 kJ  
 REF=Carson et al J. Chem Thermo. 25,(1992),261} Max Lst Sq Error Cp  
 @ 6000 K 0.33%.

CHI3 IODOFORM	g 8/99C	1.H	1.I	3.	0.G	200.000	6000.000	B	393.73205	1
		9.68729360E+00	2.99956270E-03	-1.09071270E-06	1.77574920E-10	-1.06948694E-14				2
		2.20877279E+04	-1.38894326E+01	4.17736834E+00	2.47739875E-02	-3.54747700E-05				3
		2.54962645E-08	-7.20982666E-12	2.32819472E+04	1.29496063E+01	2.53621200E+04				4

74-90-8

HCN STATWT=1 SIGMA=1 BE=1.4782216 NU=2096,713.5(2),3311 X11=-7.0741  
 X12=-2.5265 X13=-10.4434 X22=-2.6533 X23=-19.0055 X33=-52.4901 G22=5.160  
 Y111=-.1889 Y112=-.0012 Y113=-.7723 Y122=-.0747 Y123=.1240 Y133=-1.1010  
 Y222=.0285 Y223=-.0375 Y233=-.1230 Y=333=.2702 ALFAB1=.009975  
 ALFAB2=-.0035616 ALFAB3=.010446 D000=.000002909 REF=Gurvich 91  
 HF298=129.799+/-0.38 kJ REF=ATcT A (HF298=132+/-4 kJ REF=Gurvich 91) Max  
 Lst Sq Error Cp @ 6000 K 0.30%.

HCN	ATcT/AH	1.C	1.N	1.	0.G	200.000	6000.000	A	27.02538	1
		3.80231648E+00	3.14630087E-03	-1.06315727E-06	1.66185438E-10	-9.79891962E-15				2
		1.42849502E+04	1.57501632E+00	2.25901199E+00	1.00510475E-02	-1.33514567E-05				3
		1.00920479E-08	-3.00880408E-12	1.45903166E+04	8.91631960E+00	1.56111424E+04				4

Table 4 (continued)

6914-07-4

HNC STATWT=1 SIGMA=1 B0=1.512 NU=3653,464(2),2024 REF=M. JACOX 98  
 HF298=191.908+/-0.694 kJ REF=ATcT A {HF0=194.+/-9. kJ REF=Gurvich 1991}  
 Max Lst Sq Error Cp @ 400 K 0.30%.

HNC	ATcT/AH	1.N	1.C	1.	0.G	200.000	6000.000	B	27.02538	1
4.22248262E+00	2.59458082E-03	-8.58480324E-07	1.30744940E-10	-7.50339813E-15						2
2.17156730E+04	-7.79706410E-02	2.30186822E+00	1.54157449E-02	-3.13261898E-05						3
3.08816218E-08	-1.11912204E-11	2.19306327E+04	8.14749128E+00	2.30810956E+04						4

75-13-8

HNCO HYDROGEN ISOCYANATE Isocyanic Acid SIGMA=1 STATWT=1 A0=30.638 B0=0.369  
 C0=.364 NU=3538,2269,1327,777,656,577 REF=Jacox Webbook HF0=-27.63+/-1 kcal  
 REF=Shuurman et al JCP 120, (2004), 11586 {HF298=-27.9 KCAL REF=East & Allen JCP  
 99, (1993), 4638; HF0=-27.89+/-3 kcal REF=Melius RJ5 1987} Max Lst Sq Error Cp  
 @ 6000 0.33%

HNCO Isocyanic AciA	5/05H	1.N	1.C	1.O	1.G	200.000	6000.000	B	43.02478	1
5.30045051E+00	4.02250821E-03	-1.40962280E-06	2.23855342E-10	-1.32499966E-14						2
-1.61995274E+04	-3.11770684E+00	2.24009031E+00	1.45600497E-02	-1.54352330E-05						3
8.55535028E-09	-1.79631611E-12	-1.54589951E+04	1.21663775E+01	-1.42642740E+04						4

420-05-3

HOCN Cyanic Acid trans Sigma=1 STATWT=1 IA=0.120574 IB=7.71032 IC=7.8309  
 Nu=3570,2286,1228,1081,509,460 REF=Jacox Webbook HF0=-3.05+/-1 kcal  
 REF=Shuurman et al JCP 120, (2004), 11586 {HF0=-2.82+/-5 kcal REF=Melius RJ6 87}  
 Max Lst Sq Error Cp @ 6000 K 0.33%.

HOCN Cyanic Acid A	5/05H	1.N	1.C	1.O	1.G	200.000	6000.000	B	43.02478	1
5.28767714E+00	4.01746511E-03	-1.40407465E-06	2.22562614E-10	-1.31562375E-14						2
-3.77409807E+03	-2.64470976E+00	2.88943546E+00	1.16487242E-02	-1.08005006E-05						3
5.44138776E-09	-1.06857286E-12	-3.15296691E+03	9.51295652E+00	-1.85890558E+03						4

506-85-4

HCNO Fulminic Acid (Linear) SIGMA=1 STATWT=1 IB=7.127865 Nu=3309,2268,1174,  
 575(2),554(2) REF=Melius C17B 1987 HF0=40.88+/-2 kcal REF=Shuurman et al JCP  
 120, (2004), 11586 {HF0=43.62+/-3 kcal REF=Malius C17B 1987} Max Lst Sq Error  
 Cp @ 6000 K 0.33%.

HCNO Fulminic AcidA	5/05H	1.N	1.C	1.O	1.G	200.000	6000.000	B	43.02478	1
5.91979744E+00	4.00114600E-03	-1.42063343E-06	2.27569621E-10	-1.35504870E-14						2
1.80385534E+04	-8.26935223E+00	6.07949401E-01	2.82182431E-02	-4.60451618E-05						3
3.82559486E-08	-1.23226501E-11	1.90714209E+04	1.69199098E+01	2.01698706E+04						4

51060-05-0

HONC SIGMA=1 STATWT=1 IA=0.12848 IB=7.3548 IC=7.48159 Nu=3602,2229,  
 1409,995,304,250.2 REF=Melius C27 1987 HF0=56.34+/-1 kcal REF=Shuurman et al  
 JCP 120, (2004), 11586 {HF0=55.92+/-4.5 kcal REF=Melius C27 1987} Max Lst Sq  
 Error Cp @ 6000 K 0.31%.

HONC	A 5/05H	1.N	1.C	1.O	1.G	200.000	6000.000	B	43.02478	1
5.40214604E+00	3.88924878E-03	-1.35173730E-06	2.13424929E-10	-1.25801686E-14						2
2.62745253E+04	-2.27016401E+00	4.32473877E+00	6.65109255E-03	-4.35816707E-06						3
2.13098554E-09	-6.08147518E-13	2.66128773E+04	3.42337782E+00	2.81633382E+04						4

Table 4 (continued)

12347-01-2

CHN2 CYANAMIDE RADICAL HN\*-CN SIGMA=1 STATWT=2 IA=0.130787 IB=7.4960529  
 IC=7.626847 NU=3308,1738,1101,1026,437,392 HF298=76.433 kcal  
 REF=BAC/MP4 Calculations by C. Melius Private Communication. Max Lst Sq Error  
 Cp @ 6000 K 0.33%

CHN2	T 3/93C	1H	1N	2	OG	200.000	6000.000	B	41.03242	1
	0.58470159E+01	0.36667998E-02	-0.13120636E-05	0.21135472E-09	-0.12636470E-13					2
	0.36343577E+05	-0.49756817E+01	0.31861199E+01	0.10792062E-01	-0.74954818E-05					3
	0.14780067E-08	0.43976323E-12	0.37095838E+05	0.88362660E+01	0.38462359E+05					4

517-25-9

CH(NO2)3 Tri-Nitro Methane STATWT = 1 SYMNO = 3 IA = 50.830948 IB = 68.4055572  
 IC = 99.2098743 (Ir(NO2)= 5.96 ROSYM = 2 V(2) = 0.1 kcal/mole)3  
 NU = 2749,1962,1572,1261,1232,1167,1135,1064,993,884,724,708,670,619,563,490,  
 449,421,368,347,335,210,170,157. REF = A.BURCAT TAE Report # 824 1998  
 HF(298)=-3.2 kcal/mole REF=Carpenter et. al. J. Chem. Eng. Data 15, (1970),535  
 Max Lst Sq Error Cp @ 1300 K 0.50%

CH(NO2)3	T04/98C	1.H	1.O	6.N	3.G	200.000	6000.000	B	151.03556	1
	1.96645029E+01	9.80273423E-03	-3.99278141E-06	6.90498702E-10	-4.31223139E-14					2
	-9.12328532E+03	-6.52887368E+01	1.66436817E+00	6.81055678E-02	-7.81450689E-05					3
	4.46832013E-08	-1.01862362E-11	-4.52669105E+03	2.56966436E+01	-1.61029333E+03					4

2597-44-6

CHO SIGMA=1 STATWT=2 A0=24.562 B0=1.498 C0=1.403 NU=2435,1878,1087 REF=Marenich  
 & Boggs JPC 107 (2003),2343-2350 Direct summation using CCSD(T) method. Calc.  
 from their tables HF298=42.3+/-2.0 kJ HF0=41.9 kJ {HF298=42.296+/-0.3 kJ  
 REF=ATcT A} Max Lst Sq Error Cp @ 1500 K 0.63%.

CHO	T 5/03C	1.H	1.O	1.	O.G	200.000	6000.000	A	29.01804	1
	3.92001542E+00	2.52279324E-03	-6.71004164E-07	1.05615948E-10	-7.43798261E-15					2
	3.65342928E+03	3.58077056E+00	4.23754610E+00	-3.32075257E-03	1.40030264E-05					3
	-1.34239995E-08	4.37416208E-12	3.87241185E+03	3.30834869E+00	5.08749163E+03					4

17030-74-9

CHO+ FORMYL ION B0=1.367073 NU=3223,707(2),2088 HF298=833. KJ REF=JANAF

CHO+	J12/70H	1C	1O	1E	-1G	300.000	5000.000	C	29.0178	1
	0.37411880E+01	0.33441517E-02	-0.12397121E-05	0.21189388E-09	-0.13704150E-13					2
	0.98884078E+05	0.20654768E+01	0.24739736E+01	0.86715590E-02	-0.10031500E-04					3
	0.67170527E-08	-0.17872674E-11	0.99146608E+05	0.81625751E+01	0.10019345E+06					4

71080-92-7

COH HYDROXYMETHYLIDYNE SIGMA=1 STATWT=1 A0=23.428 B0=1.401 C0=1.315 NU=1108,  
 1375,3144 Calculated from tables of direct summation. HF298=218.1 kJ  
 HF0=217.8 kJ REF=Marenich and Boggs JPC 107 (2003) 2343. {HF298=218.20+/-0.83kJ  
 REF=ATcT A} Max Lst Sq Error Cp @ 900 K 0.46% @ 1500 K 0.32%

COH	C-OH	IU5/03C	1.H	1.O	1.	O.G	200.000	6000.000	A	29.01804	1
	4.23892214E+00	1.96576170E-03	-3.82075171E-07	4.80137647E-11	-3.11176347E-15					2	
	2.47261645E+04	1.99698242E+00	4.36380907E+00	-5.35204137E-03	2.31954508E-05					3	
	-2.66109040E-08	1.02711962E-11	2.50108717E+04	2.98106307E+00	2.62312512E+04					4	

Table 4 (continued)

2564-86-5

COOH CARBOXYL RADICAL Equil SIGMA=1 STATWT=2 IAIBIC=35. NU=3316,1797,1261,1088,620,615 REF=TSIV HF298=-181.32+/-2.3 kJ HF298-trans=-181.32+/-2.30 kJ HF298-cis=176.34+/-3.88 kJ REF=ATcT A {HF298=-213.+/-13 KJ REF=Gurvich 91}

Max Lst Sq Error Cp @ 6000 K 0.39%.

COOH	equilib	ATcT/AC	1.0	2.H	1.	0.G	200.000	6000.000	B	45.01744	1	
							5.39206152E+00	4.11221455E-03	-1.48194900E-06	2.39875460E-10	-1.43903104E-14	2
							-2.38606717E+04	-2.23529091E+00	2.92207919E+00	7.62453859E-03	3.29884437E-06	3
							-1.07135205E-08	5.11587057E-12	-2.30281524E+04	1.12925886E+01	-2.18076591E+04	4

2564-86-5

HCOO RADICAL CALCULATED FROM GROUP THEORY REF=Benson 1976 HF298=-36.0 kcal

Max Lst Sq Error Cp @ 1500 K 0.40%.

HCOO*	Radical	T04/97H	1.C	1.0	2.	0.G	298.150	5000.000	E	45.01774	1	
							5.97791811E+00	3.24247847E-03	-1.46666291E-06	2.91808902E-10	-2.10704956E-14	2
							-2.04910217E+04	-7.12854015E+00	-3.01936623E+01	2.54607495E-01	-6.43484728E-04	3
							6.92943698E-07	-2.65871657E-10	-1.59887826E+04	1.47958586E+02	-1.81158000E+04	4

36058-28-3

HCS RADICAL STATWT=2 A0=0.657 B0=0.671 C0=30.500 NU=2983,1096,816

T0=3063. STATWT=2 HF0=71.7 kcal REF=ab-initio calc by Ching-Len Yu & S.H.

Bauer Private Communication Max Lst Sq Error Cp @ 6000 K 0.58%

HCS		T05/97H	1.C	1.S	1.	0.G	200.000	6000.000	B	45.08494	1	
							3.61707294E+00	3.87413811E-03	-1.52693796E-06	2.56534366E-10	-1.56455118E-14	2
							3.48552427E+04	6.60648943E+00	3.51963223E+00	2.08544960E-03	6.12130414E-06	3
							-9.93060979E-09	4.40938577E-12	3.49593934E+04	7.53361036E+00	3.61380016E+04	4

2465-56-7

CH2 METHYLENE RADICAL SINGLET SIGMA=2 STATWT=1 T0=0 IA=0.1391 IB=0.2498

IC=0.3960 NU=2806,1353,2865. T0(b 1B1)=8350. NU=3000,570,3000 A0=73.8

B0=8.59 C0=7.2 HF298=428.8+/-1.6 kJ HF0=428.3+/-1.6 kJ REF=Ruscic et al

JPCRD IUPAC Task Group 2003. {HF298=429.04+/-0.27 kJ REF=ATcT A} Max Lst Sq Error Cp @ 1300 K 0.40%

CH2(1)	SINGLET	IU6/03C	1.H	2.	0.	0.G	200.000	6000.000	B	14.02658	1	
							3.13501686E+00	2.89593926E-03	-8.16668090E-07	1.13572697E-10	-6.36262835E-15	2
							5.05040504E+04	4.06030621E+00	4.19331325E+00	-2.33105184E-03	8.15676451E-06	3
							-6.62985981E-09	1.93233199E-12	5.03662246E+04	-7.46734310E-01	5.15727280E+04	4

2465-56-7

CH2 METHYLENE RAD TRIplet This is for applications where triplet methylene is not equilibrated with single methylene. Only HF0 is identical to the one given for the equilibrium Singlet and Triplet. HF298 is 0.005 kJ lower than given for the equilibrium HF1000=1.1 kJ lower and HF3000 is 6.8 kJ lower than the

equilibrium STATWT=3 SIGMA=2 A0=73.811 B0=8.450 C0=7.184 NU=3031,963,3190 T0=3500 SIGMA=2 HF298=391.2+/-1.6 HF0=390.7 +/-1.6 kJ REF=Ruscic et al JPCRD 2003 IUPAC Task Group {HF298=391.46+/-0.27 REF=ATcT A} Max Lst Sq Error Cp @ 6000 K 0.27%

CH2	TRIplet RAD	IU3/03C	1.H	2.	0.	0.G	200.000	6000.000	B	14.02658	1	
							3.14631886E+00	3.03671259E-03	-9.96474439E-07	1.50483580E-10	-8.57335515E-15	2
							4.60412605E+04	4.72341711E+00	3.71757846E+00	1.27391260E-03	2.17347251E-06	3
							-3.48858500E-09	1.65208866E-12	4.58723866E+04	1.75297945E+00	4.70504920E+04	4



Table 4 (continued)

2465-56-7

CH2 METHYLENE RADICAL Equilibrium SINGLET + TRIPLET T0=0 SIGMA=2. STATWT=3  
 A0=73.811 B0=8.450 C0=7.184 NU=3031,963,3190. T0=3147. SIGMA=2 STATWT=1  
 A0=20.118 B0=11.205 C0=7.069 NU=3147,1353,2865 T0=11497. SIGMA=2 STATWT=1  
 A0=73.8 B0= 8.59 C0=7.2 Nu=3000,570,3000 HF298=319.2+/-1.6 kJ  
 HF0=390.7+/-1.6 kJ REF=Ruscic et al JPCRD 2005 IUPAC Task Group {HF298=391.46  
 +/-0.27 kJ REF=ATcT A} Max Lst Sq Error Cp @ 6000 K 0.52%  
 CH2 EQUILBRIUM IU3/03C 1.H 2. 0. 0.G 200.000 6000.000 B 14.02658 1  
 3.11049513E+00 3.73779517E-03-1.37371977E-06 2.23054839E-10-1.33567178E-14 2  
 4.59715953E+04 4.62796405E+00 3.84261832E+00-7.36676871E-06 6.16970693E-06 3  
 -6.96689962E-09 2.64620979E-12 4.58631528E+04 1.27584470E+00 4.70504920E+04 4

74-97-5

CH2BrCl Halon 1011 SIGMA=1 IAIBIC=469.E-116 NU=3001,1421,1232,743,608,236,  
 3065,1136,852 HF298=-45+/-15 KJ REF=TSIV 1979 Max Lst Sq Error Cp @ 6000 K .41%  
 CH2BRCL HALON1011 RUS 79C 1H 2BR 1CL 1G 200.000 6000.000 B 129.38358 1  
 0.65082153E+01 0.57744846E-02-0.20744896E-05 0.33492192E-09-0.20051184E-13 2  
 -0.79549405E+04-0.49946731E+01 0.30310057E+01 0.10607707E-01 0.63407360E-05 3  
 -0.18341110E-07 0.88847421E-11-0.68113680E+04 0.13983350E+02-0.54122251E+04 4

74-95-3

CH2Br2 DiBromoMethane SIGMA=2 STATWT=1 Ia=3.1852 Ib=69.6197 Ic=72.2609  
 Nu=168.5,583.6,640,815,1109,1209,1430,3121,3208 HF298=4.937 kJ HF0=26.329 kJ  
 REF=Martin & Burcat JPC 108 (2004),7752 Max Lst Sq Error Cp @ 6000 K 0.37%  
 CH2Br2 W2 T09/04C 1.BR 2.H 2. 0.G 200.000 6000.000 B 173.83458 1  
 6.67087098E+00 5.51238897E-03-1.95323046E-06 3.12443170E-10-1.85854530E-14 2  
 -1.94784246E+03-4.98511911E+00 3.07810878E+00 1.23681783E-02 8.40317756E-07 3  
 -1.25546148E-08 6.79189724E-12-8.59489686E+02 1.41666382E+01 5.93795666E+02 4

6806-86-6

CH2CL RADICAL REF=TSIV HF298=116.87 KJ SIGMA=2 STATWT=2 NU=2950,3050,826.3,1391,  
 1250,396.6 IAIBIC=11.E-117 MAX LST SQ ERROR CP @ 1300 K 0.52%  
 CH2CL L 8/84C 1H 2CL 1 0G 300.000 5000.000 B 49.47979 1  
 0.47707529E 01 0.43237582E-02-0.14223033E-05 0.20599472E-09-0.10714865E-13 2  
 0.12277027E 05 0.46459579E 00 0.33185844E 01 0.65915734E-02 0.10332604E-06 3  
 -0.43136268E-08 0.21676541E-11 0.12780980E 05 0.84271412E 01 0.14056558E 05 4

593-70-4

CH2ClF CLOROFLUOROMETHANE FC-31 TRC DATA EXTRAPOLATED TO 5000 K USING WILHOIT'S  
 POLYNOMIALS. HF298=-63.2 Kcal  
 CH2CLF GC-31 P12/75C 1.H 2.CL 1.F 1.G 298.150 5000.000 C 68.47820 1  
 0.59572783E 01 0.60879700E-02-0.20813759E-05 0.31346215E-09-0.17084878E-13 2  
 -0.34280781E 05-0.48930445E 01 0.20975533E 01 0.12551896E-01 0.27147036E-06 3  
 -0.91319841E-08 0.44713573E-11-0.32973617E 05 0.16155014E 02-0.31803671E 05 4

75-09-2

CH2Cl2 DICHLOROMETHANE SIGMA=2 STATWT=1 IAIBIC=1865.4 Nu=2998,1467,712,280,  
 1153,3065,898,1268,758 REF=Gurvich 1991 HF298=-22.8 Kcal REF=TRC 12/81  
 {HF298=-95.0+/-0.30 kJ REF=Gurvich 91; HF298=-95.446+/-0.74 kJ REF=ATcT A}  
 Max Lst Sq Error Cp @ 6000 K 0.43%  
 CH2CL2 tpis91C 1.H 2.CL 2. 0.G 200.000 6000.000 B 84.93198 1  
 6.29318149E+00 5.98773270E-03-2.15635738E-06 3.48717095E-10-2.09014331E-14 2  
 -1.39806830E+04-5.90810756E+00 3.09078884E+00 8.35269259E-03 1.25182071E-05 3  
 -2.46845519E-08 1.11752358E-11-1.28332020E+04 1.20563837E+01-1.14733400E+04 4

Table 4 (continued)

86013-71-0

CH2DNO2 Nitro-Methane D STATWT = 1 SYMNO = 1 IA = 6.60202 IB = 8.90396  
 IC = 14.75046 I(red) = 0.619102 ROSYM = 2 V(2) = 0.104 kcal/mole  
 NU = 463,579,651,893,957,1099,1254,1304,1338,1480,1557,2221,2997,3082.

REF = McKee JACS 107, (1985), 1900. HF298= -12.555 kcal REF =A. BURCAT

TAE Report # 824a, 1998 Max Lst Sq Error Cp @ 1300 K 0.60%

\*\*\* WARNING \*\*\* THIS COMPOUND CONTAINS 5 ELEMENTS BUT THE FORMULA LINE NO 1 CAN  
 ACCOMODATE ONLY FOUR. See 9-THERM POLYNOMIALS\*\*\*\*

NITRO-METHANE D	T04/98	WARNING!	G	200.000	6000.000	B	62.04652	1
7.42983565E+00	1.02242244E-02	3.76339564E-06	6.17531100E-10	3.73902847E-14				2
-9.68557204E+03	-1.23529524E+01	3.23582229E+00	6.54117396E-03	3.47848512E-05				3
-5.08832580E-08	2.07922157E-11	7.79017302E+03	1.29867207E+01	-6.31809439E+03				4

676-55-1

CH2D2 METHANE-D2 STATWT=1. SIGMA=2. A0=4.303 B0=3.506 C0=3.05 NU=2974,  
 2202,1435,1033,1331,3013,1090,2234,1234 REF=BURCAT MAX LST SQ ERROR CP @ 1300K  
 0.95% . HF298=-81.75 KJ

CH2D2	T05/79C	1H	2D	2	OG	300.000	5000.000	B	18.0551	1
0.35087013E+01	0.81863180E-02	0.27852266E-05	0.41648370E-09	0.22470558E-13						2
-0.11595125E+05	0.18880228E+01	0.23866291E+01	0.57553649E-02	0.64751221E-05						3
-0.67107635E-08	0.13974620E-11	0.10846535E+05	0.94605669E+01	-0.98322090E+04						4

3744-29-4

CH2F RADICAL STATWT=2 IAIBIC=2.8E-117 NU=2900,3000,1163,1500,1350,500

REF=TSIV 1979 HF298=-32. KJ Max Lst Sq Error Cp @ 6000 K 0.47%

CH2F	RUS 79C	1H	2F	1	OG	200.000	6000.000	C	33.02528	1
0.40610825E+01	0.52432553E-02	0.18726751E-05	0.30101543E-09	0.17961659E-13						2
-0.54531615E+04	0.34407775E+01	0.39006976E+01	0.18878812E-03	0.14670620E-04						3
-0.17625373E-07	0.65799837E-11	0.51179668E+04	0.56574728E+01	-0.38486934E+04						4

75-10-5

CH2F2 DIFLUOROMETHANE FC-32 SIGMA=2 IA=1.650 IB=7.720 IC=8.832  
 NU=529,1090,1116,1176,1262,1435,1508,2949,3012 REF=Zachariah, Westmoreland,  
 Burgess, Tsang& Melius JPC 100, (1996), 8737-8747 HF298=-108.2 Kcal REF=TRC/81  
 {HF298=-452.3 kJ REF=Gurvich 1991; HF298=-452.59+/-1.0 kJ REF=ATcT A} Max  
 Lst Sq Error Cp @ 6000 K 0.55%.

CH2F2	FC-32	T 9/99C	1.H	2.F	2.	O.G	200.000	6000.000	B	52.02339	1
5.06948195E+00	7.23193135E-03	-2.64021025E-06	4.30854708E-10	-2.59873096E-14							2
-5.67270077E+04	-2.34590394E+00	4.25023157E+00	-6.84861262E-03	4.85583334E-05							3
-5.83442752E-08	2.24503933E-11	-5.57351602E+04	5.76716418E+00	-5.44480432E+04							4

15845-29-1

CH2N (H2C=N\*) RADICAL SIGMA=2 T0(STATWT)=0(2) A0=1.140 B0=1.31 C0=9.48

NU=3103,2820,1725,1337,954,913 T0(STATWT)=35075(4) HF298=57.4 kcal

REF=Ching-Len Yu & S.H. Bauer Private Communication Max Lst Sq Error Cp @  
 400 K 0.59%.

H2CN RADICAL	T05/97H	2.C	1.N	1.	O.G	200.000	6000.000	B	28.03362	1
3.80315523E+00	5.47197456E-03	-1.95314927E-06	3.13362513E-10	-1.86249463E-14						2
2.73218196E+04	3.31721893E+00	3.97799541E+00	-3.43275678E-03	2.59134226E-05						3
-3.04692133E-08	1.16272702E-11	2.76769528E+04	4.43029598E+00	2.88846366E+04						4

Table 4 (continued)

15691-95-9

CH2N (H\*C=NH) RADICAL trans SIGMA=1 T0(STATWT)=0(2) A0=1.150 B0=1.26  
 C0=12.75 NU=3304,2873,1584,1194,977,913 T0(STATWT)=30000(2) HF298=71.4 kcal  
 REF=Ching-Len Yu & S.H. Bauer Private Communication Max Lst Sq Error Cp @  
 400 K 0.54%

HCNH trans	T05/97H	2.C	1.N	1.	0.G	200.000	6000.000	B	28.03362	1
4.04014620E+00	5.16591818E-03	-1.82276886E-06	2.90299166E-10	-1.71614663E-14						2
3.42988370E+04	2.58896150E+00	3.97114548E+00	-3.88875657E-03	2.92918929E-05						3
-3.57482385E-08	1.40303899E-11	3.47237453E+04	5.06390351E+00	3.59296699E+04						4

54980-11-9

CH2N (H\*C=NH) RADICAL cis SIGMA=1 T0(STATWT)=0(2) A0=1.150 B0=1.27  
 C0=12.08 NU=3295,2845,1567,1099,924,873 T0(STATWT)=30000(2) HF298=76.4 kcal  
 REF=Ching-Len Yu & S.H. Bauer Private Communication Max Lst Sq Error Cp @  
 400 K 0.55

HCNH cis	T05/97H	2.C	1.N	1.	0.G	200.000	6000.000	B	28.03362	1
4.21964804E+00	5.00385006E-03	-1.76392053E-06	2.80725924E-10	-1.65851919E-14						2
3.67706419E+04	1.67138658E+00	3.68324269E+00	-1.38553482E-03	2.40042191E-05						3
-3.11573905E-08	1.25791818E-11	3.72527355E+04	6.21248890E+00	3.84457533E+04						4

3858-51-7

CH2NO H2N-C(\*)=O RADICAL STATWT=2 SIGMA=2 IA=0.6363 IB=7.397796 IC=8.0341  
 NU=3539,3390,1839,1589,1207,1060,593,520,188.7 HF298=-5.57 +/-2.37 KCAL  
 REF= C. Melius Database BAC/MP4 C37 Max Lst Sq Error Cp @ 6000 K 0.37%

H2NCO	T09/96H	2N	1C	1O	1G	200.000	6000.000	B	44.03302	1
0.57886741E+01	0.60938325E-02	-0.21165797E-05	0.33404486E-09	-0.19684582E-13						2
-0.50210948E+04	-0.44063740E+01	0.35677914E+01	0.10193381E-01	-0.15289951E-05						3
-0.47571551E-08	0.26052647E-11	-0.42980380E+04	0.75824281E+01	-0.28029168E+04						4

2683-96-7?

CH2NO CH2=N-O\* RADICAL STATWT=2 SIGMA=2 IA=0.8304 IB=6.6914 IC=7.5218  
 NU=3095,2977,1469,1301,1112,1035,835,712,360.8 HF298=41.45+/-5 KCAL  
 REF=C. MELIUS DATABASE BAC/MP4 C42 Max Lst Sq Error Cp @ 6000 K 0.44 %.

CH2NO CH2=N-O*	T 9/96C	1H	2N	1O	1G	200.000	6000.000	C	44.03302	1
0.61088065E+01	0.61700384E-02	-0.22263482E-05	0.36051980E-09	-0.21629499E-13						2
0.18374401E+05	-0.74217824E+01	0.31022300E+01	0.63256777E-02	0.18394585E-04						3
-0.30856607E-07	0.13425502E-10	0.19544369E+05	0.99247330E+01	0.20858331E+05						4

2683-96-7

CH2NO H2C\*N=O RADICAL STATWT=2 SIGMA=2 IA=2.596 IB=3.041 IC=5.0754  
 NU=3040,2952,1505,1304,1188,1111,983,897,846 HF298=53.52+/-2 KCAL  
 REF=C. MELIUS DATABASE BAC/MP4 D93X Max Lst Sq Error Cp @ 200 K 0.82%.

H2CNO H2C*N=O	T 9/96H	2C	1N	1O	1G	200.000	6000.000	C	44.03302	1
0.54028152E+01	0.69057001E-02	-0.25162977E-05	0.41014066E-09	-0.24718300E-13						2
0.24528690E+05	-0.44574262E+01	0.38781858E+01	-0.66530886E-02	0.53947610E-04						3
-0.68176813E-07	0.27181746E-10	0.25716857E+05	0.74618774E+01	0.26932156E+05						4

16787-85-2

\*CH2NO2 Nitro Methylene Radical SYMNO = 1 STATWT = 2 IA = 6.34509  
 IB = 6.7566103 IC = 13.1017 IRED=0.3267 V(2)= 0.08 kcal/mole ROSYM = 2  
 NU = (457,555),693,719,986,1095,1297,1419,1461,3055,3200 HF298= 36.44 kcal  
 REF=McKee, J. Am. Chem. Soc. 107, (1985),1900 Max Lst Sq Error Cp @ 6000 K 0.44%

*CH2NO2 RADICAL	T04/98C	1.H	2.N	1.O	2.G	200.000	6000.000	B	60.03242	1
7.67214886E+00	7.04674142E-03	-2.55301211E-06	4.14646979E-10	-2.49316782E-14						2
1.52307521E+04	-1.22510821E+01	2.46754293E+00	1.56130407E-02	4.71686464E-06						3
-2.05123642E-08	1.02705094E-11	1.69015807E+04	1.59016345E+01	1.83372153E+04						4

Table 4 (continued)

38082-43-8 ??

\*CH2ONO2 METHYL-NITRATE-RADICAL STATWT = 2 SYMNO = 1 IA = 6.5230882  
 IB = 16.246015 IC = 22.69382 Ir(NO2) = 5.96 ROSYM = 2 V(2) = 9.1 kcal  
 Ir(CH2) = 0.345711 ROSYM = 2 V(2) = 2.3 kcal NU= 3142,3009,1727,1412,  
 1306,1165,1120,921,766,718,683,608,364. HF298 = 23.65 kcal  
 REF = Melius Database 1988 P73BJ Max Lst Sq Error Cp @ 1300 K 0.56%  
 \*CH2ONO2 RADICAL T05/98C 1.H 2.O 3.N 1.G 200.000 6000.000 B 76.03182 1  
 1.03913885E+01 7.66103917E-03-3.02728077E-06 5.16124915E-10-3.19767406E-14 2  
 7.78486241E+03-2.54151556E+01 2.98654023E+00 2.47990510E-02-1.17175684E-05 3  
 -5.36820166E-09 4.80947389E-12 1.00202588E+04 1.36939353E+01 1.19010741E+04 4

420-04-2

CH2N2 CYANAMIDE H2N-CN SIGMA=1 STATWT=1 IA=0.2674823 IB=8.1221516  
 IC=8.319017 NU =412,475,615,1035,1182,1611,2324,3380,3473  
 HF298= 32.478+/-4.8 KCAL REF=C. MELIUS, BAC/MP4 Database N62Z Max Lst Sq  
 Error Cp @ 6000 K 0.38%  
 CH2N2 CYANAMIDE T 3/93C 1H 2N 2 OG 200.000 6000.000 B 42.04036 1  
 0.54262217E+01 0.63845441E-02-0.22119323E-05 0.34832646E-09-0.20489145E-13 2  
 0.14263617E+05-0.33915332E+01 0.24205497E+01 0.17026593E-01-0.17728435E-04 3  
 0.11218736E-07-0.30107729E-11 0.15000886E+05 0.11611217E+02 0.16343471E+05 4

151-51-9

CH2N2 CARBODIIMIDE HN=C=NH SIGMA=2 STATWT=1 IA=0.2246383 IB=7.89834  
 IC=7.903817 IR=0.05859 INT. ROTATION BARRIER V(3)=1601.8 cm-1  
 NU=3416,3412,2102,1241,913,905,746,511 HF298=35.613+/-3.56 Kcal  
 REF=C.MELIUS BAC/MP4 Database N62Y Max Lst Sq Error Cp @ 200 K 0.5%  
 H2CN2 HN=C=NH T 3/93H 2C 1N 2 OG 200.000 6000.000 B 42.04036 1  
 0.64734743E+01 0.51023160E-02-0.17738598E-05 0.28010178E-09-0.16511234E-13 2  
 0.15445903E+05-0.93929437E+01 0.16502481E+01 0.17225336E-01-0.62645743E-05 3  
 -0.90652062E-08 0.65197171E-11 0.16733605E+05 0.15528105E+02 0.17921055E+05 4

334-88-3

CH2N2 DIAZOMETHANE H2C=N=N STATWT=1 SIGMA=2 IA=0.2985 IB=7.179138  
 IC=7.47764 NU= 405,532,595,1115,1181,1419,2061,3024,3139  
 HF298=68.447+/-5.85 KCAL REF= C. MELIUS BAC/MP4 Database N62X MAX LST SQ  
 ERROR CP @ 6000 K 0.45%  
 CH2N2 H2C=N=N T 3/93C 1H 2N 2 OG 200.000 6000.000 B 42.04036 1  
 0.56157835E+01 0.65328561E-02-0.23376828E-05 0.37633930E-09-0.22483577E-13 2  
 0.32222744E+05-0.54835013E+01 0.25553699E+01 0.15039976E-01-0.11279972E-04 3  
 0.45140426E-08-0.66460339E-12 0.33104359E+05 0.10402408E+02 0.34443671E+05 4

157-22-2

CH2N2 CYCLO DIAZIRENE H2(CNN) STATWT=1 SIGMA=2 IA=1.94049 IB=3.39497  
 IC=4.76825 NU=879,980,1050,1054,1127,1478,1789,2964,3061  
 HF298=76.516+/-4.54 kcal REF= C. MELIUS BAC/MP4 Database N62 MAX LST SQ  
 ERROR CP @ 200 K 0.75%  
 H2CN2 CY T 3/93H 2C 1N 2 OG 200.000 6000.000 B 42.04036 1  
 0.49500072E+01 0.73057703E-02-0.26589670E-05 0.43302613E-09-0.26081126E-13 2  
 0.36251846E+05-0.28322509E+01 0.40367917E+01-0.75951605E-02 0.53236385E-04 3  
 -0.65261005E-07 0.25586745E-10 0.37284686E+05 0.59240768E+01 0.38504126E+05 4

Table 4 (continued)

625-76-3

CH<sub>2</sub>(NO<sub>2</sub>)<sub>2</sub> Di Nitro Methane STATWT = 1 SYMNO = 2 IA = 13.497367 IB = 49.930024  
 IC = 50.708 (Ir(NO<sub>2</sub>) = 5.96 ROSYM = 2 V(2) = 0.08 kcal)x2  
 NU = 2962,2875,1959,1951,1602,1555,1358,1275,1063,971,915,895,746,638,585,568,  
 430,412,194. REF = A.BURCAT TAE Report # 824 1998 HF298= -14.7 kcal  
 REF=Knobel et.al., Bull Acad. Sci. USSR Div. Chem. Sci. (1971),425. Max Lst Sq  
 Error Cp @ 1300 K 0.62%

CH <sub>2</sub> (NO <sub>2</sub> ) <sub>2</sub>	T10/98C	1.H	2.N	2.O	4.G	200.000	6000.000	B	106.03796	1
1.14912019E+01	1.18834901E-02	-4.59405883E-06	7.73301202E-10	-4.75226143E-14						2
-1.22791660E+04	-2.79393135E+01	2.13762234E+00	3.16667350E-02	-1.09883048E-05						3
-1.02396987E-08	6.93005788E-12	-9.32805967E+03	2.20134081E+01	-7.39728499E+03						4

50-00-0

CH<sub>2</sub>O FORMALDEHYDE SIGMA=2 A0=9.40546 B0=1.295407 C0=1.134216 NU=2782.4,1746.1,  
 1500.1,1167.2,2843.2,1249.1 HF298=-108.7 KJ REF=TSIV

CH <sub>2</sub> O	L 8/88H	2C	1O	1	OG	200.000	6000.000	B	30.02628	1
0.31694807E+01	0.61932742E-02	-0.22505981E-05	0.36598245E-09	-0.22015410E-13						2
-0.14478425E+05	0.60423533E+01	0.47937036E+01	-0.99081518E-02	0.37321459E-04						3
-0.37927902E-07	0.13177015E-10	-0.14308955E+05	0.60288702E+00	-0.13059098E+05						4

64-18-6

CH<sub>2</sub>O<sub>2</sub> METHANOIC(FORMIC) ACID HCOOH MONOMER STATWT=1 SIGMA=1 IA=1.0953  
 IB=6.9125 IC=8.0078 BROT=24.96 ROSYM=1 V(1)=2011. V(2)=3123. V(3)=192.  
 NU=3570,2943,1770,1387,1229,1105,625,1033 NEL=100 HF298=-90.48KCAL  
 REF=CHAO & ZWOLINSKI JPCRD 7. (1978),363 {HF298=-378.941+/-0.31 kJ for eq. mix  
 REF=ATcT A} Max Lst Sq Error Cp @ 6000 K 0.47%

HCOOH FORMIC ACID	L 8/88H	2C	1O	2	OG	200.000	6000.000	B	46.02568	1
0.46138316E+01	0.64496364E-02	-0.22908251E-05	0.36716047E-09	-0.21873675E-13						2
-0.47514850E+05	0.84788383E+00	0.38983616E+01	-0.35587795E-02	0.35520538E-04						3
-0.43849959E-07	0.17107769E-10	-0.46770609E+05	0.73495397E+01	-0.45531246E+05						4

865-36-1

CH<sub>2</sub>S SIGMA=2 T0(STATWT)=0(1) A0=0.555 B0=0.59 C0=9.27 NU=3025,2971,1456,  
 1059,991,990 T0(STATWT)=14507.(3) REF=JACOX HF0=28.3 kcal REF=Ching-Len Yu &  
 S.H. Bauer Private Communication Max Lst Sq Error Cp @ 400 K 0.59%.

H <sub>2</sub> CS	T05/97H	2.C	1.S	1.	OG	200.000	6000.000	B	46.09288	1
4.18881491E+00	5.12826276E-03	-1.86326118E-06	3.12838130E-10	-1.93704551E-14						2
1.20948373E+04	2.65102700E+00	3.98890561E+00	-4.48092826E-03	3.23152359E-05						3
-3.98563874E-08	1.57804583E-11	1.25888504E+04	5.99167863E+00	1.37931688E+04						4

2229-07-4

CH<sub>3</sub> METHYL-RAD STATWT=1. SIGMA=6. IA=IB=.2923 IC=.5846 NU=3004,606.4,3161(2),  
 1396(2) HF298=146.7 +/-0.3 KJ HF0=150.0+/-0.3 kJ REF= Ruscic et al JPCRD 2003.  
 {HF298=146.582+/-0.1 kJ REF=ATcT A} Max Lst Sq Error Cp @ 6000 K 0.44%.

METHYL RADICAL	IU0702C	1.H	3.	0.	OG	200.000	6000.000	B	15.03452	1
0.29781206E+01	0.57978520E-02	-0.19755800E-05	0.30729790E-09	-0.17917416E-13						2
0.16509513E+05	0.47224799E+01	0.36571797E+01	0.21265979E-02	0.54583883E-05						3
-0.66181003E-08	0.24657074E-11	0.16422716E+05	0.16735354E+01	0.17643935E+05						4

Table 4 (continued)

14531-53-4

CH3+ Methylcarbonium ion Polynomial made from table calculated by Ruscic's ACTIVE TABLES generator. HF298=1101.792 +/-0.097 kJ REF=B. Ruscic Active Tables ver 1.25 Argonne Nat. Labs. HF0=1099.37 kJ Thermal Electron Convention.

Max Lst Sq Error Cp @ 6000 K 0.50%

CH3+	A12/04C	1.H	3.E	-1.	0.G	200.000	6000.000	A	15.03397	1	
						2.41723886E+00	6.40287629E-03	-2.21301978E-06	3.46738910E-10	-2.02364572E-14	2
						1.31474291E+05	6.78764161E+00	4.73043702E+00	-8.66259820E-03	3.12269215E-05	3
						-3.13568798E-08	1.09957173E-11	1.31269897E+05	-3.03197684E+00	1.32514363E+05	4

74-83-9

CH3Br METHYL-BROMIDE SIGMA=3 STATWT=1 IA=0.5376 IB=IC=8.8669 Nu=606,962(2), 1324,1470(2),3071,3178(2) HF298=-36.443+/-2 kJ HF0=-21.034 kJ REF=Martin & Burcat JPC 108 (2004),7752 {HF298=-9.0 KCAL REF=Stull Westrum Sinke; HF298=-36.410+/-0.2 kJ REF=ATcT A} Max Lst Sq Error Cp @ 6000 K 0.48%.

CH3Br	T09/04C	1.BR	1.H	3.	0.G	200.000	6000.000	B	94.93852	1	
						4.14293955E+00	7.61096796E-03	-2.67015354E-06	4.24035809E-10	-2.50883825E-14	2
						-6.20545949E+03	3.21432559E+00	3.61367184E+00	-8.86540422E-04	2.94669395E-05	3
						-3.76504049E-08	1.49390354E-11	-5.61401651E+03	8.24978857E+00	-4.38301716E+03	4

74-87-3

CH3CL METHYL CHLORIDE SIGMA=3 STATWT=1 IAIBIC=3039.28 Nu=2968,1356,731, 3039(2),1452(2),1017(2) HF298=-81.87+/-0.6 kJ HF0=-73.94 kJ REF=Gurvich 91 {HF298=-82.562+/-0.35 kJ REF=ATcT A; HF298=-81.966 kJ REF=TRC 12/81; HF298=-83.68 kJ REF=Kromkin Khimicheskaya Fizika 22,(2003),30} Max Lst Sq Error Cp @ 6000 K 0.54%.

CH3CL	tpis91C	1.H	3.CL	1.	0.G	200.000	6000.000	B	50.48722	1	
						3.97883949E+00	7.91729094E-03	-2.81713927E-06	4.51715634E-10	-2.69086155E-14	2
						-1.16761879E+04	2.58272676E+00	3.96611858E+00	-5.05692958E-03	4.02006413E-05	3
						-4.82781901E-08	1.86721580E-11	-1.10729538E+04	5.70446517E+00	-9.84664159E+03	4

593-53-3

CH3F METHYL FLUORIDE FC-41 SIGMA=3 IAIBIC=5.834315

NU=2965,1468(2),1459,1049,1182(2),3007(2) REF=Gurvich 91 HF298=-239.56+/-2.65 kJ REF=ATcT A {HF298=-237.66 kJ REF=TRC/81} Max Lst Sq. Error Cp @ 6000 K 0.60%

CH3F	FC-41	ATcT/AC	1.H	3.F	1.	0.G	200.000	6000.000	B	34.03292	1
						3.31313831E+00	8.59220132E-03	-3.07900691E-06	4.96094438E-10	-2.96530154E-14	2
						-3.04944219E+04	4.75449384E+00	5.03521799E+00	-1.46116013E-02	6.06434127E-05	3
						-6.60574176E-08	2.42831624E-11	-3.00795919E+04	3.07681862E-01	-2.88110785E+04	4

16056-34-1

CH3Hg MethylMercury SIGMA=3 STATWT=1 IA=0.519687 IB=10.8654273 IC=10.865433 Nu=404,830(2),1205,1425(2),3075,3231(2) HF298=45+/-2 kcal REF=Lee & Wright Chem. Phys. Lett 376 (2003), 418-423. Inertia Mom=MOPAC 2000. Max Lst Sq Error Cp @ 6000 K 0.43%

CH3Hg	T04/04C	1.H	3.HG	1.	0.G	200.000	6000.000	C	215.62452	1	
						4.65149496E+00	7.06884557E-03	-2.45450648E-06	3.86970344E-10	-2.27759227E-14	2
						2.07368599E+04	2.31971273E+00	3.28241059E+00	5.11441711E-03	1.41087840E-05	3
						-2.24934858E-08	9.61790250E-12	2.13540400E+04	1.06664448E+01	2.26447500E+04	4

Table 4 (continued)

74-88-4

CH3I METHYL-IODIDE SIGMA=3 IA=0.53569 IB=IC=11.09756 NU=2933,1252,533,  
3060(2),1437(2)882(2) REF=Kudchadker & Kudchadker JPCRD 4,(1975),457  
HF298=14.3+/-1.4 kJ REF=NIST WEBBOOK 2000. {HF298=14.382+/-0.35 kJ  
REF=ATcT A} Max Lst Sq Error Cp @ 6000 K 0.49%

CH3I	g	8/99C	1.H	3.I	1.	0.G	200.000	6000.000	B	141.93899	1
4.44377329E+00	7.45523940E-03	-2.63962017E-06	4.21796322E-10	-2.50645631E-14							2
-1.90140790E+02	2.47913765E+00	3.27037586E+00	3.04938761E-03	2.00286679E-05							3
-2.82751858E-08	1.15828787E-11	4.82743383E+02	1.03200626E+01	1.71988488E+03							4

2053-29-4

CH3N METHANIMINE (CH2NH) SIGMA=2 A0=6.545 B0=1.156 C0=0.979 NU=3263,3024,2914,  
1638,1452,1344,1058,1127,1061 REF=M.E. Jacox JPCRD 1988, 17, p.418 HF298=20.08  
KCAL REF=Bauer & Wilcox B3LYP/6-31G(d) calculations, private communication  
(Melius MP4/G2 1997 HF298=20.35+/-1.03 KCAL) Max Lst Sq Error Cp @ 6000 K 0.57%.

CH3N	(H2C=NH)	A12/04H	3.C	1.N	1.	0.G	200.000	6000.000	B	29.04156	1
3.44258358E+00	8.37600036E-03	-2.97819078E-06	4.77352867E-10	-2.84295062E-14							2
8.40771949E+03	3.95595397E+00	4.79302577E+00	-1.26841692E-02	5.69766521E-05							3
-6.34985251E-08	2.37023330E-11	8.85023146E+03	1.10277996E+00	1.01045906E+04							4

27770-42-9

CH3N Methyl-N Radical Triplet Ground State. STATWT=2 SIGMA=3 IA=0.5229835  
IB=IC=3.0573634 REF=Melius N62R Nu=2989(2),2943,1490(2),1349,1040,903(2)  
REF=NIST Webbook 2002 (Jacox) HF298=76.47 kcal REF=G2 Melius Max Lst Sq Error  
Cp @ 400 K and 6000 K 0.57%

CH3N	Methyl-N Rad	T09/02C	1.H	3.N	1.	0.G	200.000	6000.000	B	29.04122	1
3.87086792E+00	8.06656758E-03	-2.88308716E-06	4.63684143E-10	-2.76798427E-14							2
3.66640085E+04	2.20218960E+00	4.12712382E+00	-6.90772784E-03	4.47646681E-05							3
-5.27072008E-08	2.02134894E-11	3.72568026E+04	4.24579036E+00	3.84809784E+04							4

865-40-7

CH3NO NITROSOMETHYL or METHYL-NITROSYL SIGMA=1 IA=1.317537 IB=7.1010932  
IC=7.9046 IR=0.3863 NU=2970,2943,2874,1760,1437,1435,1389,1154,983,891,567  
ROSYM=3 V(3)=412.7cm-1 HF298=18.882+/-1.74 KCAL. REF=C.Melius BAC/MP4  
Database C47Y Max Lst Sq Error Cp @ 6000 K 0.58%

CH3NO	T12/92C	1H	3N	1O	1G	200.000	6000.000	B	45.04096	1
0.50677397E+01	0.93871079E-02	-0.33958317E-05	0.55076729E-09	-0.33095301E-13						2
0.71852464E+04	-0.10709779E+01	0.52463494E+01	-0.68175691E-02	0.46713959E-04						3
-0.53482743E-07	0.19916692E-10	0.79241319E+04	0.18687355E+01	0.95017371E+04						4

75-12-7

CH3NO FORMAMIDE O=CH-NH2 SIGMA=1 IA=1.1101014 IB= 7.2322785 IC=8.34238  
IR=0.21065 NU=3547,3426,2870,1784,1597,1396,1231,1056,1036,602,552  
INTERNAL ROTOR ROSYM=2 V(3)=7998.3 cm-1 HF298=-46.669+/-2.5 KCAL.  
REF=C.Melius BAC/MP4 Database C47X Max Lst Sq Error Cp @ 200 K 0.46%

OCHNH2	T12/92N	1C	1H	3O	1G	200.000	6000.000	B	45.04096	1
0.50996641E+01	0.96197778E-02	-0.33675100E-05	0.52625772E-09	-0.30639100E-13						2
-0.25835964E+05	-0.22514334E+01	0.31136723E+01	0.29491209E-02	0.32396676E-04						3
-0.44756760E-07	0.18144841E-10	-0.24750380E+05	0.10806345E+02	-0.23484619E+05						4

Table 4 (continued)

75-17-2

CH3NO FORMALDEHYDE-OXIME CH2=N-OH NU=3650,3110,2973,1647,1410,1318,1166,893,  
530,953,774,400 A0=2.258 B0=0.396 C0=0.336 SIGMA=2 REF= M.E. JACOX JPCRD 19  
(1990) P.1485 Max Lst Sq Error Cp @ 6000 K .45% HF298=~7. KCAL REF=NIST 1991.  
CH2NOH T12/92C 1H 3N 1O 1G 200.000 6000.000 B 45.04096 1  
0.61695525E+01 0.84795279E-02-0.29867632E-05 0.47595261E-09-0.28239453E-13 2  
0.88797203E+03-0.86718905E+01 0.25862255E+01 0.10725212E-01 0.14452581E-04 3  
-0.28351956E-07 0.12697967E-10 0.21970777E+04 0.11543250E+02 0.35225167E+04 4

136597-55-2

CH3NO FORMIMIDIC-ACID HN-CH-OH SIGMA=1 IA=1.137793 IB=7.1567938 IC=829458  
IR=0.11946 NU=3614,3381,2988,1718,1394,1335,1175,1067,1049,819  
INT ROT (-NH) ROSYM=2 V(3)=4189.8 cm-1 INT ROT (OH) ROSYM=2 IR=0.126761  
V(3)=8897. cm-1 HF298=-35.477+/-2.6 Kcal REF=C.Melius BAC/MP4 Database C47  
Max Lst Sq Error Cp @ 200 K 0.89%  
NCH3O T12/92N 1C 1H 3O 1G 200.000 6000.000 B 45.04096 1  
0.47124724E+01 0.10365763E-01-0.37841833E-05 0.60778864E-09-0.36085700E-13 2  
-0.20246735E+05-0.47729078E+00 0.43010649E+01-0.11793465E-01 0.73237860E-04 3  
-0.88185655E-07 0.34305951E-10-0.19099774E+05 0.70251243E+01-0.17852618E+05 4

463-62-7

CH3NO CH2-NH=O SIGMA=1 IA=1.0784185 IB=6.89888 IC=7.977299 IR=0.2474  
V(3)=13234. cm-1 ROSYM=2 NU=3283,3130,3020,1663,1406,1382,1244,1030,1028,888,  
715 HF298=14.109+/-2.73 Kcal REF=C.Melius BAC/MP4 Database D45 Max Lst Sq  
Error Cp @ 200 K 0.84%  
H3CNO T12/92H 3C 1N 1O 1G 200.000 6000.000 B 45.04096 1  
0.51586790E+01 0.95358020E-02-0.33500983E-05 0.53311574E-09-0.31736144E-13 2  
0.45908024E+04-0.32378122E+01 0.39607020E+01-0.82834871E-02 0.64408406E-04 3  
-0.79465373E-07 0.31225515E-10 0.58604280E+04 0.78294069E+01 0.70998839E+04 4

75-52-5

CH3NO2 Nitro-Methane STATWT =1 SYNMO = 3 IA = 6.45024 IB = 8.24944  
IC = 14.181 I(red)=0.47695 V(2) = 0.0 kcal/mole ROSYM =2 NU= 598,639,666,  
928,1083,1157,1380,1400,1440,1481,1561,2484,2767,2962. REF=McKean & Watt J. Mol  
Struct. 61(1976),164 HF(298)= -19.3 kcal/mole REF=Knobel, Mirishnichenko  
& Lebedev, Bull.Acad Sci USSR Div. Chem Sci 1971,425 Max Lst Sq Error Cp @  
1300 K 0.56%  
CH3NO2 T01/00C 1.H 3.N 1.O 2.G 200.000 6000.000 B 61.04036 1  
6.73034758E+00 1.09601272E-02-4.05357875E-06 6.67102246E-10-4.04686823E-14 2  
-1.29143475E+04-1.01800883E+01 3.54053638E+00 1.86559899E-03 4.44946580E-05 3  
-5.87057133E-08 2.30684496E-11-1.11385976E+04 1.06884657E+01-9.71208165E+03 4

624-91-9

CH3NO2 Methyl-Nitrite CH3ONO SIGMA=1 STATWT=1 IA=3.8980 IB=10.8775  
IC=14.25354 Ir(CH3)=0.50617 ROSYM=3 [V(3)=811. cm-1 as in CH3ONO2]  
Ir(NO)=1.8102 ROSYM=1 [V(3)=412.7 cm-1 as in CH3NO] Nu=3004,2979,2905,1748,  
1469,1462,1440,1194,1148,1094,903,788,355 REF=Melius D30G 1987 HF298=-65.44+/-1  
kJ REF=Ray & Gershon JPC 66,(1962),1750 {HF300=-15.31 kcal REF=Melius D30G}  
HF298(liq)=-67.15+/-1 kJ REF=Webbook Max Lst Sq Error Cp @ 1300 K 0.54%.  
CH3ONO A 5/05C 1.H 3.O 2.N 1.G 200.000 6000.000 B 61.04006 1  
6.93605239E+00 9.97319424E-03-3.60642537E-06 5.83462161E-10-3.50058729E-14 2  
-1.08381899E+04-6.98144573E+00 6.15261387E+00-2.91937431E-03 4.14526828E-05 3  
-4.93954776E-08 1.85608328E-11-9.85260262E+03 8.04057190E-01-7.87057806E+03 4



Table 4 (continued)

598-58-3

CH3ONO2 Methyl-Nitrate SYMNO = 1 STATWT = 1 IA = 6.67244 IB = 17.20275  
 IC = 23.3497 Ir (NO2) = 5.96 ROSYM = 2 V(2) = 9.1 kcal/mole  
 Ir (CH3) = 0.53436 ROSYM = 3 V(3) = 2.32 kcal/mole NU=3008,2940,2907,1672,  
 1468,1435,1434,1287,1176,1136,1017,854,759,657,578,340. REF =Brand & Cawthon  
 JACS 77, (1955),319. HF298=-29.16 kcal REF = Roy & Ogg J. Phys. Chem. 63(1959),  
 1522. Max Lst Sq Error Cp @ 1300 K 0.66%  
 CH3ONO2 T05/98C 1.H 3.N 1.O 3.G 200.000 6000.000 B 77.03976 1  
 9.77845489E+00 1.10069541E-02-4.25928645E-06 7.18198185E-10-4.42041793E-14 2  
 -1.88804487E+04-2.39163197E+01 3.91363583E+00 1.52137945E-02 1.73479131E-05 3  
 -3.37074473E-08 1.44322204E-11-1.66103232E+04 9.44208392E+00-1.46737980E+04 4

64287-49-6

CH3N2 CH3N=N\* METHYL DIAZINE RADICAL STATWT=2 SIGMA=3 IA=1.20736 IB=7.14898  
 IC=7.83945 NU=2972,2971,2888,1507,1453,1449,1375,1096,1035,821,445,147.9  
 HF298=247.7+/-12. KJ REF=C. MELIUS DATABASE BACMP4 #840 A67F Max Lst Sq Error Cp  
 @ 6000 K 0.58%  
 CH3N2 CH3N=N\* T 9/96C 1H 3N 2 0G 200.000 6000.000 B 43.04830 1  
 0.57393539E+01 0.92314020E-02-0.33396566E-05 0.54160230E-09-0.32522545E-13 2  
 0.27235968E+05-0.53905119E+01 0.46506054E+01-0.14932994E-02 0.37619849E-04 3  
 -0.46522472E-07 0.17885496E-10 0.28216313E+05 0.35837652E+01 0.29785394E+05 4

624-90-8

CH3N3 MethylAzid CH3-N=NN SIGMA=1 STATWT=1 IA=1.8392 IB=15.8708 IC=17.1758  
 Ir=0.50969 ROSYM=3 (V(3)=685 cm-1 est from East & Radom JCP 106, (1997),6655)  
 Nu=3174,3098,3038,2265,1523,1521,1475,1349,1158,1120,926,665,573,247  
 HF298=297.29 kJ HF0=309.93 kJ REF=Burcat G3B3 calc {G2 HF298=71.0 kcal  
 REF=Rogers & McLaferty JCP 103(18), (1995),8302} Max Lst Sq Error Cp @ 1300 K  
 0.54%.  
 CH3N3 MethylAzyd A11/04C 1.H 3.N 3. 0.G 200.000 6000.000 B 57.05474 1  
 6.41280183E+00 1.07448898E-02-3.85726225E-06 6.22339742E-10-3.72381596E-14 2  
 3.29519708E+04-6.94516757E+00 4.37960260E+00 7.61069318E-03 1.69547382E-05 3  
 -2.46175363E-08 9.55803332E-12 3.40058496E+04 5.84234573E+00 3.57555570E+04 4

2143-68-2

CH3O METHOXI RADICAL SYMNO=3. A0=5.2 B0=C0=0.93 T0 STATWT=3 NU=2840,1417,  
 1047,2774(2),1465,1210,914,653 T0=61.97 STATWT=1 Specific calculations perfo-  
 rmed and the polynomials were calculated from tabular values obtained.  
 HF298=21.0+/-2.1 kJ HF0=28.4 +/-2.1 kJ REF=Ruscic et al IUPAC Group JPCRD  
 2003 {HF298=20.257+/-0.42 kJ REF=ATcT A} Max Lst Sq Error Cp @ 200 K 0.93%.  
 CH3O METHOXY RA IU1/03C 1.H 3.O 1. 0.G 200.000 6000.000 A 31.03392 1  
 4.75779238E+00 7.44142474E-03-2.69705176E-06 4.38090504E-10-2.63537098E-14 2  
 3.78111940E+02-1.96680028E+00 3.71180502E+00-2.80463306E-03 3.76550971E-05 3  
 -4.73072089E-08 1.86588420E-11 1.29569760E+03 6.57240864E+00 2.52571660E+03 4

2597-43-5

H3CO HYDROXYMETHYLENE RAD (CH2OH) STATWT=2. SIGMA=1. IA=.4274 IB=2.789  
 IC=3.2164 NU=3650,3169,3071,1459,1334,1176,1048,420,234 HF298=-17.0+/-0.7  
 kJ. HF0=-10.7+/-0.7 Polynomials calculated from original Tables of Johnson &  
 Hudgens JPC 100 (1996),19874 extrapolated to 6000 K REF=Ruscic et al JPCRD  
 2003 IUPAC Group {HF298=-17.179+/-0.37 kJ REF=ATcT A} Max Lst Sq Error Cp @  
 200 & 6000 K 0.38%  
 CH2OH RADICAL IU2/03C 1.H 3.O 1. 0.G 200.000 6000.000 B 31.03392 1  
 5.09314370E+00 5.94761260E-03-2.06497460E-06 3.23008173E-10-1.88125902E-14 2  
 -4.03409640E+03-1.84691493E+00 4.47834367E+00-1.35070310E-03 2.78484980E-05 3  
 -3.64869060E-08 1.47907450E-11-3.50072890E+03 3.30913500E+00-2.04462770E+03 4

Table 4 (continued)

18682-95-6

CH2OH+ Hydroxymethylene Ion From original tables of Johnson JPC 100, (1996), 19874 extrapolated from 2000 K using Wilhoit's polynomials. HF298=716. +/-0.3 kJ REF=ATcT A {HF298=716.4+/-1.8 kJ REF= Johnson, ibid} Max Lst Sq Error Cp @ 6000 K 0.48%.

CH2OH+	ATcT/AC	1.H	3.O	1.E	-1.G	298.150	6000.000	B	31.03337	1	
						3.15788623E+00	8.47226665E-03	-2.90024459E-06	4.52234730E-10	-2.64240920E-14	2
						8.46086423E+04	6.46292180E+00	3.54817212E+00	-2.88791348E-03	2.98391223E-05	3
						-3.33577513E-08	1.20140893E-11	8.50297180E+04	7.01728608E+00	8.61626241E+04	4

1455-13-6

CH3OD Methanol-d1. SIGMA=1 IA=0.788756 IB=3.58065 IC=3.811689 IR=0.0993 NU=2718,3000,2843,1473,1456,864,1230,1040,2960,1473,1160 ROSYM=3 V(3)=130.46 cm-1. REF= Shimanouchi + Chem3D. HF0=-194.494 kJ REF=based on HF0(CH3OH)=-190.114 kJ. Max Lst sq Error Cp @ 6000 K 0.61%.

CH3OD	T06/02C	1.H	3.O	1.D	1.G	200.000	6000.000	B	33.04832	1	
						3.76904744E+00	1.04379143E-02	-3.74701222E-06	6.04357037E-10	-3.61480018E-14	2
						-2.66333524E+04	3.94139691E+00	5.23836494E+00	-1.25811165E-02	6.09285288E-05	3
						-6.76337252E-08	2.50761065E-11	-2.61145985E+04	9.40935211E-01	-2.46954899E+04	4

2143-58-0

CH3O2 METHYLPEROXIDE RAD (CH3OO) SIGMA=1 STATWT=2 IA= 1.6128 IB= 7.4232 IC=8.4958 NU=3038,3025,2937,1443,1433,1395,1173,1116,1088,885,471,131 REF= Janoscheck IUPAC Sheets HF298=9.0+/-5.1 kJ JPC 102, (1998) 1770. MAX LST SQ ERROR CP @ 6000 K 0.53 %

CH3OO PEROXYMETH	T04/02C	1.H	3.O	2.	0.G	200.000	6000.000	B	47.03362	1	
						5.92505819E+00	9.00194542E-03	-3.24254309E-06	5.24362718E-10	-3.14263003E-14	2
						-1.53258958E+03	-4.93669747E+00	4.76597792E+00	-3.51077148E-03	4.54394152E-05	3
						-5.66763729E-08	2.21591482E-11	-4.82401289E+02	4.76095141E+00	1.08244503E+03	4

7175-75-9

CH3S RADICAL SIGMA=3 STATWT=2 A=5.6800 B=C=0.44958 NU=2960,2706(2),1496(2),1313,727,586(2) T0=26397 REF=NIST Webbook 2000 HF298=29.78 kcal REF=Nicovich et al. J. Chem. Phys. 96, (1992),2518 Max Lst Sq. Erroe Cp @ 1300 0.57%.

CH3S	IU3/03H	3.C	1.S	1.	0.G	200.000	6000.000	B	47.10052	1	
						4.62809340E+00	7.50242892E-03	-2.70631691E-06	4.37671177E-10	-2.61526827E-14	2
						1.30328459E+04	4.15868210E-02	2.56437070E+00	1.15796385E-02	-4.50119584E-06	3
						-5.02342418E-10	6.95252997E-13	1.37469790E+04	1.12504946E+01	1.49857923E+04	4

74-82-8

CH4 METHANE Same as the Anharmonic but calculated Using the RRHO method rather than the NRRAO2. Max Lst Sq Error Cp @ 6000. K 0.62%.

CH4	RRHO	g 8/99C	1.H	4.	0.	0.G	200.000	6000.000	B	16.04246	1
						1.91178600E+00	9.60267960E-03	-3.38387841E-06	5.38797240E-10	-3.19306807E-14	2
						-1.00992136E+04	8.48241861E+00	5.14825732E+00	-1.37002410E-02	4.93749414E-05	3
						-4.91952339E-08	1.70097299E-11	-1.02453222E+04	-4.63322726E+00	-8.97226656E+03	4

Table 4 (continued)

74-82-8

CH4 METHANE STATWT=1. SIGMA=12. IA=IB=IC=0.52410356 NU=2916.7,1533.295(2),  
3019.491(3),1310.756(3) X11=-26 X12=-3 X13=-75 X14=-4 X22=-.4,X23=-9 X24=-20  
X33=-17 X34=-17 X44=-11 ALFA1=.01 ALFA2=-.09 ALFA3=.04 ALFA4=.07 D0=1.10864E-4  
HF298=-74.6+/-0.3 kJ HF0=66.63 kJ REF=TSIV 91 MAX LST SQ ERROR CP @ 1300K  
0.54%.

CH4	ANHARMONIC	g	8/99C	1.H	4.	0.	0.G	200.000	6000.000	B	16.04246	1	
								1.65326226E+00	1.00263099E-02	-3.31661238E-06	5.36483138E-10	-3.14696758E-14	2
								-1.00095936E+04	9.90506283E+00	5.14911468E+00	-1.36622009E-02	4.91453921E-05	3
								-4.84246767E-08	1.66603441E-11	-1.02465983E+04	-4.63848842E+00	-8.97226656E+03	4

49784-84-1

CH4N CH3NH\* METHYL AMINO RADICAL STATWT=2 SIGMA=3 IA=0.6587 IB=3.3113  
IC=3.4543 NU=3257,2937,2871,2830,1468,1458,1406,1303,1016,966,965,252.6  
HF298=187.6+/-4.77 kJ REF=C. MELIUS DATABASE BACMP4 #999 N38X Max Lst Sq Error  
Cp @ 6000 K 0.57 %

CH4N	CH3NH*	T	9/96C	1H	4N	1	0G	200.000	6000.000	B	30.04950	1	
								0.43023153E+01	0.10277337E-01	-0.36593760E-05	0.58702457E-09	-0.34979453E-13	2
								0.20473126E+05	0.13025403E+00	0.47462749E+01	-0.71705198E-02	0.50242579E-04	3
								-0.58589231E-07	0.22243219E-10	0.21124201E+05	0.17162390E+01	0.22559203E+05	4

10507-29-6

CH4N \*CH2-NH2 MethenylAmine AminoMethyl Radical SIGMA=1 STATWT=2 Ia=0.5825  
Ib=3.0764 Ic=3.5317 Ir=0.15172 ROSYM=2 V(3)=1980. cm-1 Nu=3609,3508,3255,  
3150,1687,1497,1347,1226,958,794,687 HF298=153.49 kJ HF0=164.618 kJ  
REF= Janoschek & Rossi Int. J. Chem Kinet 36, 2004, p. Max Lst Sq Error Cp @  
200 K 0.46%.

CH2NH2	A10/04C	1.H	4.N	1.	0.G	200.000	6000.000	B	30.04920	1			
								5.25073259E+00	8.44869513E-03	-2.88246667E-06	4.49128757E-10	-2.62206805E-14	2
								1.61865807E+04	-3.71361484E+00	2.77841738E+00	6.26037288E-03	2.29355197E-05	3
								-3.62922633E-08	1.55578225E-11	1.72156009E+04	1.09949826E+01	1.84604986E+04	4

57-13-6

CH4N2O Urea (NH2)2C=O IAIBIC=936.8E-117 SIGMA=2 NU=3548,3448,3440(2),1734,  
1594(2),1394,1014,1000,790,618,600,578,542,410,233,228 HF298=-235.5 kJ  
REF=Dorofeeva & Tolmach Thermochim. Acta 240, (1994),47-66. Max Lst Sq Error  
Cp @ 6000 K 0.38 %

(NH2)2C=O Urea	T10/99C	1.H	4.N	2.O	1.G	200.000	6000.000	B	60.05564	1			
								8.96505812E+00	1.08623207E-02	-3.73612748E-06	5.85618314E-10	-3.43401569E-14	2
								-3.19075377E+04	-2.11968192E+01	1.27019759E+00	3.79235458E-02	-4.13652154E-05	3
								2.49128013E-08	-6.09879982E-12	-3.00691642E+04	1.71177671E+01	-2.83239782E+04	4

556-88-7

CH4N4O2 NITROGUANIDINE (PICRITE) (NH2)2C=N-NO2 REF= Dorofeeva & Tolmach  
Thermochim. Acta 240, (1994),47-66. Data estimated by Dorofeeva and extrapolated  
to 5000 K using Wilhoit's polynomials. HF298=1.+/-20. kJ Max Lst Sq  
Error Cp @ 1200 K 0.49%

Nitroguanidine	T10/99C	1.H	4.N	4.O	2.G	298.150	5000.000	D	104.06852	1			
								1.38288509E+01	1.52703007E-02	-5.55748705E-06	9.62860873E-10	-6.41418016E-14	2
								-5.38226605E+03	-4.25512674E+01	5.74393403E-01	6.18916652E-02	-7.09491928E-05	3
								4.52102784E-08	-1.22867606E-11	-2.25858616E+03	2.33882854E+01	1.20271670E+02	4

Table 4 (continued)

67-56-1

CH<sub>3</sub>OH liquid METHANOL DATA TAKEN FROM TRC 12/84 HF298=-57.101 kcal

{HF298=-239.389+/-0.14 kJ REF=ATcT A}

CH <sub>3</sub> OH(L)	P12/84C	1.H	4.O	1.	0.C	175.610	390.000	B	32.04186	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			2
0.00000000E+00	0.00000000E+00	1.21754995E+01	-4.19673868E-02	1.42400437E-04						3
-1.60999972E-07	2.14794684E-10	-3.15401115E+04	-4.68827360E+01	-2.87341046E+04						4

67-56-1

CH<sub>4</sub>O METHANOL (CH<sub>3</sub>OH) STATWT=1. SIGMA=1. IA=.6578 IB=3.4004 IC=3.5306

Brot=28.182 ROSYM=3 V3=373.21 V6=-0.521 cm-1 NU=3681,3000,2844,1477,1455,  
 1345,1060,1033,2960,1477,1165 HF298=-201. KJ REF=CHEN WILHOIT & ZWOLINSKI  
 JPCRD 6, (1977), 105 {HF298=-201.166+/-0.18 kJ REF=ATcT A} MAX LST SQ ERROR Cp  
 @ 1300 K 0.82%.

CH <sub>3</sub> OH Methyl alc	T06/02C	1.H	4.O	1.	0.G	200.000	6000.000	B	32.04216	1
3.52726795E+00	1.03178783E-02	-3.62892944E-06	5.77448016E-10	-3.42182632E-14						2
-2.60028834E+04	5.16758693E+00	5.65851051E+00	-1.62983419E-02	6.91938156E-05						3
-7.58372926E-08	2.80427550E-11	-2.56119736E+04	-8.97330508E-01	-2.41746056E+04						4

3031-73-0

CH<sub>4</sub>O<sub>2</sub> PEROXYMETHANE (CH<sub>3</sub>OOH) SIGMA=1 STATWT=1 A=1.434544 B=0.350826 C=0.301985

Ir(CH<sub>3</sub>)=0.4282 ROSYM(CH<sub>3</sub>)=3 V(3)=1120 cm-1 Ir(OH)0.138 ROSYM(OH)=1 V(0)=780.7  
 V(1)=1111.1 V(2)=555.6 V(3)=52.6 cm-1. NU=3604,2957,2955,2861,1509,1453,1450,  
 1348,1145,1115,1003,800,415 REF=Dorofeeva et al JPCRD 30, (2001), 475  
 HF0=-27.3+/-1. kcal HF298=-126.733 kJ REF=Matthews et al JCP 122, (2005), #221101  
 {HF298=-139.0+/-5 kJ HF0=-126.2 kJ REF=Dorofeeva et al JPCRD 30, (2001), 475  
 HF298=-33.4+/-1.2 Kcal REF=Lay et. al JPC 100 (1996), 8240} Max Lst Sq Error Cp  
 @ 6000 K 0.37%

CH <sub>4</sub> O <sub>2</sub>	A 7/05C	1.H	4.O	2.	0.G	200.000	6000.000	B	48.04126	1
7.76538058E+00	8.61499712E-03	-2.98006935E-06	4.68638071E-10	-2.75339255E-14						2
-1.82979984E+04	-1.43992663E+01	2.90540897E+00	1.74994735E-02	5.28243630E-06						3
-2.52827275E-08	1.34368212E-11	-1.68894632E+04	1.13741987E+01	-1.52423685E+04						4

74-93-1

CH<sub>3</sub>SH METHANETHIOL SIGMA=1 IA=0.797364 IB=6.4954022 IC=6.76794 IR=0.181954

NU=2970(2), 2892, 2599, 1460, 1449, 1358, 1088, 964, 778, 692 POT BARRIER V(3)=454.7cm-1  
 ROSYM=2 HF298=-5.38+/-1 KCAL REF=C. Melius BAC/MP4 Database, S6B Max Lst Sq  
 Error Cp @ 6000 K 0.55%

CH <sub>4</sub> S	T 4/93C	1H	4S	1	0G	200.000	6000.000	B	48.10876	1
0.46777426E+01	0.95699729E-02	-0.34209825E-05	0.55016476E-09	-0.32838372E-13						2
-0.48206134E+04	0.10108699E+01	0.42867053E+01	-0.12993254E-04	0.29820894E-04						3
-0.37118619E-07	0.14368072E-10	-0.41817048E+04	0.56301215E+01	-0.27073057E+04						4

74-89-5

CH<sub>5</sub>N METHYLAMINE (CH<sub>3</sub>NH<sub>2</sub>) STATWT=1. SIGMA=1. IA=.81375 IB=3.8663 IC=3.7089

IR=0.5288 POT BARRIER V(3)=1980. ROSYM=6 NU=3361,2961,2820,1623,1473,1430,  
 1130,1044,780,3427,2985,1485,1419,1195 REF=Dewar & Rzepa J. Mol Struct 40,  
 (1977), 145. HF298=-5.5 kcal REF=Stull, Westrum & Sinke Max Lst Sq Error Cp @  
 1300 K 0.83%.

CH <sub>5</sub> N	T09/81C	1H	5N	1	0G	300.000	5000.000	C	31.0574	1
0.44235811E+01	0.11449948E-01	-0.36999727E-05	0.52389848E-09	-0.26375054E-13						2
-0.49847539E+04	-0.41469345E+00	0.27267694E+01	0.10014653E-01	0.67409546E-05						3
-0.98750093E-08	0.30637376E-11	-0.40688989E+04	0.10215076E+02	-0.27676911E+04						4

Table 4 (continued)

51891-74-8

CH5N2 METHYL HYDRAZINE RADICAL CH3N\*NH2 SIGMA=6 STATWT=2 IA=1.779 IB=7.9946  
 IC=9.1582 NU=3442,3308,2951,2880,2822,1647,1464,1455,1414,1316,1230,1073,1031,  
 932,755,453,385,143.9 HF298=51.43+/-1.3 kcal REF=C.MELIUS DATABASE N86A

Max Lst Sq Error Cp @ 6000 K 0.54%

CH5N2 CH3N*NH2	T 9/96C	1H	5N	2	OG	200.000	6000.000	B	45.06418	1
0.62727186E+01	0.13750206E-01	-0.48829875E-05	0.78213769E-09	-0.46564024E-13						2
0.22861878E+05	-0.96381311E+01	0.42113439E+01	0.34130124E-02	0.41788037E-04						3
-0.55495848E-07	0.21958966E-10	0.24203232E+05	0.48609693E+01	0.25880433E+05						4

113-00-8

CH5N3 GUANIDINE (NH2)2C=NH SIGMA=4 IAIBIC=1010.E-117 NU=3450,3400(3),3260,  
 1670,1640,1611,1450,1300,1284,1000(2),800(2),600,550,400(2),230(2)

REF= Dorofeeva & Tolmach Thermochim. Acta 240, (1994),47-66.

HF298=15.+/-10. kJ Max Lst Sq Error Cp @ 1200 K 0.49%

CH5N3 GUANIDINE	T10/99C	1.H	5.N	3.	O.G	200.000	6000.000	B	59.07092	1
8.64673050E+00	1.38037583E-02	-4.78895966E-06	7.55059297E-10	-4.44582536E-14						2
-5.52365417E+03	-2.09594729E+01	2.30997765E+00	2.84093787E-02	-1.07395307E-05						3
-7.11224938E-09	5.50455394E-12	-3.64916310E+03	1.24181134E+01	-1.80407504E+03						4

60-34-4

CH6N2 METHYLHYDRAZINE CH3-NH-NH2 SIGMA=1 STATWT=1 IA=2.2902 IB=8.6563 IC=9.9766  
 Ir(CH3)=0.48591 V(3)=1283 cm-1 ROSYM=3 Ir(NH2)=0.31424 V(3)=1301 cm-1 ROSYM=2  
 NU=3366,3358,3314,2967,2951,2850,2784,1597,1479,1465,1449,1282,1210,1118,1124,  
 1108,968,888,777,425 REF=Durig,Harris & Wertz J. Chem. Phys 50, (1969), 1449  
 HF298=26.15 kcal HF0=31.12 kcal REF=Burcat G3B3 calc {HF298=22.6 kcal REF=NIST  
 1991.} Max Lst Sq Error Cp @ 200 K 0.69%

CH3-NH-NH2	A10/04C	1.H	6.N	2.	O.G	200.000	6000.000	B	46.07182	1
6.63737309E+00	1.56702023E-02	-5.47121574E-06	8.65945432E-10	-5.11109616E-14						2
9.95613633E+03	-1.05806558E+01	3.36546357E+00	9.16487019E-03	4.07415430E-05						3
-6.18270852E-08	2.62064026E-11	1.14982139E+04	9.75314576E+00	1.31591158E+04						4

1631-78-3

CH6Sn Methyl Stanum TriHydrid CH3SnH3 SIGMA(external)=3 STATWT=1 IA=1.82075  
 IB=IC=12.3944 Ir=0.3706 ROSYM=3 V(3)=182 cm-1 Nu=2945.4(2),2870,1792.5,  
 1780(2),1438(2),1250,778(2),710(2),685,480.5,395(2) HF298=118.407 +/-4.2 kJ  
 HF0=136.091 kJ REF=Allendorf & Melius JPC A 109, (2005),4939 Max Lst Sq Error  
 Cp @ 1300 K 0.59%.

CH3SnH3	A 6/05SN	1.C	1.H	6.	O.G	200.000	6000.000	B	136.76834	1
8.60498921E+00	1.18186923E-02	-4.32757434E-06	7.07531801E-10	-4.27280043E-14						2
1.05182949E+04	-1.95089930E+01	1.58461850E+00	3.06017263E-02	-2.34105881E-05						3
9.64970928E-09	-1.66455492E-12	1.25969742E+04	1.71692137E+01	1.42410316E+04						4

507-25-5

CI4 TetraIodoMethane SIGMA=12 STATWT=1 IA=IB=IC=256.1162 Nu=178,90(2),  
 555(3),125(3) HF298=260.41 kJ HF0=265.53 KJ REF=Kudchadker JPCRD 4 (1975),457  
 Max Lst Sq Error Cp @ 700 K 0.17%.

CI4	T07/03C	1.I	4.	0.	O.G	200.000	6000.000	B	519.62858	1
1.23995148E+01	6.31312113E-04	-2.51112588E-07	4.33028327E-11	-2.71172423E-15						2
2.74438944E+04	-2.41335716E+01	6.28824380E+00	3.15849627E-02	-6.20355760E-05						3
5.59794766E-08	-1.89968017E-11	2.84879357E+04	4.12330502E+00	3.13202053E+04						4

Table 4 (continued)

2074-87-5

CN CYANID RADICAL REF=TSIV T0=0 WE=2068.435 WEXE=12.9765 WEYE=-3.082E-2  
 WEZE=-1.228E-3 BE=1.89931 ALFAB1=1.72786E-2 ALFAB2=-4.74E-5 ALFAB3=-4.512E-7  
 ALFAB4=3.533E-10 ALFAB5=-7.87E-12 DE=6.3782E-6 BETA1=-4.39E-8 BETA2=-9.65E-9  
 BETA3=-6.9E-10 T0=9240.041 WE=1813.474 WEXE=12.8272 WEYE=5.61E-3 WEZE=4.192E-4  
 BE=1.71547 ALFAB1=1.73452E-2 ALFAB2= 9.583E-6 ALFAB3=2.756E-6 ALFAB4=4.323E-8  
 ALFAB5=3.324E-9 ALFAB6=1.6E-10 ALFAB7=-3E-12 DE=6.1534E-6 BETA1=-0.781E-8  
 BETA2=6.83E-10 BETA3=-1.164E-10 T0=25752. WE=2163.9 WEXE=20.2 BE=1.985  
 ALFAB1=2.3E-2 DE=6.543 BETA1=8.7E-8 REF Gurvich 1991 HF298=438.68+/-2 kJ  
 HF0=435.4 kJ REF=Huang, Barts & Halpern J.Phys.Chem. 96, (1992), 425.  
 {HF298=438.807+/-0.52 REF=ATcT A} Max Lst Sq Error Cp @ 1300 K 0.51%  
 CN Cyanogen IU8/03C 1.N 1. 0. 0.G 200.000 6000.000 B 26.01744 1  
 3.39912850E+00 7.46548662E-04-1.41493852E-07 1.86747736E-11-1.26032540E-15 2  
 5.16569715E+04 4.67148681E+00 3.61256069E+00-9.53015737E-04 2.13757271E-06 3  
 -3.05001808E-10-4.70518097E-13 5.17084034E+04 3.98238722E+00 5.27611901E+04 4

22400-26-6

NCO SIGMA=1 STATWT=2 B0=0.390 NU=1363,534(2),218 T0=95.589 SIGMA=1 STATWT=2  
 B0=0.39 NU=1267,534(2),1921 T0=22754.02 STATWT=2 B0=0.402 Nu=2338,681(2),  
 1289 T0=31751.1 STATWT=4 B0=0.356 Nu=2303,681(2),1047 REF=Jacox JPCRD 27,  
 (1998),115 HF0=30.49+/-1 kcal REF=Allen & Schaefer JCP,120,(2004).11586.  
 {HF298=31.5 kcal REF= East & Allen J.Phys.Chem. 99 (1993), 4638} Max Lst Sq  
 Error Cp @ 1300 K 0.42  
 CNO (NCO) A 5/05N 1.C 1.O 1. 0.G 200.000 6000.000 A 42.01684 1  
 5.08064474E+00 2.37443587E-03-9.07098904E-07 1.52286713E-10-9.31009234E-15 2  
 1.35781204E+04-2.15734434E+00 2.77405177E+00 9.24523481E-03-9.91773586E-06 3  
 6.68461303E-09-2.09520542E-12 1.42369570E+04 9.75458670E+00 1.53995606E+04 4

2468-81-7

CNN SIGMA=1 STATWT=3 B0=0.414 NU=1235,396(2),1419 T0=23850. SIGMA=1  
 STATWT=6 B0=0.425 V1=1325,1807,525(2) T0=39950 SIGMA=1 STATWT=3 B0=0.425  
 Nu=1450,525(2),1807 REF=Jacox & Gurvich 91 HF298=591.87+/-3.19 kJ REF=ATcT A  
 {REF=Gurvich 91 HF298=632.83+/-100. kJ} Max Lst Sq Error Cp @ 1300 K 0.35%  
 CNN ATcT/AC 1.N 2. 0. 0.G 200.000 6000.000 B 40.02418 1  
 5.72167248E+00 1.80419618E-03-7.05032324E-07 1.20228712E-10-7.39252170E-15 2  
 6.91704579E+04-5.69345952E+00 3.07913306E+00 8.94074202E-03-7.89902287E-06 3  
 3.51606879E-09-7.03248477E-13 6.99329325E+04 8.06302282E+00 7.11851931E+04 4

2669-76-3

CN2 NCN SIGMA=2 STATWT=3 B0=.397 NU=1197,437(2),1466.5 T0=30383.74  
 STATWT=6 B0=0.396 NU=1254,534(2),1466 REF=JACOX JPCRD (1998) & gURVICH 91  
 HF298=465.89+/-1.78 kJ REF=ATcT A {HF0=500.+/-25 kJ REF=Gurvich 1991}  
 Max Lst Sq Error Cp @ 1300 K 0.36%.  
 NCN ATCT/AN 2.C 1. 0. 0.G 200.000 6000.000 B 40.02418 1  
 5.68743460E+00 1.82663439E-03-7.07551130E-07 1.19517763E-10-7.31862017E-15 2  
 5.40184049E+04-6.31950475E+00 2.79807986E+00 1.00008861E-02-9.59242059E-06 3  
 4.75565678E-09-1.04348512E-12 5.48304555E+04 8.62129570E+00 5.60333682E+04 4

Table 4 (continued)

509-14-8

C(NO2)4 Tetra-Nitro-Metane SYMNO = 4 Ia = 81.178919 Ib = 109.0935512  
 Ic = 119.96637 (Ir(NO2) = 5.96 ROSYM = 2 V(2) = 0.2 kcal/mole)x4  
 NU = 1985,1565,1213,1192(2),1146,1129,1015,791,701,687,672,646,640,594,562,  
 491,481,408,378,357,354,344,333,206,191,183,146,138. REF =A.BURCAT TAE  
 Report # 824 1998 HF298=19.69 kcal REF = Lebedev et. al. Russ. J. Phys.  
 Chem. 49, (1975), 1133 Eng. Transl. Max Lst Sq Error Cp @ 1300 K 0.45%.  
 C(NO2)4 T10/98C 1.0 8.N 4. 0.G 200.000 6000.000 B 196.03316 1  
 2.63028700E+01 9.03437992E-03-3.84962536E-06 6.80136488E-10-4.29929370E-14 2  
 2.32054355E+02-9.52181326E+01 1.50837189E+00 9.93550200E-02-1.38531389E-04 3  
 9.75231469E-08-2.77303820E-11 6.08687871E+03 2.77172777E+01 9.90833615E+03 4

630-08-0

CO CARBON-MONOXIDE CALCULATED FROM TSIV TABLE. REF=TSIV 79 HF298=-110.53+/-  
 0.17 kJ {HF298=-110.538+/-0.026 REF=ATcT A} Max Lst Sq Error Cp @ 1300 K 0.12%.  
 CO RUS 79C 10 1 0 0G 200.000 6000.000 A 28.01040 1  
 0.30484859E+01 0.13517281E-02-0.48579405E-06 0.78853644E-10-0.46980746E-14 2  
 -0.14266117E+05 0.60170977E+01 0.35795335E+01-0.61035369E-03 0.10168143E-05 3  
 0.90700586E-09-0.90442449E-12-0.14344086E+05 0.35084093E+01-0.13293628E+05 4

463-58-1

COS CARBON OXIDE SULFIDE SIGMA=1 B0=0.20287 cm-1 NU=2064,859,524(2) x11=-4.0  
 x22=-0.4 x33=-7.0 x12=-6.8 x23=-11.5 x13=-4.5 ALFA1=0.0006044  
 ALFA2=0.0003539 ALFA3=0.001838 A000=0 C000=0 D000=4.37E-8 HF298=-138.407+/-1.0  
 KJ REF=JANAF  
 COS J 3/61C 10 1S 100 0G 300.000 5000.000 A 60.0764 1  
 0.52392000E 01 0.24100584E-02-0.96064522E-06 0.17778347E-09-0.12235704E-13 2  
 -0.18480455E 05-0.30910517E 01 0.24625321E 01 0.11947992E-01-0.13794370E-04 3  
 0.80707736E-08-0.18327653E-11-0.17803987E 05 0.10792556E 02-0.16646069E-05 4

124-38-9

CO2 CARBON-DIOXIDE SIGMA=2 B0=0.39027 NU=1333.5,667(2),2351 X11=-3.014  
 X12=-5.058 X12=-19.048 X22=1.521 X23=-12.616 X33=-12.597 G22=-1.422  
 Y111=.0184 Y112=-.0667 Y113=-.0944 Y122=-.0657 Y123=.0880 Y133=.0268  
 Y222=.0105 Y223=-.0168 Y233=.0320 Y333=.0115 W0=51.834 ALPHA1=.00115  
 ALPHA2=-.000715 ALPHA3=.00311 D000=.129E-6 T0=30000 STATWT=3; T0=33000  
 STATWT=6 T0=36000 STATWT=3; T0=45000 STATWT=2; REF=Gurvich Vol 2 1991 p.27  
 HF298=-393.51 kJ {HF298=-393.472+/-0.014 kJ REF=ATcT A} Max Lst Sq Error Cp  
 @ 1400 K 0.4%  
 CO2 L 7/88C 10 2 0 0G 200.000 6000.000 A 44.00980 1  
 0.46365111E+01 0.27414569E-02-0.99589759E-06 0.16038666E-09-0.91619857E-14 2  
 -0.49024904E+05-0.19348955E+01 0.23568130E+01 0.89841299E-02-0.71220632E-05 3  
 0.24573008E-08-0.14288548E-12-0.48371971E+05 0.99009035E+01-0.47328105E+05 4

12326-85-1

CP CARBON PHOSPHIDE Calculated from Original Tables of Gurvich  
 HF298=520.141+/-10. kJ REF=Gurvich 1991 {HF298=449.9+/-9 kJ REF=JANAF 1985}  
 Max Lst Sq Error Cp @ 6000 K 0.93%  
 CP tps91C 1.P 1. 0. 0.G 200.000 6000.000 A 42.98446 1  
 4.07734620E+00-1.69581233E-04 5.46807741E-07-1.50294846E-10 1.15819322E-14 2  
 6.12471476E+04 2.56975201E+00 3.70277049E+00-2.93989206E-03 1.25276124E-05 3  
 -1.45997217E-08 5.62509067E-12 6.15029321E+04 5.35023631E+00 6.25607288E+04 4

Table 4 (continued)

2944-05-0  
 CS CARBON SULFIDE SIGMA=1 Be=0.820046 WE=1285.08 WEXE=6.44 WEYE=-.00077  
 ALPHAA1=.0059115 ALPHA2=-4.7E-06 DE=1.348E-06 BETA1=-3.6E-09 STATWT=1  
 T0=27661.0 WE=1135.1 WEXE=7.73 BE=0.7851 ALPHA1=.0072 DE=1.5E-06 STATWT=6  
 T0=31339.4 WE= 828.4 WEXE=4.85 WEYE=-.0056 BE=0.6489 ALPHA1=.006 DE=1.6E-06  
 STATWT=3 T0=35675. WE=795.6 WEXE=4.91 BE=.6367 ALPHA1=.0062 DE=1.6E-06  
 STATWT=6 T0=38681.9 WE=752.8 WEXE=4.95 BE=.6227 ALPHA1=.0062 DE=1.7E-06  
 STATWT=3 T0=38895.7 WE=1077.3 WEXE=10.66 BE=.7881 ALPHA1=.0092 DE=1.9D-06  
 STATWT=2. T0=39300. WE=665. BE=.57 STATWT=2.  
 T0=39345. WE=720. BE=.58 STATWT=1.  
 T0=56504. WE=462.4 WEXE=7.46 WEYE=-.108 WEZE=.0377 STATWT=1.  
 BE=.58 REF=Gurvich 91 HF298=278.55 kJ H0=275.307+/-3.8 kJ REF=Prinslow  
 JCP 94, (1991), 3563 {HF298=280.3+/-25 kJ REF=JANAF76} Max Lst Sq Error Cp @  
 2200 K 0.18%  
 CS g11/01C 1.S 1. 0. 0.G 200.000 6000.000 A 44.07670 1  
 3.76959667E+00 7.30980640E-04-2.42920716E-07 2.88070971E-11-5.21956199E-17 2  
 3.22498707E+04 3.42022942E+00 3.73124786E+00-3.09803648E-03 1.24828276E-05 3  
 -1.41633372E-08 5.33370965E-12 3.24420956E+04 4.54855088E+00 3.35016830E+04 4

75-15-0  
 CS2 CARBON DISULFIDE SIGMA=2 B0=0.1090917 cm-1 D0=1.12E-8 g22=-0.779  
 NU=664.465,395.982(2),1535.353 x11=-0.957 x22=0.940 x33=-6.54 x12=-2.261  
 x23=-6.45 x13=-7.685 W0=30.13 ALFAB1=0.000152 ALFAB2=-0.0002229  
 ALFAB3=0.0007117 STATWT=1 T0=24000. STATWT=3 T0=26187. STATWT=3.  
 T0=26500 STATWT=3. T0=28000. STATWT=3. T0=30200. STATWT=2.  
 HF298=116.7+/-1. KJ REF=Gurvich 91 {HF298=116.9 kJ REF=TRC 6/2001} Max Lst  
 Sq Error Cp @ 1200 K 0.25%  
 CS2 g 6/95C 1.S 2. 0. 0.G 200.000 6000.000 A 76.14270 1  
 5.94905043E+00 1.69288150E-03-6.74333823E-07 1.16460519E-10-6.37363519E-15 2  
 1.20171256E+04-6.17036834E+00 2.17230835E+00 1.81263444E-02-3.08080090E-05 3  
 2.65150564E-08-8.92801520E-12 1.28063739E+04 1.19826948E+01 1.40357038E+04 4

12070-15-4  
 C2 CALCULATED FROM Gurvich 91 TABLES HF298=824.35+/-1.61 kJ HF0=816.288 kJ  
 REF=ATcT A {HF298=830.457+/-10 kJ REF=Gurvich 91} Max Lst Sq Error Cp @ 700 K  
 \*\*\*2.57%\*\*\* @ 1000 K \*\*\*1.06%\*\*\*  
 C2 ATCT/AC 2. 0. 0. 0.G 200.000 6000.000 A 24.02140 1  
 4.12492246E+00 1.08348338E-04 1.57252585E-07-4.24046828E-11 3.25059373E-15 2  
 9.81882961E+04 7.97432262E-01-1.96261001E+00 5.76822247E-02-1.58039636E-04 3  
 1.72462711E-07-6.57913199E-11 9.82538219E+04 2.33201223E+01 9.91459509E+04 4

749252-44-6  
 C2Br Bromoacetylnyl Radical SIGMA=1 STATWT=2 IA= 0.687 IB=191.413 IC=192.100  
 NU=1699,609,238.6 HF298=149.06 kcal REF=Martin & Burcat JPC 108 (2004), 7752  
 HF0=626.39 kJ Max Lst Sq Error Cp @ 1300 K 0.28%  
 C2BR T04/04C 2.BR 1. 0. 0.G 200.000 6000.000 B 103.92540 1  
 5.63149447E+00 1.35149684E-03-5.17926114E-07 8.72035662E-11-5.37264882E-15 2  
 7.31493364E+04 2.73049339E+00 3.72784585E+00 8.95599534E-03-1.43282460E-05 3  
 1.26601774E-08-4.46887642E-12 7.36036331E+04 1.21059784E+01 7.50094762E+04 4



Table 4 (continued)

624-61-3

C2Br2 DIBROMOACETYLENE SIGMA=2 IB=151.8586 Nu=2264,845,333(2),292,142.4(2)  
 HF298=80.14 kcal REF=Martin & Burcat JPC 108 (2004),7752 Max Lst Sq Error  
 Cp @ 1200 K 0.25%.

C2BR2	T04/04C	2.BR 2.	0.	0.G	200.000	6000.000	B 183.83000	1
					8.39108965E+00	1.99841963E-03-7.46939907E-07	1.23760780E-10-7.54233761E-15	2
					3.76118385E+04-1.32670171E+01	4.11906993E+00	2.42469785E-02-4.74614882E-05	3
					4.45811398E-08-1.57269122E-11	3.83606241E+04	6.46248110E+00	4.03277836E+04 4

124-73-2

C2Br2F4 1,2 DIBROMO TETRAFLUORO ETHANE, HALON 2402 SIGMA=2 IA=39.179  
 IB=155.14416 IC=163.61 IR=26.4159 NU=(scaled by .89) 1229,1221,1200,1121,  
 1023,754,631,526,487,333.5,326,306,298.5,264,194,182,121 ROSYM=3 POT BARRIER  
 V(3)=5141.4 cm-1 (estim). REF=M.Karni Gaussian 89 calc 5/93 + Burcat  
 HF298=-189.0+/- 1.0 Kcal REF=Kolosov & Papina Russ. Chem. Rev 52, (1983),  
 p.754. Max Lst Sq Error Cp @ 1300 K 0.34%

C2BR2F4	T 8/95C	2BR 2F 4	OG	200.000	6000.000	C 259.82361	1
					0.16927925E+02	0.52040023E-02-0.21650634E-05	0.37666686E-09-0.23550019E-13 2
					-0.10111059E+06-0.69271880E+02	0.43050634E+01	0.50253865E-01-0.66832698E-04 3
					0.44622030E-07-0.12028279E-10-0.98117172E+05-0.65395609E+01-0.95107950E+05		4

777890-19-4 ##!##

C2Br3 TRIBROMOVINYL RADICAL SIGMA=1 STATWT=2 IA=60.3526 IB=142.4985  
 IC=202.85297 Nu=1671,742,787,470,405,243,158.4,152.2,79.6 HF298=92.11 kcal  
 REF=Martin & Burcat JPC 108 (2004),7752 Max Lst Sq Error Cp @ 1200 K 0.25%

C2Br3	T11/03C	2.BR 3.	0.	0.G	200.000	6000.000	B 263.73400	1
					1.10410172E+01	1.97324973E-03-7.65383213E-07	1.29884873E-10-8.04561971E-15	2
					4.26969165E+04-1.96376081E+01	4.22906724E+00	3.26663033E-02-5.79628181E-05	3
					5.02432370E-08-1.68050665E-11	4.40592174E+04	1.28181434E+01	4.63512871E+04 4

79-28-7

C2Br4 TERABROMOETHYLENE SIGMA=4 IA=131.96466 IB=152.0377 IC=284.0036  
 Nu=1573,885,773,643,489,272,248,214,189.4,144.3,116.3,56.2 HF298=45.43 kcal  
 REF=Martin & Burcat JPC 108 (2004),7752 Max Lst Sq Error Cp @ 1200 K 0.23%.

C2BR4	T11/03C	2.BR 4.	0.	0.G	200.000	6000.000	B 343.63800	1
					1.37363260E+01	2.30038169E-03-8.96871866E-07	1.52690680E-10-9.47880890E-15	2
					1.82943948E+04-3.32035520E+01	5.56028685E+00	3.66494584E-02-6.05261466E-05	3
					4.93947860E-08-1.57953370E-11	2.00189683E+04	6.27251873E+00	2.28611331E+04 4

777890-20-7 ##!##

C2Br5 PENTABROMOETHANE RADICAL SIGMA=3 STATWT=2 IA=198.2898 IB=225.4931  
 IC=290.7000 Ir=60.339 ROSYM=3 V(3)=2000 cm-1 Nu=1081,855,677,607,517,367,  
 254,203,199,156,142,137.4,107.7,81.3 HF298=67.7 kcal REF=Martin & Burcat  
 JPC 108 (2004),7752 Max Lst Sq Error Cp @ 1200 K 0.16%.

C2BR5	T11/03C	2.BR 5.	0.	0.G	200.000	6000.000	B 423.54200	1
					1.76288893E+01	6.60830066E-04-3.20496475E-07	6.11899398E-11-4.07154671E-15	2
					2.83290269E+04-4.82304769E+01	7.27020629E+00	4.31652804E-02-7.08697245E-05	3
					5.53591923E-08-1.68986132E-11	3.05063018E+04	1.88590203E+00	3.40677683E+04 4

Table 4 (continued)

594-73-0

C2Br6 HEXABROMOETHANE SIGMA=6 IA=264.1493 IB=306.1776 IC=306.1776 Ir=67.241  
 ROSYM=3 V(3)=20.89 kcal Nu=912,747(2),639(2),555,254.5,223,200(2),163.6(2),  
 134.3,132.5(2),100(2) HF298=39.55 kcal REF=Martin & Burcat JPC 108 (2004),  
 7752 Max Lst Sq Error Cp @ 1200 K 0.14%.

C2BR6 T11/03C 2.BR 6. 0. 0.G 200.000 6000.000 B 503.44600 1  
 1.94778939E+01 2.36200538E-03-9.24677034E-07 1.49363153E-10-8.77275567E-15 2  
 1.36096514E+04-5.73648381E+01 7.93869722E+00 5.44456034E-02-9.44881560E-05 3  
 7.78030724E-08-2.46434044E-11 1.58083744E+04-2.68266179E+00 1.99025559E+04 4

90894-95-4

C2Cl RADICAL STATWT=2 IB=13.5 NU=800,359(2),2050 REF=TSIV 1979 Max Lst Sq Error  
 Cp @ 1300 K 0.32 % HF298=494.09 KJ

C2CL RUS 79C 2CL 1 0 0G 200.000 6000.000 B 59.47470 1  
 0.56234123E+01 0.18105201E-02-0.68417616E-06 0.11416613E-09-0.69911780E-14 2  
 0.57535699E+05-0.37681711E+01 0.25669685E+01 0.16082406E-01-0.28879777E-04 3  
 0.26238319E-07-0.91509851E-11 0.58152495E+05 0.10748857E+02 0.59425029E+05 4

7572-29-4

C2Cl2 DICHLOROACETYLENE SIGMA=2 B0=0.046368 cm-1 NU=2200,410,925,380(2),  
 165(2) {F298=209.6=-42 KJ} REF=JANAF HF298=226.6+/-14 kJ REF=Manion JPCRD  
 31 (2002),123. OLD (1976) L Polynomial adjusted for new HF298.

C2CL2 TT8/03C 2CL 20 00 0G 300.000 5000.000 C 94.9274 1  
 0.81728547E 01 0.23659892E-02-0.96552505E-06 0.17736148E-09-0.12135203E-13 2  
 0.24554808E 05-0.14916744E 02 0.50229482E 01 0.14082667E-01-0.18095669E-04 3  
 0.11610348E-07-0.28817478E-11 0.25272100E 05 0.59684170E 00 0.27253560E+05 4

598-88-9

C2Cl2F2 1,2-DichloroDifluoroEthylene-trans E SIGMA=2 STATWT=1 IA=19.7543  
 IB=56.2005 IC=75.9547 Nu=1785,1252,1209,870,641,538,422(2),365,290,177,135  
 HF298=-341.486 kJ HF0=-339.297 kJ REF=Burcat G3B3 calc {HF298=-324.1 kJ  
 REF=Gurvich 1991; HF298=-334.9 kJ REF=G3 calc Novak, JOC 65,(2000),5057} Max  
 Lst Sq Error Cp @ 1200 K 0.36%.

C2Cl2F2 1,2-trans A 4/05C 2.CL 2.F 2. 0.G 200.000 6000.000 B 132.92361 1  
 1.22451924E+01 3.78046914E-03-1.46578504E-06 2.48660756E-10-1.53990929E-14 2  
 -4.54146822E+04-3.27309402E+01 2.62914166E+00 4.10399887E-02-6.21784729E-05 3  
 4.85226879E-08-1.52202072E-11-4.32183738E+04 1.45010690E+01-4.10710346E+04 4

311-81-9

C2Cl2F2 1,2-DichloroDifluoroEthylene-cis Z SIGMA=2 STATWT=1 IA=27.4349  
 IB=45.4569, IC=72.8918 Nu=1774,1234,1183,954,561,527,431,413,346,330,168,147  
 HF298=-339.548 kJ HF0=-337.369 kJ REF=Burcat G3B3 calc {HF298=-325.2 kJ  
 REF=Gurvich 1991; HF298=-334.9 kJ REF=G3 calc Novak, JOC 65,(2000),5057} Max  
 Lst Sq Error Cp @ 1200 K 0.37%.

C2Cl2F2 1,2-cis A 4/05C 2.CL 2.F 2. 0.G 200.000 6000.000 B 132.92361 1  
 1.22715086E+01 3.75606497E-03-1.45678851E-06 2.47184023E-10-1.53096826E-14 2  
 -4.51855503E+04-3.28645807E+01 2.63832423E+00 4.13848978E-02-6.34470202E-05 3  
 5.01025619E-08-1.58761044E-11-4.29950573E+04 1.43921216E+01-4.08380453E+04 4

76-14-2

C2Cl2F4 DICHLOROTETRAFLUOROETHANE FC-114 SIGMA=2 TRC DATA EXTRAPOLATED TO  
 6000 K USING WILHOIT'S POLYNOMIALS HF298=-900.4 KJ Max Lst Sq Error Cp @ 1200 K  
 0.29%.

C2CL2F4 P 6/89C 2CL 2F 4 0G 200.000 6000.000 C 170.92101 1  
 0.18371829E+02 0.35022641E-02-0.14461714E-05 0.25677130E-09-0.16390256E-13 2  
 -0.11490699E+06-0.64188919E+02 0.15529390E+01 0.61192651E-01-0.77774410E-04 3  
 0.46109224E-07-0.10412101E-10-0.11087452E+06 0.19780366E+02-0.10829261E+06 4

Table 4 (continued)

90177-25-6

C2CL3 TRICHLOROVINYL RADICAL STATWT=2 IAIBIC=9.9E-113 NU=625,950,850,1600,  
300,200(2),400,450 HF298=190.28 kJ REF=TSIV 1979 Max Lst Sq Error Cp @ 1200  
K 0.3%

C2CL3	RUS 79C	2CL	3	0	OG	200.000	6000.000	C 130.38010	1
0.10595050E+02	0.24399967E-02	0.95037713E-06	0.16169666E-09	0.10033459E-13					2
0.19234142E+05	0.22503828E+02	0.26913275E+01	0.34419583E-01	0.54507749E-04					3
0.43131421E-07	0.13498250E-10	0.20955741E+05	0.15941066E+02	0.22885293E+05					4

76-13-1

C2CL3F3 TRICHLOROTRIFLUOROETHANE CCl2F-CClF2 FC-113 SIGMA=1 TRC DATA  
EXTRAPOLATED TO 6000 K USING WILHOIT'S POLYNOMIALS HF298=-705.8 KJ  
{HF298= -726.8+/-4.3 kJ REF=Kolesov & Papina Russ Chem Rev. 52,(1983), 425.}  
Max Lst Sq Error Cp @ 1300 K 0.36%

CCl2F-CClF2	P 6/89C	2CL	3F	3	OG	200.000	6000.000	C 187.37531	1
0.18530350E+02	0.34300395E-02	0.14462044E-05	0.25941090E-09	0.16648746E-13					2
-0.91474377E+05	0.62171585E+02	0.24748737E+01	0.60785666E-01	0.83261974E-04					3
0.55593237E-07	0.14834855E-10	0.87694606E+05	0.17547918E+02	0.84887744E+05					4

354-58-5

C2CL3F3 111-TRICHLORO 222-TRIFLUORO ETHANE CF3-CCl3 (FC-113A) SIGMA=9 TRC  
DATA EXTRAPOLATED TO 6000 K USING WILHOIT'S POLYNOMIALS HF298=-740.5 KJ Lst Sq  
Error Cp @ 1200 K 0.35%.

C2CL3F3	FC-113A	P 6/89C	2CL	3F	3	OG	200.000	6000.000	C 187.37531	1
0.18413343E+02	0.35473766E-02	0.15023623E-05	0.27024166E-09	0.17375093E-13					2	
-0.95640066E+05	0.63672664E+02	0.29342707E+01	0.56805544E-01	0.73255691E-04					3	
0.45121198E-07	0.10894098E-10	0.91909696E+05	0.13640335E+02	0.89073199E+05					4	

127-18-4

C2CL4 TETRACHLOROETHYLENE DATA TAKEN FROM TRC/12/82 EXTRAPOLATED USNG WILHOIT'S  
POLYNOMIALS. {HF298=-12.13 KJ REF=TRC} HF298=-24.2+/-4.0 kJ REF=Manion JPCRD  
32 (2002),123. Old (1987) L Polynomial with HF298 adjusted

C2CL4	TT8/03C	2.CL	4.	0.	O.G	298.150	5000.000	C 165.83400	1
0.12935937E 02	0.34309200E-02	0.15067194E-05	0.29346993E-09	0.21070896E-13					2
-0.73449128E 04	0.34693855E 02	0.41434792E 01	0.37422372E-01	0.54369793E-04					3
0.39112863E-07	0.11176384E-10	0.54009520E 04	0.83314072E 01	0.29105744E 04					4

7094-17-9

C2CL5 PENTACHLOROETHYL RADICAL STATWT=2 IAIBIC=8.3E-112 NU=550,800,850,725,775  
1000,250,300,400,175,300,165,225,250 ROSYM=3 IR=24.6 V(1)=1150 1/CM REF=TSIV 79  
Max Lst Sq Error Cp @ 1200 K 0.20% HF298=39.0 KJ

C2CL5	RUS79 C	2CL	5	0	OG	200.000	6000.000	C 201.28550	1
0.17153955E+02	0.13960259E-02	0.64226587E-06	0.11840383E-09	0.76901280E-14					2
-0.10091822E+04	0.51540891E+02	0.29430292E+01	0.63377422E-01	0.10845541E-03					3
0.87020632E-07	0.26867241E-10	0.17951146E+04	0.16297364E+02	0.46905951E+04					4

Table 4 (continued)

67-72-1

C2Cl6 HEXACHLOROETHANE SIGMA=2(ext) STATWT=1 IA=99.0743 IB=IC=121.1808  
 IR=25.1120 ROSYM=3 V(3)=5796. cm-1 REF=Burcat G3B3 calc NU=975,431,170,675,  
 372,778(2),271(2),114(2),859(2),340(2),223(2) REF=Shimanouchi HF298=-161.11 kJ  
 HF0=-159.695 kJ REF=Burcat G3B3 calc  
 {HF298=-33.2 kcal REF=Chao, Rodgers, Wilhoit & Zwolinski JPCRD 3, (1974), 141;  
 HF298=-148.2+/-5.7 kJ REF=Manion JPCRD 31 (2002), 123.} Max Lst Sq Error Cp @  
 6000 K 0.19%.

C2Cl6	A 4/05C	2.CL 6.	0.	0.G	200.000	6000.000	B 236.73760	1
1.88630387E+01	3.24136618E-03	-1.36977241E-06	2.36702848E-10	-1.46489708E-14				2
-2.57902776E+04	-6.06433678E+01	3.83016650E+00	6.99619400E-02	-1.19578126E-04				3
9.72583947E-08	-3.05156890E-11	-2.28701227E+04	1.08683334E+01	-1.94972404E+04				4

1070-74-2

C2D2 ACETYLENE-D2 STATWT=1. SIGMA=2. IB=3.2838 NU=2701,1762,2439,505(2),  
 537(2) X11=15.43,X12=12.1,X13=58.78,X14=10.87,X15=6.92,X22=6.31,X23=.91,X24=  
 8.34,X25=.56,X34=5.54,X35=3.13,X44=-3.66,X45=7.7,X55=1.24,X33=14.3,G44=-0.75,  
 G55=-1.36 REF=SHIMANOUCI MAX LST SQ ERROR CP @ 1300K 0.55% . HF0=53.22 KCAL  
 derived from HF0 of C2H2 in JANAF 1971.

C2D2	T 8/80C	2D 2	0	OG	300.000	5000.000	A 28.0502	1
0.57631445E+01	0.39823391E-02	-0.14399011E-05	0.21952536E-09	-0.12146185E-13				2
0.24641469E+05	-0.92791763E+01	0.37629929E+01	0.83192550E-02	-0.22101658E-05				3
-0.40820787E-08	0.27229842E-11	0.25258297E+05	0.13356880E+01	2.6723643 E+04				4

4789-21-3

C2D2O KETENE-D2 SIGMA=2 IA=.5974 IB=9.1958 IC=9.7932 NU=2267,2120,1228,  
 927,2383,855,371,542,432 REF=B.MOORE & PIMENTEL MAX LST SQ ERROR CP @ 1300 K  
 0.65 %. HF298=9.54 KCAL derived from Benson's value for C2H2O

C2D2O	T10/82C	2D 20	1	OG	300.000	5000.000	B 44.0496	1
0.68584700E+01	0.55908523E-02	-0.19912059E-05	0.31183456E-09	-0.17762101E-13				2
0.21307729E+04	-0.11521992E+02	0.34471798E+01	0.11882458E-01	-0.17057137E-05				3
-0.64614767E-08	0.35897769E-11	0.32729224E+04	0.69639057E+01	0.48011892E+04				4

683-73-8

C2D4 ETHYLENE-D4 STATWT=1. SIGMA=4. IA=1.1487 IB=3.793 IC=4.942 NU=2247,  
 1515,981,728,2289,1009,720,780,2345,586,2200,1078 REF=BURCAT MAX LST SQ ERROR  
 CP @ 1300K 0.86% . HF298=30.27 KJ.

C2D4	T12/79C	2D 4	0	OG	300.000	5000.000	B 32.0784	1
0.67207203E 01	0.84912479E-02	-0.30327419E-05	0.47564219E-09	-0.27109157E-13				2
0.62753809E 03	-0.14424983E 02	0.13294621E 01	0.17719518E-01	-0.13082199E-05				3
-0.10431190E-07	0.53182406E-11	0.24874675E 04	0.15025264E 02	0.36406234E+04				4

1632-89-9

C2OD4 ETHANAL-D4 (ACETALDEHIDE-D4) STATWT=1 SIGMA=1 IA=2.4015 IB=9.7752  
 IC=11.109 IR=.64048 POT BARRIER V(3)=1161. NU=2265,2130,2060,1737,1045,938,  
 1028,1151,747,436,2225,1028,573,670 REF=CHAO,WILHOIT & HALL MAX LST SQ ERROR  
 CP @ 1300 K 0.85 %. HF298=-43.16 KCAL.

C2OD4	T 8/81C	2D 40	1	OG	300.	5000.	B 48.0778	1
0.85226345E+01	0.92743672E-02	-0.33571869E-05	0.53372684E-09	-0.30898383E-13				2
-0.25431613E+05	-0.19829504E+02	0.24537258E+01	0.18615011E-01	0.81830109E-06				3
-0.12927025E-07	0.59826883E-11	-0.23262375E+05	0.13648181E+02	-0.21718827E+05				4

Table 4 (continued)

1632-99-1

C2D6 ETHANE-D6 STATWT=1. SIGMA=6. SIGMA BARRIER=3. IA=2.0942 IB=IC=6.0986  
 NU=2083,1155,843,2087,1077,2226(2),1041(2),970(2),2235(2),1081(2),594(2)  
 POTENTIAL BARRIER V0=2.87 IR=.5235 REF=BURCAT MAX LST SQ ERROR CP @ 1300 K  
 0.92 % . HF298=-110.68 KJ.

C2D6	T05/80C	2D	6	0	OG	300.000	4000.000	B	36.1066	1
	0.87366476E+01	0.11772312E-01	0.42297552E-05	0.66704353E-09	0.38247847E-13					2
	-0.17392641E	05-0.25919988E	02	0.81539208E	00	0.24633620E-01	0.28606987E-07			3
	-0.16559884E-07	0.79903445E-11	0.14620465E	05	0.17542796E	02-0.13311668E+05				4

65844-97-5 and 64919-23-9 or 1681-47-6

C2D6N2 AZOMETHANE-D6 (CD3NNCD3) STATWT=1 SIGMA=2 IA=3.147 IB=24.215  
 IC=25.133 IR=0.765 POT BARRIER V0=1700. NU=2234,2127,1569,1122,1044,1034,761,  
 523,2225,1027,803,2239,1049,896,261,2240,1115,1112,1051,921,900,304,(191,166  
 TORSIONAL FREQ) REF=PAMIDIMUKKALA,ROGERS &SKINNER MAX LST SQ ERROR CP @ 1300K  
 0.9 % . HF298=28.5 KCAL.

C2D6N2	L 8/84C	2D	6N	2	OG	300.000	5000.000	B	64.12001	1
	0.13025591E	02	0.13045497E-01	0.47310468E-05	0.75233886E-09	0.43511835E-13				2
	0.86393672E	04-0.43220398E	02	0.23340378E	01	0.30852020E-01	0.74860048E-06			3
	-0.23019155E-07	0.11133473E-10	0.12308605E	05	0.15217487E	02	0.14341845E	05		4

17222-37-6

C2D6O DIMETHYL-ETHER-D6 SIGMA=2 SIGMA BARRIER=3 IA=3.2656 IB=11.2126  
 IC=12.3437 IR=9.271 V(3)=2500. NU=2248(2),2054(2),1059(4),1057(2),1033,827,  
 362,2202,1162,872,2184,931,950 REF=KANAZAWA AND NUKADA MAX LST SQ ERROR @  
 1300 K 0.86 % . HF0=-45.9 KCAL derived from HFO of C2H6O by Stull,Westrum & Sinke

C2D6O	T12/82C	2D	6O	1	OG	300.000	5000.0	B	52.10601	1
	0.10630716E+02	0.12416139E-01	0.44895924E-05	0.71285688E-09	0.41213699E-13					2
	-0.29983387E+05	0.32492361E+02	0.16130285E+01	0.27251996E-01	0.22420198E-06					3
	-0.19127672E-07	0.92674445E-11	0.26856473E+05	0.16893214E+02	0.25195712E+05					4

22533-50-2

C2F RADICAL STATWT=2 IB=7.8 NU=1100,400(2),2175 HF298=353.847 kJ REF=TSIV 91  
 Max Lst Sq Error Cp @ 1300 K 0.37%

C2F	tpis91C	2.F	1.	0.	OG	200.000	6000.000	C	43.01980	1
	5.26094396E+00	2.14579712E-03	8.07509859E-07	1.34379596E-10	8.21353206E-15					2
	4.07468230E+04	3.14254580E+00	2.70218031E+00	1.27931571E-02	2.04432188E-05					3
	1.78526199E-08	6.17934124E-12	4.13318085E+04	9.33996365E+00	4.25578275E+04					4

689-99-6

C2F2 DIFLUOROACETYLENE SIGMA=2 IB=23.7 NU=2400,770,1375,370(2),250(2)  
 HF298=-147.+/-20 KJ REF=Gurvich 91 Max Lst Sq Error Cp @ 1300 K 0.35%.

C2F2	tpis91C	2.F	2.	0.	OG	200.000	6000.000	C	62.01821	1
	7.52427784E+00	2.82972830E-03	1.06007796E-06	1.75914064E-10	1.07321882E-14					2
	-1.99676214E+04	1.41326234E+01	2.91334535E+00	2.41841544E-02	4.29053931E-05					3
	3.87359940E-08	1.34689906E-11	1.90338319E+04	7.79800602E+00	1.73991838E+04					4

4605-17-8

C2F3 TRIFLUOROVINYL RADICAL STATWT=2 IAIBIC=5.2E-114 NU=925,1350,1250,1800,  
 500(2),250,550,300 HF298=-228.181+/-20 kJ REF=Gurvich 91 {HF298=-244 kJ  
 REF=Orlov Zaripov Lebedev Russ Chem Bul 47,(1998),621.} Max Lst Sq Error Cp  
 @ 1300 K 0.42%.

C2F3	tpis91C	2.F	3.	0.	OG	200.000	6000.000		81.01661	1
	9.28002368E+00	3.72628116E-03	1.44027826E-06	2.43838247E-10	1.50793717E-14					2
	-3.08448687E+04	1.92329718E+01	2.41464240E+00	2.68291562E-02	3.39283388E-05					3
	2.31906358E-08	6.71131007E-12	2.90990246E+04	1.53576825E+01	2.74437210E+04					4

Table 4 (continued)

116-14-3

C2F4 TETRAFLUOROETHYLENE FC-1114 SIGMA=4 IAIBIC=16300. NU=1872,1340,1337,778,551,218,394,406,1186,190,508,558 HF298=-675.34+/-2.0 kJ REF=ATcT A {HF298=-659.5+/-2.5 kJ REF=Gurvich 91; HF298=-658.6+/-2.9 REF=JANAF 69 & TRC 94} Max Lst Sq Error Cp @ 1300 K 0.43%

C2F4	FC-1114	ATcT/AC	2.F	4.	0.	0.G	200.000	6000.000	B	100.01501	1
1.14178412E+01	4.59161071E-03	-1.77520928E-06	3.00598731E-10	-1.85921260E-14							2
-8.54207001E+04	-3.16445526E+01	1.99308667E+00	3.84734406E-02	-5.32322754E-05							3
3.92122720E-08	-1.19302747E-11	-8.31300869E+04	1.53134111E+01	-8.12242694E+04							4

3369-48-0

C2F5 PENTAFLOROETHYL RADICAL SIGMA=1 STATWT=2 IA=21.788 IB=33.994 IC=41.428 IR=5.128 ROSYM=3 V(3)=881. 1/CM NU=1398,1273,1227,1184,1117,820,703,604(2),514,419,366,227,211 HF298=-213.0 Kcal REF=Chen Rauk & Tschuikow-Roux J. Chem. Phys. 95 (1991), 2774 {HF298=-212.66+/-1.3 kcal REF=Chen et al JPCRD 4, (1975), 441} Max Lst Sq Error Cp @ 1300 K 0.36%

C2F5	T01/92C	2F	5	0	0G	200.000	6000.000	B	119.01402	1
0.14093289E+02	0.44836847E-02	-0.17454011E-05	0.29629851E-09	-0.18397296E-13						2
-0.11234658E+06	-0.42296047E+02	0.19562988E+01	0.44980179E-01	-0.54414843E-04						3
0.31961057E-07	-0.73732181E-11	-0.10934658E+06	0.18665321E+02	-0.10718515E+06						4

76-16-4

C2F6 HEXAFLUOROETHANE (FC-116) SIGMA=6 STATWT=1 IA=29.9923 IB=IC=45.8147 IR=7.4980 V(3)=1595. cm-1 REF=Burcat G3B3 calc NU=1251(2),1250(2),1228,1117,807,714,619(2),520(2),372(2),348,220(2) REF=Shimanouchi HF298=-1347.38+/-4.1 kJ REF=ATcT A {HF298=-1351.52 kJ REF=Burcat G3B3 calc HF298=-1343.9+/-5.0 KJ REF=JANAF} Max Lst Sq Error Cp @ 1300 K 0.38%

C2F6	FC-116	ATcT/AC	2.F	6.	0.	0.G	200.000	6000.000	B	138.01182	1
1.70284831E+01	4.64174937E-03	-1.92155485E-06	3.37538839E-10	-2.13452416E-14							2
-1.68391922E+05	-5.98112608E+01	1.56503771E+00	5.10909623E-02	-5.07167534E-05							3
1.88993955E-08	-7.73770882E-13	-1.64377996E+05	1.89556430E+01	-1.62051642E+05							4

927-84-4

C2F6O2 CF3-OO-CF3 SIGMA=18 Calculated Using THERM (97) Extrapolated 1000-5000K Using Wilhoit's Polynomials HF298=360.2+/-3. kcal REF=Levy & Kennedy JACS 94 (1972) 3302 Max Lst Sq Error Cp @ 1000K 0.30%

CF3-O-O-CF3	T10/97C	2F	60	2	0G	298.150	5000.000	F	170.01122	1
1.87994539E+01	8.78358323E-03	-3.68712829E-06	6.99609239E-10	-4.92829440E-14						2
-1.88252514E+05	-5.97973365E+01	9.11006951E+00	2.71182010E-02	-1.23579087E-06						3
-2.30183402E-08	1.25085439E-11	-1.85129629E+05	-7.65920017E+00	-1.81258643E+05						4

2122-48-7

C2H ETHYNYL RADICAL SIGMA=1 STATWT=2 B0=1.457 NU=3328,372(2),1841 T0=4000 STATWT=4 B0=1.457 NU=3460,560(2),1850 REF=Kiefer, Sidhu, Kern, Xie, Chen, Harding 1992 HF298=568.522+/-4 kJ REF= NIST Webbook 1999. {HF298=568.056+/-0.3 kJ REF=ATcT A; HF298=567.4+/-1.5 kJ REF=Szalay Tajti & Stanton Mol Phys 103, (2005), xxx} MAX LST SQ ERROR Cp @ 400 K 0.34 %

C2H ETHYNYL RAD	T07/00C	2.H	1.	0.	0.G	200.000	6000.000	B	25.02994	1
3.66459586E+00	3.82189487E-03	-1.36509398E-06	2.13253692E-10	-1.23098939E-14						2
6.72238503E+04	3.91355399E+00	2.90180321E+00	1.32859725E-02	-2.80508233E-05						3
2.89300812E-08	-1.07446930E-11	6.71171170E+04	6.17234595E+00	6.83770805E+04						4

Table 4 (continued)

593-61-3

C2HBr BROMOACETYLENE SIGMA=1 IB=21.0049 NU=3325,2085,618(3),295(2)  
 HF298=67.50 kcal HF0=289.07 kJ REF=Martin & Burcat JPC 108 (2004),7752 Max  
 Lst Sq Error Cp @ 1300 K 0.27%  
 BROMOACETYLENE T02/04C 2.H 1.BR 1. 0.G 200.000 6000.000 B 104.93334 1  
 6.55399311E+00 3.37962726E-03-1.18362410E-06 1.87797808E-10-1.11059116E-14 2  
 3.17495713E+04-8.20269727E+00 1.10795098E+00 3.21065018E-02-6.02244383E-05 3  
 5.45400888E-08-1.86034151E-11 3.26428366E+04 1.67414085E+01 3.39671249E+04 4

777890-18-3 ##!##

C2HBr2 DIBROMOVINYL RADICAL SIGMA=1 STATWT=2 IA=1.3539 IB=141.3108  
 IC=142.6657 NU=3156,1647,1167,714,692,684,222.7,168.3,151.5 REF=IR(NIST) +  
 B97-1/Aug-VTZ calc HF298=79.73 kcal REF=Martin & Burcat JPC 108 (2004),7752  
 Max Lst Sq Error Cp @ 6000 K 0.29%  
 DIBROMOVINYL Rad T02/04C 2.H 1.BR 2. 0.G 200.000 6000.000 B 184.83734 1  
 8.72858939E+00 3.86564166E-03-1.40557002E-06 2.28856470E-10-1.37851228E-14 2  
 3.70537064E+04-1.22420089E+01 3.90735018E+00 2.01719356E-02-2.29185829E-05 3  
 1.32196024E-08-2.97657283E-12 3.82376740E+04 1.19225925E+01 4.01214648E+04 4

598-16-3

C2HBr3 TriBromoEthylene SIGMA=1 IA=53.9874 IB=141.5181 IC=195.5043  
 Nu=3102,1536,1218,835,770,704,[511,425,239.5,167(2),108.2] REF=NIST Webbook  
 2000 IR + B97-1/Aug-VTZ[] HF298=34.46 kcal REF=Martin Burcat JPC 108 (2004),  
 7752 Max Lst Sq Error Cp @ 1300 K 0.29%  
 C2HBR3 T02/04C 2.H 1.BR 3. 0.G 200.000 6000.000 B 264.74134 1  
 1.13478698E+01 4.29311143E-03-1.58086118E-06 2.59583491E-10-1.57282684E-14 2  
 1.33625344E+04-2.35492301E+01 3.77338993E+00 3.25157387E-02-4.40715090E-05 3  
 3.06046323E-08-8.51827665E-12 1.51034973E+04 1.38067404E+01 1.73408463E+04 4

143962-85-0

C2HBr4 1,1,2,2-Tetrabromoethyl Radical SIGMA=1 STATWT=2 IA=130.46699 IB=197.2737  
 IC=230.0634 Ired=34.053 ROSYM=1 V(3)=4571.cm-1 NU=3159,1242,1147,1119,831,  
 631,531,502,338,235,180,129.5,106.9,77.6 HF298=52.30+/-2 kcal HF0=65.64 kcal  
 REF=Martin Burcat JPC A 108 (2004),7752 Max Lst Sq Error Cp @ 6000 K 0.34%  
 C2HBR4 1,1,2,1 A04/05C 2.H 1.BR 4. 0.G 200.000 6000.000 B 344.64534 1  
 1.43466439E+01 4.59266344E-03-1.90433791E-06 3.30906808E-10-2.06740879E-14 2  
 2.13543342E+04-3.30720905E+01 5.74443922E+00 3.53866220E-02-4.56980575E-05 3  
 2.94359085E-08-7.52371010E-12 2.33818229E+04 9.62682719E+00 2.63182316E+04 4

777890-21-8 ##!##

C2HBr4 1,1,1,2-Tetrabromoethyl Radical CBr3CHBr SIGMA=1 STATWT=2 IA=120.5543  
 IB=194.2015 IC=209.6538 Ired=29.3667 ROSYM=3 V(3)=4571.cm-1 Nu=95.3,139,142,  
 183,230,233,396,433,566,659,770,115,1244,3214 HF298=58.23+/-2 kcal  
 HF0=65.64 kcal REF= Martin & Burcat JPC 108 A (2004),7752 Max Lst Sq  
 Error Cp @ 6000 K 0.31%  
 C2HBR4 1,1,1,2 A04/05C 2.H 1.BR 4. 0.G 200.000 6000.000 B 344.64534 1  
 1.49021916E+01 4.09313174E-03-1.71942492E-06 3.00191012E-10-1.87917454E-14 2  
 2.42836440E+04-3.68514122E+01 5.49338769E+00 4.43775106E-02-7.21638780E-05 3  
 5.81949089E-08-1.83446315E-11 2.62232314E+04 8.36337126E+00 2.93023064E+04 4

Table 4 (continued)

75-95-6

C2HBr5 PENTABROMOETHANE STATWT=1 SIGMA=1 IA=194.3132 IB=194.3132  
 IC=290.9547 Ired=58.12 ROSYM=3 V(3)=4570.2 cm-1 NU=3191,1243,1158,1011,720,  
 709,621,590,476,241,200,196,160,146.2,142,110.4,105.1 HF298=27.03 kcal  
 REF=Martin Burcat JPC 108 (2004),7752 {HF298=9.9 kcal Benson est} Max Lst Sq  
 Error Cp @ 1300 K 0.30%.

C2HBR5	T02/04C	2.H	1.BR	5.	0.G	200.000	6000.000	B	424.54934	1	
						1.66081581E+01	5.06290581E-03	-2.03596140E-06	3.48536490E-10	-2.15900552E-14	2
						7.94235843E+03	-4.44034839E+01	6.69308019E+00	4.34129740E-02	-6.15643594E-05	3
						4.36743888E-08	-1.22540346E-11	1.01402274E+04	4.11773919E+00	1.36019465E+04	4

593-63-5

C2HCl CHLOROACETYLENE B0=0.188645 cm-1 NU=3340,2110,756,604(2),326(2)  
 SIGMA=1 {HF298=213.8+/-42 KJ} REF=JANAF HF298=226.4+/-10 kJ REF=Manion JPCRD  
 31,(2002),123. OLD (1982) L polynomial adjusted for new HF298

C2HCL	TT8/03C	2H	1CL	1	0G	200.000	6000.000	B	60.48264	1	
						0.65309289E+01	0.34106362E-02	-0.11975370E-05	0.19036853E-09	-0.11274117E-13	2
						0.24999035E+05	-0.94114463E+01	0.11110549E+01	0.31070093E-01	-0.56793918E-04	3
						0.50648615E-07	-0.17112722E-10	0.25927035E+05	0.15622398E+02	0.27229506E+05	4

211235-51-7

C2HClF 1,1-ChloroFluoroVinyl Radical \*CH=CFC1 STATWT=2 SIGMA=1 IA=7.3539  
 IB=16.4588 IC=23.8128 NU=3347,1716,1101,822,608.5,578,519,403,359  
 HF298=24.348+/-4.kcal REF=G3B3 calc {HF298=20.8+/-10 kcal REF=NIST-94 ;  
 Thergas est=7.51 kcal (wrong) PM3=28.02 kcal AM1=29.74 kcal} Max Lst sq Error  
 Cp @ 1300 K 0.31%.

C2HCLF 1,1-CLF	A12/04C	2.H	1.CL	1.F	1.G	200.000	6000.000	B	79.48044	1	
						8.50937039E+00	4.01863606E-03	-1.45196186E-06	2.35520678E-10	-1.41529004E-14	2
						9.20079581E+03	-1.56313584E+01	7.65226273E-01	3.63165689E-02	-5.63440044E-05	3
						4.42113186E-08	-1.36516970E-11	1.08268804E+04	2.17621692E+01	1.22523194E+04	4

359-10-4

C2HClF2 1,1-CHCl=CF2 CLORO-DIFLUORO-ETHYLENE FC-1122 SIGMA=1 IAIBIC=1.2873E 113  
 NU=1745,3130,1333,1199,845,970,433,579,201,751,572,243 HF298=-334. KJ  
 REF=TSIV 79 Max Lst sq error Cp @ 1300 K 0.39%

C2HCLF2-1,1	RUS 79C	2F	2H	1CL	1G	200.000	6000.000	B	98.47945	1	
						0.99982378E+01	0.56213876E-02	-0.20890705E-05	0.34507576E-09	-0.20992736E-13	2
						-0.43955643E+05	-0.23448017E+02	0.20480403E+01	0.29590895E-01	-0.28065357E-04	3
						0.11297923E-07	-0.10168634E-11	-0.41870475E+05	0.17086656E+02	-0.40170738E+05	4

30860-28-7

C2HClF2 cis-CHF=CFCl E-CLORO-DIFLUORO-ETHYLENE FC-1131 SIGMA=1  
 IAIBIC=1.2873E 113 NU=1716,3137,1326,1159,854,1112,361,480,224,776,523,255  
 T0=850 HF298=-323.569 KJ REF=TSIV 79 Max Lst sq error Cp @ 1300 K 0.33%

C2HCLF2 cis	RUS 79C	2F	2H	1CL	1G	200.000	6000.000	B	98.47945	1	
						0.10773817E+02	0.48843919E-02	-0.18135371E-05	0.29944899E-09	-0.18214330E-13	2
						-0.42909705E+05	-0.27423997E+02	0.18766172E+01	0.32753447E-01	-0.32851961E-04	3
						0.13358593E-07	-0.10107904E-11	-0.40667163E+05	0.17580933E+02	-0.38916184E+05	4

2837-86-7

C2HClF2 trans-CFCl=CHF Z-CHLORO-1,2-DIFLUORO-ETHYLENE SIGMA=1 IAIBIC=1.2873E 113  
 NU=1708,3120,1290,1196,696,1150,397,578,200,776,467,310 T0=900

HF298=-323.103 KJ REF=TSIV 79 Max Lst sq error Cp @ 1300 K 0.33%

C2HCLF2 trans	RUS 79C	2F	2H	1CL	1G	200.000	6000.000	B	98.47945	1	
						0.10848435E+02	0.48316495E-02	-0.17979829E-05	0.29732063E-09	-0.18103369E-13	2
						-0.42888036E+05	-0.27962648E+02	0.15000194E+01	0.34865481E-01	-0.37049162E-04	3
						0.17161874E-07	-0.23168944E-11	-0.40562524E+05	0.19158855E+02	-0.38860137E+05	4



Table 4 (continued)

354-25-6

C2HCLF4 1-CHLORO-1,1,2,2-TETRA-FLUORO-ETHANE (HCFC-124a) TRC 1989 DATA TO 1500 K  
EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS HF298=-903.3 KJ Max Lst  
Sq Error Cp @ 1400 K 0.32%.

CF2H-CCLF2 FC-124AP	89C	2F	4H	1CL	1G	200.000	5000.000	C	136.47625	1
0.14476092E+02	0.77521899E-02	-0.34676003E-05	0.68691373E-09	-0.49890490E-13						2
-0.11413815E+06	-0.44436670E+02	0.25660695E+01	0.40636569E-01	-0.30205490E-04						3
0.15001542E-08	0.49004025E-11	-0.11095106E+06	0.16810762E+02	-0.10864140E+06						4

2837-89-0

C2HCLF4 2-CHLORO-1,1,1,2-TETRAFLUORO-ETHANE (HCFC-124) TRC 1989 DATA TO 1500K  
EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS HF298=-924.7 KJ Max Lst  
Sq Error Cp @ 1400 K 0.32%.

CF3-CCLFH HCFC124 P	89C	2F	4H	1CL	1G	200.000	5000.000	C	136.47625	1
0.14310765E+02	0.77386392E-02	-0.33659964E-05	0.65591076E-09	-0.47163678E-13						2
-0.11665629E+06	-0.43664043E+02	0.25109331E+01	0.39611296E-01	-0.26968606E-04						3
-0.22740439E-08	0.64125753E-11	-0.11348471E+06	0.17136671E+02	-0.11121521E+06						4

430-58-0

C2HCL2F Diclorofluoroethylene (FC-1121) Equilibrium Mixture of 1,1- cis & trans  
as excited states. trans is 1,cis is 2 and 1,1 is 3. Sigma=1 IAIBIC=33400.  
Nu=3115,1650,1274,1097,853,815,447,766,532,326,193(2) T0=84 IAIBIC=36700.  
Nu=3106,1650,1239,1149,907,771,669,486,472,390,243,168 T0=1000. IAIBIC=39000.  
Nu=3112,1661,1295,1152,974,798,668,465,446,284,262,206 HF298=-168.648 kJ  
REF=Gurvich 91 Max Lst Sq Error Cp @ 1300 K 0.32%.

C2HCL2F	tpis91C	2.H	1.F	1.CL	2.G	200.000	6000.000	B	114.93314	1
1.09691500E+01	4.73571534E-03	-1.76548202E-06	2.92239127E-10	-1.78047046E-14						2
-2.43192990E+04	-2.66541318E+01	2.45417198E+00	3.09044162E-02	-2.99536924E-05						3
1.12271273E-08	-4.18205355E-13	-2.21462432E+04	1.65457942E+01	-2.02835765E+04						4

306-83-2

C2HCL2F3 2,2-DICHLORO-1,1,1-TRIFLUORO-ETHANE (HCFC-123) TRC 1989 DATA TO 1500 K  
EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS HF298=-743.9 KJ Max Lst Sq  
Error Cp @ 1400 K 0.3%

CF3-CCL2H HCFC123 P	89C	2F	3H	1CL	2G	200.000	5000.000	C	152.93055	1
0.15372216E+02	0.65536841E-02	-0.28223775E-05	0.54480973E-09	-0.38845129E-13						2
-0.95263745E+05	-0.49194203E+02	0.24843775E+01	0.41924396E-01	-0.29376222E-04						3
-0.37135096E-08	0.82904456E-11	-0.91811259E+05	0.17075157E+02	-0.89470095E+05						4

354-23-4

C2HCL2F3 1,2-DICHLORO-1,1,2-TRIFLUORO-ETHANE (HCFC-123a) TRC (1989) DATA TO  
1500 K EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS HF298=-710.0 KJ  
Max Lst Sq Error Cp @ 1300 K 0.28%.

CF2CL-CFCLH	P	89C	2F	3H	1CL	2G	200.000	5000.000	C	152.93055	1
0.15214490E+02	0.68034260E-02	-0.29677784E-05	0.57947261E-09	-0.41715986E-13						2	
-0.91047599E+05	-0.46292045E+02	0.22308101E+01	0.46950596E-01	-0.46338534E-04						3	
0.17532444E-07	-0.78742071E-12	-0.87769687E+05	0.19469685E+02	-0.85392885E+05						4	

812-04-4

C2HCL2F3 1,1-DICHLORO-1,2,2-TRIFLUORO-ETHANE TRC (1989) DATA TO 1500 K  
EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS HF298=-702.1 KJ Max Lst Sq  
Error Cp @ 800 K 0.29%.

CFCL2-CF2H	P	89C	2F	3H	1CL	2G	200.000	5000.000	C	152.93055	1
0.15065748E+02	0.70864071E-02	-0.30919691E-05	0.60150084E-09	-0.43128759E-13						2	
-0.90106886E+05	-0.46351547E+02	0.28807063E+01	0.42935581E-01	-0.38052765E-04						3	
0.94294010E-08	0.24256356E-11	-0.86893560E+05	0.15891141E+02	-0.84442739E+05						4	

Table 4 (continued)

79-01-6

C2HCl3 TRICHLOROETHYLENE SIGMA=1 IAIBIC=928.E-115 NU=3096,1590,1250,933,859,633,381,274,172,783,452,211 {HF298=-19.1 kJ} REF=TSIV 1979 Max Lst Sq Error Cp @ 1300 K 0.33% HF298=-17.5+/-3.0 kJ HF0=-14.0 kJ REF=Manion JPCRD 31 (2002),123 Old (1989) L Polynomial adjusted for new HF298.

C2HCL3	TT8/03C	2H	1CL	3	OG	200.000	6000.000	B	131.38804	1	
						0.10888462E+02	0.47583118E-02	-0.17617541E-05	0.29031942E-09	-0.17633485E-13	2
						-0.60360276E+04	-0.25439709E+02	0.25996860E+01	0.34238007E-01	-0.43577745E-04	3
						0.28199249E-07	-0.73014917E-11	-0.40688962E+04	0.15763417E+02	-0.21047542E+04	4

23273-90-7

C2HCl4 TETRACHLOROETHYL RADICAL (CHCl2CCl2\*) STATWT=2 SIGMA=1 IA=49.7712 IB=78.35509 IC=92.2811 IR=14.7906 ROSYM=1 V(3)=2580 cm-1 REF=Burcat G3B3 NU=1023,2984,812,778,706,618,1265,1210,382,326,314,279,231,168 REF=Skinner & Rabinovich Bull Soc Chim Belg 82, (1973),305 HF298=21.82 kJ REF=Burcat G3B3 {HF298=45. kJ REF=THERM program} Max Lst Sq Error Cp @ 1300 K 0.36%

C2HCL4	CHCl2=CCl2	A04/05C	2.H	1.CL	4.	O.G	200.000	6000.000	B	166.84014	1
						1.45236396E+01	4.29972946E-03	-1.77166296E-06	3.07646634E-10	-1.92515584E-14	2
						-2.57510890E+03	-4.04511621E+01	3.15151526E+00	4.41094266E-02	-5.75511181E-05	3
						3.73697567E-08	-9.73947933E-12	1.63836575E+02	1.62607402E+01	2.62477813E+03	4

76-01-7

C2HCl5 Pentachloroethane STATWT=1 SIGMA=1 IA=73.7496 IB=88.8265 IC=115.0446 IR=19.787 ROSYM=3 V(3)=3788 CM-1 Nu=3005,1257,1212,1020,946,911,824,775,726,586,[327,322,280,239,225,174.1,161.7] REF=Webbook 2000 IR+Burcat [] G3B3 calc. {HF298=-155.9 kJ REF=J. Manion JPCRD 31, (2002),123; HF298=-145. kJ REF=Kirkbride J. Appl. Chem. 6, (1956),11-21.} Max Lst Sq Error Cp @ 6000 K 0.42%

C2HCL5	A04/05C	2.H	1.CL	5.	O.G	200.000	6000.000	B	202.29284	1	
						1.61889108E+01	6.02755857E-03	-2.52297714E-06	4.42668370E-10	-2.78828019E-14	2
						-2.51861039E+04	-5.01366047E+01	3.85594982E+00	4.56073672E-02	-4.99565523E-05	3
						2.45552722E-08	-3.95375908E-12	-2.20748312E+04	1.21373851E+01	-1.92927785E+04	4

2713-09-9

C2HF FLUOROACETYLENE SIGMA=1 IB=8.645 NU=3357,2239,1061,583(2),367(2) HF298=41.69 HF0=41+/-25 kJ REF=Gurvich 91 {HF298=125.5+/-63 KJ REF=JANAF} Max Lst Sq Error Cp @ 1300 K 0.30 %.

C2HF	tpis91C	2.H	1.F	1.	O.G	200.000	6000.000	B	44.02774	1	
						6.20949775E+00	3.69584855E-03	-1.29973578E-06	2.06830940E-10	-1.22578311E-14	2
						2.85749388E+03	-8.93525071E+00	1.30649331E+00	2.77924488E-02	-4.86268691E-05	3
						4.25956865E-08	-1.42675759E-11	3.74175901E+03	1.39346815E+01	5.01440301E+03	4

207602-04-8

C2HF2 CHF=CF\*(E) DiFluoroEthyl Radical SIGMA=1 STATWT=2 IA=1.031 IB= 20.795 IC=21.826 NU=3052,1568,1260,1163,1049,685,518,298,296 HF298=-42.5+/-17.9 kJ REF=Zachariah, Westmoreland, Burges, Tsang & Melius J. Phys. Chem. 100, (1996), 8737. Max Lst Sq Error Cp @ 1300 K 0.40%.

C2HF2	CHF=CF(E)	T 6/02C	2.H	1.F	2.	O.G	200.000	6000.000	B	63.02615	1
						7.87499232E+00	4.77134517E-03	-1.76600789E-06	2.90903847E-10	-1.76623863E-14	2
						-8.08846630E+03	-1.36036843E+01	3.08690083E+00	1.60213261E-02	-7.49407266E-06	3
						-3.65234768E-09	3.19176449E-12	-6.67208283E+03	1.15973919E+01	-5.11154596E+03	4

Table 4 (continued)

359-11-5

C2HF3 CHF=CF2 TriFluoroEthylene SIGMA=1 IAIBIC=5043. Nu=3150,1788,1362,1264,  
 1171,929,623,485,232,750,555,305 HF298=-498.78+/-8.24 kJ REF=ATcT A  
 {HF298=-490.78 kJ REF=TRC 12/83; HF298=-491+/-9 kJ REF=Gurvich 91;  
 HF298=-485.6+/-14. kJ REF=Zachariah, Westmoreland, Burges, Tsang & Melius J.  
 Phys. Chem. 100, (1996),8737.} Max Lst Sq Error Cp @ 1300 K 0.43%.  
 C2HF3 CHF=CF2 ATcT/AC 2.H 1.F 3. 0.G 200.000 6000.000 B 82.02455 1  
 9.56303811E+00 6.03922396E-03-2.24656246E-06 3.71316848E-10-2.25981353E-14 2  
 -6.27202069E+04-2.23573620E+01 2.00354119E+00 2.74140646E-02-2.30032301E-05 3  
 7.09389407E-09 1.96148641E-13-6.06536347E+04 1.65697402E+01-5.90269300E+04 4

354-33-6

C2HF5 PENTAFLUOROETHANE (HFC-125) SIGMA=1 IA=23.1057 IB=34.8656 IC=42.1831  
 IR=6.2020 ROSYM=3 V(3)=1460. cm-1 REF=Burcat G3B3 calc Nu=3008,1393,1309,1218,  
 1111,867,725,577,523,361,246,1359,1198,1145,508,413,216 REF=Chen et al JPCRD 4,  
 (1975),441 HF298=-1120.0 kJ REF=Burcat G3B3 calc {HF298=-264. KCAL REF=Chen  
 et al JPCRD 4 (1975),441}. Max Lst Sq Error Cp @ 1300 0.42%  
 C2HF5 A 4/05C 2.H 1.F 5. 0.G 200.000 6000.000 B 120.02136 1  
 1.45281312E+01 6.80984691E-03-2.67132939E-06 4.54433791E-10-2.81433657E-14 2  
 -1.40296859E+05-4.67174252E+01 2.56680624E+00 3.63877723E-02-1.93606756E-05 3  
 -9.02362714E-09 8.52266342E-12-1.36902027E+05 1.56968804E+01-1.34704270E+05 4

2612-62-6

HCCN STATWT=3 SIGMA=1 IB=7.8 NU=3229,1735,1179,458(2),370(2)  
 HF0=609.241+/-100. KJ REF=Gurvich 89  
 HCCN RUS 91H 1.C 2.N 1. 0.G 200.000 6000.000 B 39.03668 1  
 6.56314169E+00 3.48040967E-03-1.24603080E-06 2.00764486E-10-1.20044547E-14 2  
 7.11347086E+04-9.86556141E+00 1.87184307E+00 2.60611314E-02-4.62723965E-05 3  
 4.18609731E-08-1.45352705E-11 7.20340360E+04 1.22173228E+01 7.34175107E+04 4

4471-47-0

C2HNO CYANOKETENE NC-CHO SIGMA=1 STATWT=1 IA=1.2675 IB=16.7941 IC=18.0617  
 NU=3018,2347,1800,1425,1004,932,628,313,222 HF298=10.545 kcal HF0=10.994 kcal  
 REF=Burcat G2B3 Calc Max Lst Sq Error Cp @ 1300 K 0.48%  
 NCCHO T06/04C 2.H 1.N 1.O 1.G 200.000 6000.000 B 55.03548 1  
 6.42261995E+00 6.03502826E-03-2.21102350E-06 3.61593143E-10-2.18401729E-14 2  
 2.82171279E+03-6.42840578E+00 3.63362859E+00 1.18741728E-02-5.03742673E-06 3  
 -8.99834820E-10 1.01583787E-12 3.74108769E+03 8.57237760E+00 5.30641974E+03 4

32038-80-5

C2HNO2 Nitroacetylene HCC-NO2 SIGMA=1 STATWT=1 IA=6.4119 IB=18.5936  
 IC=25.0056 Nu=3494,2241,1632,1339,935,764,715,643,611,602,273,206 REF=Burcat  
 B3LYP calc HF298=66.6 kcal G3B3 calc REF=Politzer Lane Concha JPC A 108,  
 (2004), 3493-98 Max Lst Sq Error Cp @ 1300 K 0.39%.  
 HCCNO2 A 1/05C 2.H 1.N 1.O 2.G 200.000 6000.000 B 71.03488 1  
 9.24323493E+00 6.11883233E-03-2.22735280E-06 3.63050837E-10-2.18882152E-14 2  
 3.00082130E+04-2.07147538E+01 1.34403396E+00 3.33183494E-02-3.93939158E-05 3  
 2.41124634E-08-5.90505390E-12 3.19357897E+04 1.87890785E+01 3.35142299E+04 4

Table 4 (continued)

51095-15-9

C2HO KETYL RAD SIGMA=1 STATWT=2 A0=41.5 B0=0.363 C0=0.359 REF=Endo & Hirota J. Chem. Phys. 86 (1987),4319 NU=1967,380,1063,730,610,3290 HF298=42.4 +/- 2.1 Kcal REF=Oakes, Jones, Blerbaum & Ellison J. Phys. Chem. 87 (1983),4810 {HF298=178.242+/-0.68 REF=ATcT A; HF298=178.3+/-1.5 kJ REF=Szalay, Tajti & Stanton Mol Phys. 103, (2005),xxx} MAX LST SQ ERROR CP @ 6000 K 0.32%

C2HO	T 6/94C	2H	1O	1	OG	200.000	6000.000	B	41.02934	1
	0.58469006E+01	0.36405960E-02	-0.12959007E-05	0.20796919E-09	-0.12400022E-13					2
	0.19248496E+05	-0.52916533E+01	0.23350118E+01	0.17010083E-01	-0.22018867E-04					3
	0.15406447E-07	-0.43455097E-11	0.20050299E+05	0.11976729E+02	0.21336387E+05					4

2143-69-3

CH2C VINYLIDENE RADICAL SIGMA=2 STATWT=1 IA=0.29432 IB=2.17453 IC=2.46885 NU=3344,3239,1710,1288,787,444 REF=OSAMURA, SCHAFFER, GRAY & MILER J.A.C.S. 103 (1981) 1904. HF0=414.489 kJ REF= Chen, Jonas, Kinsey & Field J Chem Phys 91, (1989),3976. {HF298=413.36+/-1.8 kJ REF=ATcT A} Max Lst Sq Error Cp @ 6000 K 0.35%.

H2C2	L12/89H	2C	2	0	OG	200.000	6000.000	B	26.03728	1
	0.42780340E+01	0.47562804E-02	-0.16301009E-05	0.25462806E-09	-0.14886379E-13					2
	0.48316688E+05	0.64023701E+00	0.32815483E+01	0.69764791E-02	-0.23855244E-05					3
	-0.12104432E-08	0.98189545E-12	0.48621794E+05	0.59203910E+01	0.49887266E+05					4

74-86-2

C2H2 ACETYLENE SIGMA=2 B0=1.1766 NU=3372.83,1973.8,3283.83,612.88(2),730.29(2) X11=-18.57,X12=-13.09 X13=-102.39 X14=-16.54 X15=-10.85 X22=-7.92 X23=-2.83 X24=-12.70 X25=-1.38 X33=-30.95 X34=-8.22 X35=-8.68 X44=3.3 X45=-5.24 X55=-2.27 G44=-1.36 G55=3.45 ALPHA1=6.83E-3 ALPHA2=6.3E-3 ALPHA3=5.6E-3 ALPHA4=-1.3E-3 ALPHA5=-2.2E-3 D0=1.598E-6 T0=25000(3),35000(6),42198(1),50000(3),54116(1) REF=TSIV HF298=228.2+/-0.8 kJ HF0=228.769 {HF298=228.264+/-0.30 kJ REF=ATcT A} Max Lst Sq Error Cp @ 6000 K 0.24%

C2H2,acetylene	g 1/91C	2H	2.	0.	0.G	200.000	6000.000	A	26.03728	1
	4.65878489E+00	4.88396667E-03	-1.60828888E-06	2.46974544E-10	-1.38605959E-14					2
	2.57594042E+04	-3.99838194E+00	8.08679682E-01	2.33615762E-02	-3.55172234E-05					3
	2.80152958E-08	-8.50075165E-12	2.64289808E+04	1.39396761E+01	2.74459950E+04					4

590-12-5

C2H2Br2 1,2-DibromoEthylene trans SIGMA=2 STATWT=1 IA=1.7831833 IB=135.958573 IC=137.741754 NU=3131,3122,1846,1150,1104,880,859,756,743,224,182.5,153.1 REF=PM3 MOPAC 2000 calc HF298=101.9+/-8. kJ HF0=121.55 kJ REF=NIST 94 + THERGAS estimates. Max Lst Sq Error Cp @ 6000 K 0.37%

DIBROMOETHYLENE	T03/04C	2.H	2.BR	2.	0.G	200.000	6000.000	B	185.84528	1
	8.71830574E+00	6.46729755E-03	-2.32172026E-06	3.74707113E-10	-2.24292533E-14					2
	8.95990052E+03	-1.45931197E+01	3.92133171E+00	1.60428828E-02	-1.49792112E-07					3
	-1.49285034E-08	8.33024182E-12	1.04003743E+04	1.08945560E+01	1.22556831E+04					4

79-27-6

C2H2Br4 1,1-2,2-TetraBromoEthane CHBr2CHBr2 SIGMA=2 STATWT=1 IA=135.0208 IB=157.5327 IC=289.8103 Ir=44.767 ROSYM=3 V(3)=4505 cm-1 Nu=112.9,142.8,179.2,180.8,222,269,574,609,649,697,1044,1151,1153,1169,1325,3196,3208 REF=G3B3LYP calc HF298=53.35 kJ HF0=89.89 kJ REF=PM3 calc Max Lst Sq Error Cp @ 6000 K 0.38%

CHBR2CHBR2	T02/04C	2.H	2.BR	4.	0.G	200.000	6000.000	B	345.65328	1
	1.38358129E+01	7.38994179E-03	-2.84169603E-06	4.75473782E-10	-2.90613149E-14					2
	1.42718237E+03	-3.42538684E+01	5.78939817E+00	3.15602244E-02	-2.76651125E-05					3
	8.64111911E-09	5.04841959E-13	3.51473595E+03	6.71486330E+00	6.41649358E+03					4

Table 4 (continued)

50663-45-1

C2H2Cl Radical SIGMA=1 STATWT=2 IA=1.4503 IB=13.2980 IC=14.7483  
 Nu=3322,3230,1651,1241,843,805,649,648,350 HF298=274.767+/-8 kJ HF0=277.937 kJ  
 REF=Burcat G3B3 calc. {HF298=275. kJ REF=Gao,Marshall et al 6th Int. Conf.  
 Chem. Kinet NIST July 2005 p.131 exper.; HF298=262.75 kJ REF=NIST 94} Max  
 Lst Sq Error Cp @ 6000 K 0.35%.

CHCL=CH\* A 8/05C 2.H 2.CL 1. 0.G 200.000 6000.000 B 61.48998 1  
 6.57992662E+00 5.50498054E-03-1.93056595E-06 3.06672838E-10-1.81536735E-14 2  
 3.05524286E+04-7.26735678E+00 1.75764780E+00 2.07031239E-02-1.84481964E-05 3  
 6.31043021E-09 1.19854774E-13 3.17529714E+04 1.70686824E+01 3.30467417E+04 4

2317-91-1

C2H2ClF 1,1-ChloroFluoroEthylene SIGMA=1 STATWT=1 IAIBIC=3182.8 E-117 Nu=3064,  
 3016,1656,1383,1186,947,836,699,607,515,432,371 REF=Gurvich 1979+1991  
 HF0=-159.0+/-15 kJ HF298=-165.393 kJ Max Lst Sq Error Cp @ 1300 K 0.42%.

C2H2ClF 1,1-FC1 T 9/02C 2.H 2.F 1.CL 1.G 200.000 6000.000 B 80.48868 1  
 8.38519082E+00 6.88965435E-03-2.50358771E-06 4.07384367E-10-2.45254671E-14 2  
 -2.31789264E+04-1.68056385E+01 9.12415579E-01 3.11141994E-02-3.24490541E-05 3  
 1.67416393E-08-3.16508383E-12-2.12920536E+04 2.09030401E+01-1.98920923E+04 4

75-35-4

C2H2Cl2 1,1-Dichloroethylene SIGMA=2 STATWT=1 IA=110.911595 IB=24.154963  
 IC=35.066515 NU=3130,3035,[1624,1390,1086,869],800,[614,593],460,372,299  
 HF298=2.2+/-1.4 kJ REF=NIST Webbook 2000, IR[] + Shimanouchi. HF Mansson et al  
 J. Chem Therm.3, (1971),547-551. Max Lst sq Error Cp @ 1300 K 0.39%.

CCL2CH2 S05/01C 2.H 2.CL 2. 0.G 200.000 6000.000 B 96.94328 1  
 8.72268524E+00 6.52268348E-03-2.35597369E-06 3.81833999E-10-2.29238459E-14 2  
 -3.05837782E+03-1.79212139E+01 1.09017479E+00 3.38342476E-02-4.14626040E-05 3  
 2.66982563E-08-6.91176950E-12-1.24744244E+03 1.99941222E+01 2.64597673E+02 4

23273-89-4

C2H2CL3 1,1,1-TrichloroEthane Radical CH2-CCl3 SIGMA=3 STATWT=2 IA=34.3659  
 IB=34.67771 IC=49.11669 Ir=0.297355 ROSYM=2 V(3)=1500.cm-1 NU=236,246,320,  
 345,353,521,581,720,737,1058,1112,1415,3061,3379 REF=Liu et al JPC A 107(2003),  
 6231 HF298=82.81+/-5.0 kJ HF0=88.91 kJ REF=Estimated according to Melius and  
 CH3CCL3 {HF298=78.62 REF=Melius CL72} Max Lst Sq Error Cp @ 6000 K 0.23%

CH2-CCl3 T08/03C 2.H 2.CL 3. 0.G 200.000 6000.000 B 132.39538 1  
 1.28942506E+01 4.86170307E-03-1.72031755E-06 2.75143478E-10-1.63718689E-14 2  
 5.45317262E+03-3.62976535E+01 8.94429907E-01 5.61578321E-02-8.89059018E-05 3  
 6.89328575E-08-2.07848100E-11 7.85604934E+03 2.11970392E+01 9.95969696E+03 4

1320-41-8 ??

C2H2F2 C2H2F2 DIFLUOROETHYLENE 1,1 cis & trans in equilibrium REF=McBride  
 SIGMA=2 IAIBIC=963.624E-117 NU=1727.6,3057,3,1393,925.5,549.7,592,3174,  
 1300.8,954.3,437,803.5,609.6 T0=1920. SIGMA=2 Nu=1716,3122,1263,1015,237,839,  
 495,3136,1374,1130,769,756 IAIBIC=1021.74 T0=2170 Nu=1694,3111,1286,1123,548,  
 875,329,788,3144,1274,1159,341 IAIBIC=671. REF=Gurvich 1991 HF298=-336.4 KJ  
 Max Lst Sq Error Cp @ 1300 K 0.71%

C2H2F2 FC-1132A tpis91C 2.H 2.F 2. 0.G 200.000 6000.000 B 64.03409 1  
 8.95189658E+00 7.14641061E-03-2.79505418E-06 4.77439020E-10-2.97191427E-14 2  
 -4.42668961E+04-2.29204220E+01 1.28301801E+00 2.31903824E-02-9.70095198E-06 3  
 -4.40973912E-09 3.38826355E-12-4.17798395E+04 1.82378552E+01-4.04593897E+04 4

Table 4 (continued)

75-38-7

C2H2F2 1,1-C2H2F2 1,1-DIFLUOROETHYLENE (FC-1132a) SIGMA=2 STATWT=1  
 IAIBIC=963.624E-117 Nu=1716,3122,1263,1015,237,839,495,3136,1374,1130,769,756  
 HF298=-336.4+/-4 kJ HF0=-329.476 kJ REF=Gurvich 1991 {HF298=-344+/-10 kJ  
 REF=Cox & Pilcher 1970; HF298=-334.0+/-0.84 kJ REF=Neugebauer & Margrave JPC 60,  
 (1956),1318} Max Lst Sq Error Cp @ 6000 K 0.44%  
 1,1-C2H2F2 RUS 91C 2.H 2.F 2. 0.G 200.000 6000.000 B 64.03409 1  
 7.93289587E+00 7.27979071E-03-2.64144142E-06 4.29432803E-10-2.58381152E-14 2  
 -4.36671380E+04-1.65082325E+01 9.11680326E-01 2.66032123E-02-1.89472374E-05 3  
 1.99409393E-09 2.41309066E-12-4.17513190E+04 1.96907967E+01-4.04593897E+04 4

1630-77-9

C2H2F2 Cis-C2H2F2 Z-DIFLUOROETHYLENE SIGMA=2 IAIBIC=1021.74E-117 NU=1716,  
 3122,1263,1015,237,839,495,3136,1374,1130,769,756 HF298=-306.4+/-5 kJ  
 REF=Gurvich 91 Max Lst Sq Error Cp @ 6000 K 0.46%  
 1,2-C2H2F2-cis RUS 91C 2.H 2.F 2. 0.G 200.000 6000.000 B 64.03409 1  
 7.64662972E+00 7.55622756E-03-2.74600447E-06 4.46890910E-10-2.69075698E-14 2  
 -4.00302113E+04-1.46982798E+01 2.69825023E+00 1.23878271E-02 1.53768601E-05 3  
 -3.23557844E-08 1.47696831E-11-3.82972358E+04 1.28259603E+01-3.68632667E+04 4

1630-78-0

C2H2F2 Trans-C2H2F2 E-DIFLUOROETHYLENE FC-1132 SIGMA=2 IAIBIC=671.E-117  
 NU=1694,3111,1286,1123,548,875,329,788,3144,1274,1159,341 HF298=-303.6+/-5 kJ R  
 EF=Gurvich 91 Max Lst Sq Error Cp @ 6000 K 0.45%  
 1,2-C2H2F2-trans RUS 91C 2.H 2.F 2. 0.G 200.000 6000.000 B 64.03409 1  
 7.73658780E+00 7.46809856E-03-2.71232867E-06 4.41227895E-10-2.65588270E-14 2  
 -3.96779496E+04-1.52286382E+01 2.82321391E+00 1.39737055E-02 8.79179901E-06 3  
 -2.39558133E-08 1.12741216E-11-3.80129641E+04 1.17612525E+01-3.65144789E+04 4

3248-58-6

CF3CH2 Beta-TRIFLUOROETHYL RADICAL SIGMA=1. IA=1.4637 IB=15.056 IC=15.413  
 IR=0.2892 CALCULATED AS FREE ROTOR NU=3113,3024,1440,1294,1277,1192,940,838,  
 598,574,523,466,364,319 REF=Chen Rauk & Tschuikow-Roux J. CHEM. PHYS. 93 (1990)  
 6620 Max Lst Sq Error Cp @ 6000 K 0.36% HF298=-123.6 Kcal  
 C2F3H2 T 1/92C 2F 3H 2 0G 200.000 6000.000 B 83.03309 1  
 0.10987821E+02 0.68153248E-02-0.24820763E-05 0.40457086E-09-0.24387675E-13 2  
 -0.66370037E+05-0.29515293E+02 0.54654037E+00 0.42697217E-01-0.49566004E-04 3  
 0.27781281E-07-0.57577830E-11-0.63872559E+05 0.22578365E+02-0.62197580E+05 4

811-97-2

C2H2F4 CF3-CFH2 1,1,1,2-TetraFluoroEthane HFC-134a SIGMA=1 STATWT=1 IA=15.280  
 IB=29.275 IC=29.690 Ir=2.409416 ROSYM=3 V(3)=1517.2 cm-1 NU=2990,2935,1464,  
 1427,1379,1298,1182,1103,973,885,842,665,549,539,408,352,225 HF298=-913.3+/-  
 17.5 kJ REF=Zachariah et al JPC 100, (1996),8737 exper vibr. + BAC/MP4 calc.  
 Max Lst Sq Error Cp @ 1300 K 0.42%  
 C2H2F4 HFC-134a T 5/03C 2.H 2.F 4. 0.G 200.000 6000.000 B 102.03089 1  
 1.25551115E+01 8.40186071E-03-3.12077291E-06 5.12284572E-10-3.10110291E-14 2  
 -1.14846319E+05-3.80374329E+01 2.29239681E+00 3.03108483E-02-5.33713985E-06 3  
 -2.19456612E-08 1.29970288E-11-1.11790431E+05 1.62830568E+01-1.09844116E+05 4

Table 4 (continued)

359-35-3

C2H2F4 CHF2-CHF2 1,1,2,2-TetraFluoroEthane HFC-134 SIGMA=2 STATWT=1 IA=15.594  
 IB=28.794 IC=32.762 IR=3.113463 ROSYM=3 V(3)=1517.2 cm<sup>-1</sup> NU=2984,2975,1460,  
 1417,1393,1337,1205,1157,1131,1120,903,768,582,502,398,240,223 HF298=-883+/-5.5  
 kJ REF=Zachariah et al JPC 100,(1996),8737 BAC/MP4 calc. Max Lst Sq Error Cp  
 @ 6000 K 0.44%

C2H2F4 HFC-134	T 5/03C	2.H	2.F	4.	0.G	200.000	6000.000	B	102.03089	1
1.19960865E+01	8.98721146E-03	-3.36363101E-06	5.54000254E-10	-3.35654907E-14						2
-1.11106791E+05	-3.53416069E+01	3.98924014E+00	1.72571738E-02	2.36853869E-05						3
-4.89142700E-08	2.21225708E-11	-1.08315425E+05	9.12364634E+00	-1.06235966E+05						4

2932-82-3

C2H2N METHYLENECYANIDE RADICAL (CH2CN) STATWT=2. SIGMA=1. IA=0.289043  
 IB=8.1423051 IC=8.4313945 NU=3095,2995,1858,1410,1006,971,571,390,362  
 REF=MELIUS A66S HF298=61.61 KCAL HF0=62.27 kcal REF=Melius {HF298=61.60 kcal  
 REF=Tumanov Denisov Neftchimia 44,(2004),139; HF298=61.47 kcal REF=Janoscheck  
 Rossi IJCK 36,(2004),661} Max Lst Sq Error Cp @ 6000 K 0.42%

CH2CN Methyl-Cya	T01/03C	2.H	2.N	1.	0.G	200.000	6000.000	B	40.04402	1
6.14873620E+00	6.06600240E-03	-2.17174620E-06	3.49750387E-10	-2.09004207E-14						2
2.86491222E+04	-6.59235995E+00	2.63064017E+00	1.73644377E-02	-1.70284117E-05						3
9.86551140E-09	-2.46033517E-12	2.95791691E+04	1.12776223E+01	3.10031788E+04						4

70971-59-4

\*CH2NC METHYLENEISOCYANIDE RADICAL STATWT=2 SIGMA=1 IA=0.2997 IB=7.4341  
 IC=7.7338 Nu=3299,3182,2042,1493,1140,1125,544,378,293 HF298=358.23 kJ  
 HF0=360.59 kJ REF=Janoschek & Rossi Int J Chem Kin 36,(2004),661 {HF298=326.4  
 +/-11.3 kJ REF=Berkowitz, Elison, Gutman JPC 98,(1994),2744.} Max Lst Sq Error  
 Cp @ 6000 K 0.41%.

CH2NC	A12/04C	2.H	2.N	1.	0.G	200.000	6000.000	C	40.04402	1
5.74237273E+00	6.28074654E-03	-2.21501557E-06	3.53105406E-10	-2.09509914E-14						2
4.08948870E+04	-4.10984142E+00	3.36758699E+00	1.31552658E-02	-1.05147237E-05						3
5.55784400E-09	-1.42571504E-12	4.15787507E+04	8.18621025E+00	4.30849202E+04						4

350610-21-8

C2H2NO Cyanoethoxy Radical NCCH2O\* SIGMA=1 STATWT=2 IA=2.0417 IB=17.2593  
 IB=18.7911 NU=2976,2957,2371,1404,1348,1171,1078,902,599,589,335,225  
 HF298=41.974 kcal HF0=43.312 kcal REF=Burcat G3B3 calc Max Lst Sq Error Cp  
 @ 6000 K 0.48%.

NCCH2O RADICAL	T06/04C	2.H	2.N	1.O	1.G	200.000	6000.000	B	56.04342	1
7.26373035E+00	7.91027386E-03	-2.87373023E-06	4.67365314E-10	-2.81206990E-14						2
1.81836123E+04	-1.08309486E+01	2.96391901E+00	1.64646465E-02	-3.33503209E-06						3
-8.15626290E-09	4.80224808E-12	1.95498379E+04	1.22143247E+01	2.11220163E+04						4

119437-64-8

C2H2NO2 Cyanoethylperoxy Radical NC-CH2-O-O\* SIGMA=1 STATWT=2 IA=2.4622  
 IB=32.7369 IB=34.6635 NU=3147,3091,2384.1493,1379,1230,1192,996,984,946,521,  
 441,364,183,59.96 HF298=42.54 kcal HF0=44.24 kcal REF=Burcat G3B3 calc  
 Max Lst Sq Error Cp @ 6000 K 0.46%.

NCCH2OO	T06/04C	2.H	2.N	1.O	2.G	200.000	6000.000	B	72.04282	1
9.10481741E+00	8.95969753E-03	-3.25670683E-06	5.29969111E-10	-3.19048942E-14						2
1.77397623E+04	-1.81425839E+01	4.25158957E+00	1.46469491E-02	9.70672093E-06						3
-2.46314402E-08	1.13320529E-11	1.94457826E+04	8.75950789E+00	2.14068370E+04						4

Table 4 (continued)

88055-17-8

C2H2(NO2)2 Di-Nitroethylene-trans(E) SYMNO = 2 STATWT = 1 IA = 13.5875  
 IB = 80.5878 IC = 94.1753 (Ir(NO2)= 5.96 ROSYM = 2 V(3) = 5.04 kcal)x2  
 NU=3398,3290,1732,1652,1644,1399,1398(2),1277,1217,1004,972.5(2),900,789,767,  
 702,643,580,421,295,169,155 HF298=9.788 kcal REF = BURCAT G3B3 calc  
 {HF298 = 14.2 kcal REF=NIST 94.} Max Lst Sq Error Cp @ 6000 K 0.49%.  
 C2H2(NO2)2 A 5/05C 2.H 2.N 2.O 4.G 200.000 6000.000 B 118.04836 1  
 1.65193214E+01 1.09827653E-02-4.28160802E-06 7.24664741E-10-4.47051889E-14 2  
 -1.84003069E+03-5.69855940E+01 4.46008116E+00 2.38752905E-02 3.45147187E-05 3  
 -7.10366591E-08 3.20870069E-11 2.35482654E+03 9.91351088E+00 4.92548472E+03 4

436-51-4

C2H2O KETENE SIGMA=2 IA=.299 IB=8.1477 IC=8.4466 NU=3070,2152,1388,1118,  
 3166,977,438,591,525 REF=MOORE & PIMENTEL JCP 38, (1963),2816 HF298=-11.4+/-0.4  
 kcal REF= Vogt, Williamson & Beauchamp JACS 100 (1978),3478 {HF298=-48.579+/-  
 0.28 kJ} MAX ERROR CP @ 6000 K 0.42%.  
 C2H2O KETENE T 6/94C 2H 2O 1 OG 200.000 6000.000 B 42.03728 1  
 0.57577901E+01 0.63496507E-02-0.22584407E-05 0.36208462E-09-0.21569030E-13 2  
 -0.79786113E+04-0.61064037E+01 0.21401165E+01 0.18088368E-01-0.17324216E-04 3  
 0.92767477E-08-0.19915011E-11-0.70430509E+04 0.12198699E+02-0.57366700E+04 4

32038-79-2

C2H2O ETHYNOL HCC-OH SIGMA=1 IA=0.121323 IB=8.4583765 IC=8.5796996  
 NU=346,383,523,600,1072,1232,2198,3339,3501 REF= M. JACOX JPCRD 19, (1990),1469  
 HF298=22.273 KCAL REF=C. Melius BAC/MP4 Calculations (Private Communication)  
 Max Lst Sq Error Cp @ 6000 K 0.31%  
 HCCOH T 4/93C 2H 2O 1 OG 200.000 6000.000 B 42.03728 1  
 0.63660255E+01 0.55038729E-02-0.18851901E-05 0.29446414E-09-0.17218598E-13 2  
 0.89184965E+04-0.82504705E+01 0.19654173E+01 0.25585205E-01-0.38773334E-04 3  
 0.31566335E-07-0.10081670E-10 0.97694090E+04 0.12602749E+02 0.11207642E+05 4

107-22-2

C2H2O2 (CHO-CHO) Trans-Cis-GLYOXAL SIGMA=2 T0=0 (trans) STATWT=1  
 IAIBIC=504.42 ROSYM=1 Brot1=4.213 Brot2=-1.117 Brot3=0.421 Brot4==0.126  
 Brot5=0.040 Brot6=-0.015 ROSYM=1 V(1)=1588. V2=1140. V(3)=-59.0 V(4)-110.9  
 V(5)=40. V(6)=0 NEL=150 REF=Dorofeeva JPCRD 30, (2001),475 NU=2843,1744,  
 1353,1066,551,801,1048,2835,1732,1312,339 REF= SCUSERIA & SCHAEFER JACS 111,  
 (1989),7761  
 T0=1555. (Cis) SIGMA=2 STATWT=1 IAIBIC=710.17 (No internal rotation for the  
 cis exited state B. McBride and Zeleznik) Nu=2841,1746,1369,827,284.5,1050,750,  
 2810,1761,1360,825,10\*\*10 (for the missing frequency or rotation!)  
 HF298=-212.082+/-0.8 kJ REF=Dorofeeva JPCRD 30, (2001),475 & ATcT A HF0=-213.38  
 kJ {HF298=-212.0+/-0.79 KJ REF=Fletcher & Pilcher Trans Faraday Soc 66(1970),  
 794} HF298=-193.249+/-0.8 for Cis only REF=ATcT A Max Lst Sq Error Cp @  
 1300 K 0.48%  
 O(CH)2O Glyoxal g 3/02C 2.H 2.O 2. 0.G 200.000 6000.000 B 58.03608 1  
 8.72506895E+00 6.33096819E-03-2.35574814E-06 3.89782853E-10-2.37486912E-14 2  
 -2.91024131E+04-2.03903909E+01 4.68412461E+00 4.78012819E-04 4.26390768E-05 3  
 -5.79018239E-08 2.31669328E-11-2.71985007E+04 4.51187184E+00-2.55074562E+04 4



Table 4 (continued)

42879-41-4

C2H2O2 Oxyranone Ethylene-oxide-Ketone CH<sub>2</sub>(-O-)-C=O SIGMA=1 STATWT=1  
 IA=3.3398 IB=10.4862 IC=13.2532 Nu=3240,3143,2034,1510,1207,1129,1073,1000,  
 954,728,535,491 HF298=-177.916 kJ HF0=-170.374 kJ REF=Burcat G3B3 calc  
 {HF298=-190+/-10 kJ BAD VALUE Rodriquez Williams JCS Perkin Trans 2, (1997), 953}  
 Max Lst Sq Error Cp @ 200 K 0.54%.

C2H2O2 Oxyranone	A 3/05C	2.H	2.0	2.	0.G	200.000	6000.000	B	58.03608	1	
						6.91336960E+00	8.18722427E-03	-2.96773847E-06	4.82153718E-10	-2.89963354E-14	2
						-2.43827377E+04	-1.12906510E+01	2.28414754E+00	1.08506892E-02	2.00544938E-05	3
						-3.70111422E-08	1.64078245E-11	-2.26733657E+04	1.49008612E+01	-2.13982823E+04	4

144-62-7

C2H2O4 HO-CO-CO-OH Oxalic Acid. SIGMA=2 STATWT=1 IAIBIC=11950. E-117  
 IR=3.6454 V(1)=700. cm-1 ROSYM=1 NU=3484(2),1826,1800,1423,1278,1195,1127,  
 851,815,666,651,608,563,460,405,264 HF298=-731.8+/-2.0 kJ HF0=-721.2 +/-2.0  
 kJ REF=Dorofeeva et al JPCRD 30 (2003), 475 Max Lst Sq Error Cp @ 1300 K 0.4%  
 C2H2O4 HO-CO-CO-OHT 5/03C 2.H 2.0 4. 0.G 200.000 6000.000 B 90.03488 1  
 1.12713463E+01 9.21013668E-03 -3.36045480E-06 5.44589862E-10 -3.26206809E-14 2  
 -9.24388026E+04 -2.98343923E+01 1.29593849E+00 4.17001626E-02 -4.49426401E-05 3  
 2.54216963E-08 -5.84215993E-12 -8.99050481E+04 2.05343663E+01 -8.80148078E+04 4

2669-89-8

C2H3 VINYL-RAD STATWT=2. SIGMA=1. A0=7.49 B0=1.07 C0=0.93 Nu=3265,3190,  
 3115,1670,1445,1185,920,825,785 REF=Ervin JACS 112 (1990), 5750} HF298=296.58  
 +/-0.92 kJ HF0=300.867 kJ REF=ATcT A {HF298=299.74+/-5 kJ REF=Ervin JACS  
 112, (1990), 5750; also Kromkin Chimicheskaya Fizika 22, (2002), 30; HF298=295.4  
 +/-1.7 kJ REF=Russell & Gutman JPC 93, (1989), 5184 also Kaiser & Wallington JPC  
 100, (1996), 4111 also Parthiban & Martin JCP 114, (2001), 6014; HF298=299.6+/-3 kJ  
 REF=Tsang Energetics of Organic Free Rad 1996; HF298=297.1+/-4.2 REF=De Moore  
 et al JPL 97-4 1997} Max Lst Sq Error Cp @ 400 K 0.54%.  
 C2H3 Vinyl Radi ATcT/AC 2.H 3. 0. 0.G 200.000 6000.000 B 27.04522 1  
 4.15026763E+00 7.54021341E-03 -2.62997847E-06 4.15974048E-10 -2.45407509E-14 2  
 3.38566380E+04 1.72812235E+00 3.36377642E+00 2.65765722E-04 2.79620704E-05 3  
 -3.72986942E-08 1.51590176E-11 3.44749589E+04 7.91510092E+00 3.56701718E+04 4

14604-48-9

C2H3+ Vinylum Ion Calculated from ATcT A tables. HF298=1122.34+/-1.17 kJ  
 HF0=1119.2 kJ REF=ATcT A Max Lst Sq Error Cp @ 6000 K 0.45%.  
 C2H3+ Vinylum ATcT/AC 2.H 3.E -1. 0.G 298.150 6000.000 B 27.04467 1  
 5.10636990E+00 6.93432850E-03 -2.51037737E-06 4.15437961E-10 -2.52447676E-14 2  
 1.32996534E+05 -4.37010064E+00 2.04325538E+00 1.91613874E-02 -2.33884102E-05 3  
 1.75610106E-08 -5.45672895E-12 1.33705367E+05 1.06437825E+01 1.34991719E+05 4

79-08-3

C2H3BrO2 Bromoacetic acid CH<sub>2</sub>Br-COOH STATWT=1 SIGMA=1 IAIBIC=28178.E-117  
 IR=2.8300 ROSYM=1 V(3)=450. cm-1. Nu=3566,3037,1808,1449,1325,1208,1047,908,  
 747,589,384,180,3076,1243,806,611,489 HF298=-383.5+/-3.1 kJ HF0=-364.6+/-3.1  
 kJ REF=Dorofeeva et al. JPCRD 30 (2001), 475. Max Lst Sq Error Cp @ 6000 K 0.42%  
 C2H3BrO2 T 6/03C 2.H 3.0 2.BR 1.G 200.000 6000.000 B 138.94802 1  
 1.00461497E+01 1.01587879E-02 -3.64523517E-06 5.84523562E-10 -3.47813484E-14 2  
 -5.01944638E+04 -2.10806685E+01 3.28778149E+00 2.29632669E-02 -1.48600560E-07 3  
 -1.95187664E-08 1.05257632E-11 -4.80901664E+04 1.51126493E+01 -4.61241853E+04 4

Table 4 (continued)

2311-14-0									
CH3CBr3 1,1,1-TRIBROMOETHANE SIGMA=3 STATWT=1 IA=80.1201 IB=80.1201 IC=134.8523									
Ir=0.5298 ROSYM=3 V(3)=2065.3 cm-1 NU=152.7(2),217,277.6(2),409.4,602.4(2),									
1062,1103(2),1440,1507(2),3074,3157(2) REF=B3LYP calc HF298=-26.3 kJ HF0=+5.238									
REF=NIST94 est. Max Lst Sq Error Cp @ 1300 K 0.37%									
CH3CBr3	T11/03C	2.BR	3.H	3.	0.G	200.000	6000.000	B	266.75722 1
1.24133808E+01	8.14476767E-03	-2.94327674E-06	4.77278219E-10	-2.86681963E-14					2
-7.78704433E+03	-3.16562586E+01	4.62366755E+00	3.19898912E-02	-3.12395319E-05					3
1.61131195E-08	-3.42366464E-12	-5.71776884E+03	8.09298025E+00	-3.16314491E+03					4
75-01-4									
C2H3CL CHLOROETHYLENE STATWT=1. SIGMA=1. IAIBIC=320. NU=3120.6,3086.4,									
3034.3,1610.9,1370,1280,1030,720.5,395,942.5,896.5,620.4 REF=Gurvich 91									
HF298=37.872+/-0.58 kJ REF=ATcT A {HF298=22.0+/-3 kJ REF=Manion JPCRD 31,									
(2002),123-172; HF298=29.0 kJ REF=Kromkin Chimicheskaya Fizika 22,(2002),30}									
Max Lst Sq Error Cp @ 200 K and 6000 K 0.48%									
C2H3CL	ATcT/AC	2.H	3.CL	1.	0.G	200.000	6000.000	B	62.49792 1
6.32341000E+00	8.52343039E-03	-3.04197672E-06	4.88915441E-10	-2.91775277E-14					2
1.85043273E+03	-7.74958634E+00	2.27191109E+00	1.25087140E-02	1.21343633E-05					3
-2.73077584E-08	1.26573716E-11	3.26236847E+03	1.47576437E+01	4.55492867E+03					4
79-11-8									
C2H3ClO2 Chloroacetic acid CH2Cl-COOH STATWT=1 SIGMA=1 IAIBIC=12284.E-117									
IR=2.4514 ROSYM=1 V(3)=450. cm-1 Nu=3566,3019,1806,1428,1354,1274,1111,891,									
792,596,397,216,3076,1193,929,611,492 HF298=-427.6+/-1.0 kJ HF0=-416.0+/-1.0									
kJ REF=Dorofeeva et al. JPCRD 30 (2001), 475. Max Lst Sq Error Cp @ 6000 K									
0.44 %									
C2H3ClO2	T 6/03C	2.H	3.O	2.CL	1.G	200.000	6000.000	B	94.49672 1
9.86255544E+00	1.03234542E-02	-3.69940268E-06	5.93409957E-10	-3.53481899E-14					2
-5.54766294E+04	-2.14716622E+01	3.46827272E+00	2.00080426E-02	7.43233801E-06					3
-2.70228098E-08	1.31588252E-11	-5.33700009E+04	1.33548825E+01	-5.14281659E+04					4
71-55-6									
C2H3Cl3 1,1,1-TriChloroEthane CH3CCL3 SIGMA=3 STATWT=1 IA=IB=36.2819									
IC=50.7099 Ir=0.5271 ROSYM=3 V(3)=1913. cm-1 NU=238,282,341(2),346,525,									
725(2),1074,1084(2),1383,1450(2),2951,3014,3735 REF=Ruscic & Burcat B3LYP-G3									
Calculations 2004 HF298=-144.6+/-2.0 kJ HF0=-133.982 kJ REF=Manion JPCRD									
(2002) {HF298=-140.42+/-4.8 kJ REF=Melius; HF298=-144.6+/-0.1 kJ REF=Kolesov									
& Papina Rus Chem. Rev. 52 (1983),754} Max Lst Sq Error Cp @ 1300 K 0.39%									
CH3CCl3	T11/03C	2.H	3.CL	3.	0.G	200.000	6000.000	B	133.40332 1
1.20555087E+01	8.44253446E-03	-3.04587523E-06	4.93404612E-10	-2.96165491E-14					2
-2.19789258E+04	-3.40314769E+01	2.56424495E+00	3.93928228E-02	-4.26660423E-05					3
2.42267750E-08	-5.60184447E-12	-1.95749809E+04	1.38735787E+01	-1.73912834E+04					4
75-02-5									
C2H3F FluoroEthylene SIGMA=1 STATWT=1 IAIBIC=94.357 Nu=3140,3094,3062,									
1655,1380,1305,1157,923,490,929,863,713 HF298=-140.1+/-2.5 kJ REF=Gurvich 91									
{HF298=-138.91 kJ REF=TRC 12/83; HF298=-136.0 kJ REF=Kromkin Chimicheskaya									
Fizika 22,(2002),30; HF298=-136.0 kJ REF=Kolesov & Papina Rus JPC eng.trans.									
44,(1970),611-613} Max Lst Sq Error Cp @ 200 K 0.62%.									
C2H3F	RUS 91C	2.H	3.F	1.	0.G	200.000	6000.000	B	46.04362 1
5.92787061E+00	8.89384427E-03	-3.17971566E-06	5.11681548E-10	-3.05632459E-14					2
-1.94885049E+04	-7.04448245E+00	2.61149895E+00	6.68683582E-03	2.76818258E-05					3
-4.33824699E-08	1.85254269E-11	-1.80934696E+04	1.26328255E+01	-1.68500609E+04					4

Table 4 (continued)

24314-99-6

C2H3F2 Alfa DIFLUOROETHYL RADICAL (CH3CF2) SIGMA=1. STATWT=2. IA=8.1022  
 IB=9.064 IC=10.2057 ROSYM=3. IR=0.50451 ROT BARR V3=790. 1/CM NU=2989,2959,  
 2886,1461,1458,1419,1260,1259,1089,981,843,524,447,357 REF=CHEN, RAUK, &  
 TSCHUIKOW-ROUX 93 1990, 1187 MAX LST SQ ERROR CP 1300 K 0.51 % HF298=-72.3 KCAL  
 C2H3F2 T12/91C 2H 3F 2 OG 200.000 6000.000 B 65.04263 1  
 0.79153881E+01 0.95796027E-02-0.34798118E-05 0.56594378E-09-0.34053931E-13 2  
 -0.39692403E+05-0.14382963E+02 0.33232137E+01 0.16181070E-01 0.34104446E-05 3  
 -0.15893036E-07 0.75253769E-11-0.38094855E+05 0.10888528E+02-0.36382565E+05 4

420-46-2

1,1,1-C2H3F3 1,1,1-TRIFLUOROETHANE (FC-143A) SIGMA=3 STATWT=1 IA=15.4810  
 IB=IC=16.3158 Ir=0.5137 ROSYM=3 V(3)=1133.2 cm-1 Nu=359.1(2),532.6(2),593.2,  
 834.9,993.2(2),1275(2),1301,1460,1515(2),3088,3171(2) HF298=-755.655 kJ  
 HF0=-742.906 kJ REF=G3B3LYP calc Ruscic & Burcat 2004 {HF298=-178.2 Kcal  
 Stull Westrum & Sinke 1969} Max Lst Sq Error Cp @ 1300 K 0.45%  
 C2H3F3 FC-143A T11/03C 2.H 3.F 3. OG 200.000 6000.000 B 84.04043 1  
 1.00540918E+01 1.02515900E-02-3.70172133E-06 5.99863654E-10-3.60117460E-14 2  
 -9.50222221E+04-2.72330585E+01 1.75260632E+00 3.04395701E-02-1.49788607E-05 3  
 -5.70775683E-09 5.66225345E-12-9.26184281E+04 1.62401353E+01-9.08838885E+04 4

84658-62-8

CH3CD3 1,1,1-Deuterated Ethane SIGMA=3 STATWT=1 IA=1.5687 IB=IC=5.0989  
 Ir=0.34867 ROSYM=3 V(3)=1063.3 cm-1 NU=686.3(2),918.3,1105(2),1145(2),1158,  
 1443,1534(2),2191,2306,3049,3112(2) HF298=-107.57 kJ HF0=-92.313 kJ  
 REF=G3B3LYP  
 calc Ruscic & Burcat 2004 Max Lst Sq Error Cp @ 1300 K 0.64%  
 CH3CD3 T11/03C 2.H 3.D 3. OG 200.000 6000.000 B 33.08753 1  
 5.72054997E+00 1.42190397E-02-5.14923700E-06 8.35625242E-10-5.02013874E-14 2  
 -1.59059093E+04-9.00312825E+00 3.37893166E+00 2.96664746E-03 4.53525569E-05 3  
 -5.95543887E-08 2.34320292E-11-1.43709688E+04 7.43314023E+00-1.29376235E+04 4

593-66-8

C2H3I Ethylene Iodide SIGMA=1 STATWT=1 IA=5.56149 IB=94.8920 IC=100.45348  
 Nu=3115,3067,3011,1598,1353,1251,1084,980,946,553,[531,311] REF=IR Webbook  
 + [] B3LYP/6-31G\* calc. HF298=128.876 kJ HF0=137.906 kJ REF=NIST 94 est.  
 Max Lst Sq Error Cp @ 6000 K 0.47%.  
 C2H3I A 8/05C 2.H 3.I 1. OG 200.000 6000.000 C 153.94969 1  
 6.44273647E+00 8.41887780E-03-3.00447900E-06 4.82844717E-10-2.88126081E-14 2  
 1.27974246E+04-4.03486413E+00 2.74108792E+00 1.25141822E-02 8.60970302E-06 3  
 -2.16359126E-08 1.00821068E-11 1.40875324E+04 1.64780120E+01 1.54990733E+04 4

75-05-8

C2H3N METHYLCYANIDE (CH3CN) STATWT=1. SIGMA=3. IA=0.520332 IB=IC=9.02306  
 NU=3009(2),2954,2267,1448(2),1385,1041(2),920,362(2) REF=MELIUS R4A+ Shimanouchi  
 MAX LST SQ ERROR CP @ 1300K 0.55% HF298=74.04+/-0.37 kJ REF= An & Mansson J  
 Chem Thermo 15 (1983), 287 (NIST) {HF298=19.62 KCAL HF0=21.41 kcal REF=Melius}  
 Max Lst Sq Error Cp @ 6000 K 0.55%  
 CH3CN Methyl-Cya T01/03C 2.H 3.N 1. OG 200.000 6000.000 B 41.05196 1  
 5.09921882E+00 9.69585649E-03-3.48051966E-06 5.61420173E-10-3.35835856E-14 2  
 6.60967324E+03-3.36087178E+00 3.82392803E+00 4.08201943E-03 2.16209537E-05 3  
 -2.89807789E-08 1.12962700E-11 7.44430382E+03 5.52656156E+00 8.90492212E+03 4

Table 4 (continued)

593-75-9

C2H3N METHYLISOCYANATE (CH3NC) STATWT=1. SIGMA=3. IA=0.520798 IB=IC=8.23484  
 NU=3014(2), 2966, 2166, 1467(2), 1429, 1129(2), 945, 263(2) REF=MELIUS R4B+ Shimanouchi  
 LST SQ ERROR CP @ 1300K 0.57% HF298=163.5+/-7.2 kJ REF=(NIST) Baghal-Vayjoee,  
 Collister & Pritchard Can J. Chem 55, (1977), 2634 {HF298=44.82 kcal HF0=46.46  
 kcal REF=Melius} Max Lst Sq Error Cp @ 6000 K 0.57%.

CH3NC Methyl-Iso	T01/03C	2.H	3.N	1.	0.G	200.000	6000.000	B	41.05196	1	
						4.97319556E+00	9.82585931E-03	-3.53150585E-06	5.70121357E-10	-3.41242359E-14	2
						1.74116304E+04	-2.23784096E+00	5.06585777E+00	-2.94992510E-03	3.52827212E-05	3
						-4.04524450E-08	1.48573373E-11	1.80461340E+04	4.42065468E-01	1.96641976E+04	4

107-16-4

C2H3NO CYANOMETHANOL NC-CH2-OH STATWT=1 SIGMA=1 IA=2.3575 IB=17.4351  
 IC=19.2646 Ir(OH)=0.14242 ROSYM=2 V(3)=1399. cm-1 NU=3751, 3031, 3004, 2383,  
 1530, 1477, 1266, 1264, 1089, 1044, 900, 578, 373, 233 HF298=-10.881 kcal HF0=-9.765  
 kcal REF=Burcat G3B3 calc. Max Lst sq Error Cp @ 6000 K 0.44%.

NCCH2OH	T06/04C	2.H	3.N	1.O	1.G	200.000	6000.000	B	57.05136	1	
						7.59341176E+00	9.44576002E-03	-3.33630854E-06	5.32676082E-10	-3.16483188E-14	2
						-9.13477281E+03	-1.33107264E+01	2.90218571E+00	1.63746784E-02	5.68147561E-06	3
						-2.10178429E-08	1.02633942E-11	-7.58531275E+03	1.22670504E+01	-5.97871721E+03	4

180330-47-6

C2H3NO2 CYANOMETHYLPEROXIDE NC-CH2-O-OH SIGMA=1 STATWT=1 IA=2.5577  
 IB=34.3766 IC=36.1945 Ir(OH)=0.1531 ROSYM=1 V(3)=447.7 cm-1 Ir(OOH)=4.3879  
 ROSYM=3 V(3)=1165. cm-1 NU=3702, 3082, 3041, 2382, 1526, 1416, 1387, 1237, 1073, 1048,  
 972, 945, 529, 403, 377, 202 HF298=7.045 kcal HF0=9.421 kcal REF=Burcat G3B3 calc  
 Max Lst Sq Error Cp @ 6000 K 0.43%

NC-CH2-O-OH	A08/04C	2.H	3.N	1.O	2.G	200.000	6000.000	B	73.05076	1	
						9.50764347E+00	1.00845926E-02	-3.63251862E-06	5.84207205E-10	-3.48052126E-14	2
						-2.03333938E+02	-1.92980150E+01	4.71323293E+00	1.82104447E-02	1.77781876E-06	3
						-1.68344816E-08	8.64210464E-12	1.34399499E+03	6.62658109E+00	3.54516141E+03	4

3638-64-0

C2H3NO2 Nitroethylene STATWT=1 IA = 6.77795 IB = 17.4725 IC = 24.2505  
 Ir = 5.96 ROSYM = 2 V(2) = 5.04 kcal/mole NU=3103, 3094, 3013, 1699, 1628,  
 1479, 1378, 1264, 1066, 1026, 966, 904, 828, 654, 544, 536, 323. HF298 = 7.955 kcal  
 REF = Melius Database 1988 D39 Max Lst Sq Error Cp @ 6000 0.52%

NITROETHYLENE	T11/97C	2.H	3.N	1.O	2.G	200.000	6000.000	B	73.05136	1	
						1.00660026E+01	1.04932532E-02	-3.92096997E-06	6.47758885E-10	-3.93529661E-14	2
						-3.10704319E+02	-2.61804452E+01	2.75930739E+00	1.70703761E-02	2.37349272E-05	3
						-4.77968933E-08	2.14789743E-11	2.29629458E+03	1.46559809E+01	4.00308858E+03	4

3170-69-2

C2H3O Acetyl Radical CH3\*CO SIGMA=1 STATWT=2 A=2.9436 B=0.334 C=0.3186  
 BROT=10.51589 ROSYM=3 V(3)=92 1/cm NU=2904, 2903, 2826, 1886, 1405, 1402, 1325,  
 1025, 925, 817, 454 REF=NIMLOS SODERQUIST & ELLISON JACS 111, (1989), 7675  
 HF298=-10.3+/-1.8 KJ REF=Niiaranen, Gutman & Krasnoperov J. Phys. Chem. 96  
 (1992) 5881.; Ruscic et al JPCRD 2003 Max Lst Sq Error Cp @ 6000 K 0.62%

CH3CO RADICAL	IU2/03C	2.H	3.O	1.	0.G	200.000	6000.000	B	43.04462	1	
						0.53137165E+01	0.91737793E-02	-0.33220386E-05	0.53947456E-09	-0.32452368E-13	2
						-0.36450414E+04	-0.16757558E+01	0.40358705E+01	0.87729487E-03	0.30710010E-04	3
						-0.39247565E-07	0.15296869E-10	-0.26820738E+04	0.78617682E+01	-0.12388039E+04	4

Table 4 (continued)

15762-97-9

C2H3O+ Acetylium ion [CH3CO]+ Polynomial made from table calculated by Ruscic's ACTIVE TABLES generator. HF298=669.952 +/-0.85 kJ REF=B. Ruscic Active Tables ver 1.25 Argonne Nat. Labs. HF0=670.927 kJ Thermal Electron Convention Max Lst Sq Error Cp @ 6000 K 0.54%

C2H3O+ Acetylium A12/04C	2.H	3.O	1.E	-1.G	200.000	6000.000	A	43.04407	1
5.38190942E+00	9.45572763E-03	-3.39695691E-06	5.48225731E-10	-3.28062322E-14					2
7.81860765E+04	-4.94235171E+00	3.31517723E+00	6.97633081E-03	1.75092244E-05					3
-2.69576366E-08	1.11130038E-11	7.91710835E+04	7.74260291E+00	8.05762456E+04					4

4400-01-5

C2H3O (CH2CHO) RADICAL SIGMA=1 SIGMA ROT=2 STATWT=2 IA=1.226 IB=7.7552 IC=8.7646 IR=.2902 INT ROT POTENTIAL V(2)=2000. NU=3005,2822,1743,1441,1400,1352,1113,509,2967,867,763 REF= BURCAT,MILLER & GARDINER MAX LST SQ ERROR CP @ 1300 K 0.74 %. HF298=6.22 KCAL derived from Benson & O'Neal NSRDS-NBS 1970 CH2CHO T04/830 1H 3C 2 OG 300. 5000. B 43.0451 1

0.59756699E+01	0.81305914E-02	-0.27436245E-05	0.40703041E-09	-0.21760171E-13					2
0.49032178E+03	-0.50320879E+01	0.34090624E+01	0.10738574E-01	0.18914925E-05					3
-0.71585831E-08	0.28673851E-11	0.15214766E+04	0.95714535E+01	0.30474436E+04					4

31586-84-2

C2H3O OXIRANE (ETHYLENE OXIDE) RADICAL SIGMA=1 STATWT=2 IA=2.8160 IB=3.5503 IC=5.6365 Nu=3204,3144,3114,1551,1366,1195,1133,1089,1049,949,817,793 HF298=164.473 kJ HF0=172.90 kJ REF=Burcat G3B3 calc {HF298 = 139.83 KJ est of THERM}. Max Lst Sq Error Cp @ 200 K \*\*\* 1.0% \*\*\* @ 6000 K 0.51%.

C2H3O Oxyrane Rad A 1/05C	2.H	3.O	1.	0.G	200.000	6000.000	B	43.04462	1
5.60158035E+00	9.17613962E-03	-3.28028902E-06	5.27903888E-10	-3.15362241E-14					2
1.71446252E+04	-5.47228512E+00	3.58349017E+00	-6.02275805E-03	6.32426867E-05					3
-8.18540707E-08	3.30444505E-11	1.85681353E+04	9.59725926E+00	1.97814471E+04					4

74-85-1

C2H4 ETHYLENE STATWT=1. SIGMA=4. A0=4.86596 B0=1.001329 C0=0.828424 NU=3021,1625,1344,1026,3083,1222,949,940,3105,826,2989,1444 REF=CHAO & ZWOLINSKY, JPCRD 4, (1975), 251 HF298=52.5 kJ HF0=61.025 kJ REF=TRC 4/1988 {HF298=52.574 +/-0.21 kJ REF=ATcT A} MAX LST SQ ERROR Cp 20K 0.80 .

C2H4 g 1/00C	2.H	4.	0.	0.G	200.000	6000.000	B	28.05316	1
3.99182724E+00	1.04833908E-02	-3.71721342E-06	5.94628366E-10	-3.53630386E-14					2
4.26865851E+03	-2.69081762E-01	3.95920063E+00	-7.57051373E-03	5.70989993E-05					3
-6.91588352E-08	2.69884190E-11	5.08977598E+03	4.09730213E+00	6.31426266E+03					4

106-93-4

C2H4Br2 1,2-DIBROMOETHANE CH2BrCH2Br SIGMA=2 STATWT=1 IA=2.97631 IB=144.7450 IC=146.6523 Ir=23.5621 ROSIM=3 V(3)=3189 cm-1. REF=G3B3LYP calc Nu=3037,3013,2974,2972,1441,1440,1255(2),1186,1087,1053,933,753,660,589,193,190 REF=Shimanouchi, NIST Webbook HF298=-37.5 kJ REF=CRC-2001 HF0=-10.49 kJ {HF298=-37.55+/-1.24 kJ REF=ATcT A} Max Lst Sq Error Cp @ 6000 K 0.55%.

1,2-Dibromoethan T 1/04C	2.BR	2.H	4.	0.G	200.000	6000.000	B	187.86116	1
9.36432367E+00	1.10025521E-02	-4.09730912E-06	6.76535723E-10	-4.11107071E-14					2
-8.49220956E+03	-1.85401970E+01	4.62116185E+00	9.41442414E-03	3.26665289E-05					3
-5.17217094E-08	2.19245862E-11	-6.50317454E+03	9.40527055E+00	-4.51018761E+03					4

Table 4 (continued)

557-91-5

C2H4Br2 1,1 DIBROMOETHANE CH3CHBr2 SIGMA=1 STATWT=1 IA=16.2092 IB=70.0012  
 IC=83.7991 Ir=0.52735 ROSYM=3 V(3)=1583 cm<sup>-1</sup> REF=G3B3LYP calcs. NU=3023,2996,  
 2985,2937,1443(2),1383,1260,1172,1070,1045,966,620,545,342,275,172.(253=rot)  
 HF298=-41 kJ REF=Kudchadker JPCRD 8 (1979),519-526 {HF298=-35.9+/-7.6 kJ  
 REF=ATcT A; HF298=-36.61+/-8 kJ REF=Burcat G3B3 calc} Max Lst Sq Error Cp @  
 6000 K 0.45%

1,1-Dibromoethan	T 1/04C	2.BR	2.H	4.	0.G	200.000	6000.000	B	187.86116	1	
						9.71735483E+00	1.04888147E-02	-3.76966967E-06	6.08752081E-10	-3.64504552E-14	2
						-8.90539717E+03	-2.04307602E+01	3.77828749E+00	1.88134528E-02	9.12256669E-06	3
						-2.83028599E-08	1.35973544E-11	-6.92491898E+03	1.20528601E+01	-4.93113846E+03	4

16519-99-6

C2H4Cl Beta-CHLOREETHYL RADICAL (CH2ClCH2) STATWT=2 SIGMA=1 IA=2.61729  
 IB=14.31277 IC= 15.9312 IR=0.292687 NU=1006,3002,2992,2946,2921,676,1446,  
 1444,1368,1324,1236,1140,954,336 POTENTIAL BARRIER V3=650 cm<sup>-1</sup> ROSYM=3  
 REF=Skinner & Rabinovitch HF298=90.12 KJ REF=Bozzelli & Ritter's program  
 Max Lst Sq Error Cp @ 6000 K 0.54%

C2H4CL	T 7/93C	2H	4CL	1	0G	200.000	6000.000	B	63.50646	1	
						0.59979919E+01	0.11113997E-01	-0.39890576E-05	0.64350472E-09	-0.38503835E-13	2
						0.80972298E+04	-0.45621917E+01	0.45895607E+01	0.64757653E-03	0.38470903E-04	3
						-0.49101872E-07	0.19121765E-10	0.91898417E+04	0.61950714E+01	0.10838883E+05	4

107-06-2

C2H4Cl2 1,2-Dichloroethane CH2ClCH2Cl SIGMA=2 STATWT=1 IA=2.8887 IB=56.9756  
 IC=58.8017 Ir=8.85066 ROSYM=3 V(3)=3028.5 cm<sup>-1</sup> REF=G3B3LYP calc. Nu=3005(2),  
 2983,1957,1461,1445,1304,1264,1232,1123,1052,989,773,754,728,300,222  
 HF298=-130.069+/-0.59 kJ REF=ATcT A {HF298=-130.21 kJ REF=Burcat G3B3 calc;  
 HF298=-125.4 +/-1.0 kJ REF=Webbook 2003} Max Lst Sq Error Cp @ 1300 K 0.65%

1,2-Dichloroethan	ATcT/AC	2.CL	2.H	4.	0.G	200.000	6000.000	B	98.95856	1	
						9.68476700E+00	1.12630298E-02	-4.31576920E-06	7.25209500E-10	-4.45818752E-14	2
						-1.99525878E+04	-2.39965067E+01	4.68235340E+00	3.93962518E-03	5.07306234E-05	3
						-7.03930514E-08	2.83531047E-11	-1.75372415E+04	6.96581596E+00	-1.56436158E+04	4

90584-32-0

C2H4CL2O2 Alfa CHLOROPEROXYETHANE CH3CCl2O-OH SIGMA=3 IA=46.623 IB=38.942  
 IC=35.485 IR(C-C)=0.5163539 IR(C-O)=4.310 IR(O-O)=0.144446 V(3)(C-C)=1601.9  
 cm<sup>-1</sup> V(3)(C-O)=2973. cm<sup>-1</sup> V(3)(O-O)=1916.7 cm<sup>-1</sup> NU=3651,3009,2995,2922,1465,  
 1462,1439,1413,1194,1132,1099,1066,924,734,563,549,406,352,299,288,269  
 HF298=-55.3 KCAL REF=Lay et al JPC 100,(1996),8240 Max Lst Sq Error Cp @ 1300 K  
 0.44%

C2H4O2CL2	T01/97C	2.H	4.O	2.CL	2.G	200.000	6000.000	B	130.95796	1	
						1.55129087E+01	1.03537432E-02	-3.85668118E-06	6.37648016E-10	-3.88430532E-14	2
						-3.39225403E+04	-5.01703472E+01	2.43416999E+00	4.58166561E-02	-3.41051998E-05	3
						5.34704665E-09	3.11610278E-12	-3.03007573E+04	1.74771898E+01	-2.78278816E+04	4

52067-19-3

C2H4F Alfa-FLUOROETHYL RADICAL (CH3CHF) STATWT=2. SIGMA=1. IA=1.7795 IB=8.7444  
 IC=9.927 ROSYM=3. IR=0.48875 INT ROT BARRIER V3=587. 1/CM NU=3023,2958,2926,  
 2862,1469,1454,1416,1349,1162,1096,1031,887,647,392 REF=CHEN, RAUK &  
 TSCHUIKOW-ROUX 1990 MAX LST SQ ERROR CP @ 6000 K 0.55% HF298=-17.26 KCAL.

C2H4F	T12/91C	2H	4F	1	0G	200.000	6000.000	B	47.05216	1	
						0.60065274E+01	0.11133004E-01	-0.40017964E-05	0.64613341E-09	-0.38678848E-13	2
						-0.11429867E+05	-0.55288750E+01	0.46163442E+01	0.74570459E-03	0.37958220E-04	3
						-0.48405526E-07	0.18830447E-10	-0.10343617E+05	0.51147332E+01	-0.86855197E+04	4

Table 4 (continued)

624-72-6

C2H4F2 1,2-DiFluoroEthane CH2FCH2F HFC-152 SYMNO=2 STATWT=1 IA=2.6303  
 IB=21.7818 IC=23.3466 Ir=2.9183 ROSYM=3 V(3)=2518 cm-1 Nu=274,459,824,  
 1087(2),1095,1195,1243,1312,1383,1481,1550,1561,1061,1066,3101,3127 REF=Burcat  
 G3B3 calc HF298=-450.36+/-4.92 kJ REF=ATcT A {HF298=-447.55 kJ REF=Burcat  
 G3B3 calc; HF298=-420.7 kJ REF=PM3} Max Lst Sq Error Cp @ 1300 K 0.60%.  
 C2H4F2 HFC-152 ATcT/AC 2.H 4.F 2. 0.G 200.000 6000.000 B 66.04997 1  
 7.68600535E+00 1.27375243E-02-4.68389556E-06 7.64130145E-10-4.60215127E-14 2  
 -5.78342759E+04-1.56217664E+01 5.49451903E+00-7.55640919E-03 7.44060634E-05 3  
 -9.07531624E-08 3.48667319E-11-5.59623700E+04 2.04301464E+00-5.41655491E+04 4

75-37-6

C2H4F2 1,1-DiFluoroEthane CH3CHF2 HFC-152a SYMNO=1 STATWT=1 IA=8.9734  
 IB=9.3724 IC=16.3619 Ir=0.5060 ROSYM=3 V(3)=1142 cm-1 Nu=3031,3019,2990,  
 2978,2955,[1515],1461,1426,1414,1373,[1177],1138,956,938,573,\$60.5,377]  
 REF=G3B3 freq IR spectra + B3LYP [] {HF298=-497.0+/-4. kJ REF=Webbook 2003;  
 HF298=-505.42+/-8 kJ REF=Burcat G3B3 calc} Max Lst Sq Error Cp @ 6000 K 0.53%.  
 C2H4F2 HFC-152a ATcT/AC 2.H 4.F 2. 0.G 200.000 6000.000 B 66.04997 1  
 6.73610406E+00 1.29812933E-02-4.62479857E-06 7.42212362E-10-4.42411608E-14 2  
 -6.33699802E+04-9.30130576E+00 3.12218189E+00 1.39706689E-02 1.53431350E-05 3  
 -2.94461261E-08 1.28007103E-11-6.19286294E+04 1.15409834E+01-6.02933907E+04 4

557-75-5

C2H4O Vinyl Alcohol IA=1.363243 IB=7.9930197 IC=9.3562625 NU=412,470.5,693.4,  
 922,926.3,1029,1054.3,1293,1315.3,1434.7,1645.4,2964.6,3022,3050,3461  
 BROT=6.414 INT ROT POTENTIAL V(3)=1067. V(6)=-1.49 Ref= Ab-Initio Calc Karni,  
 Oref & Burcat TAE Report 643 1989. HF298=-29.8 KCAL REF=Holm & Losing JACS 104  
 (1982) 2648. Max Lst Sq Error Cp @ 6000 K 0.5%  
 C2H4O L 8/89C 2H 4O 1 0G 200.000 6000.000 B 44.05316 1  
 0.68220305E+01 0.11059739E-01-0.39224574E-05 0.62778505E-09-0.37355714E-13 2  
 -0.18038769E+05-0.83716090E+01 0.30137746E+01 0.10203771E-01 0.25405637E-04 3  
 -0.42341002E-07 0.18267561E-10-0.16497347E+05 0.13873511E+02-0.14995857E+05 4

75-21-8

C2H4O OXYRANE (ETHYLENE OXIDE) SIGMA=2 IA=3.2793 IB=3.8059 IC=5.9511  
 NU=3006,1498,1271,1120,877,3063,1300,860,3006,1472,1151,892,3065,1142,822  
 REF=SHIMANOUCI HF298=-52.635 kJ FROM JANAF 1985. HF0=-40.082 kJ {HF298=-53.668  
 kJ REF=Burcat G3B3 calc 1/2005} Max Lst Sq Error Cp @ 200 K \*\*\*1.17%\*\*\* @  
 6000 K 0.59%.  
 C2H4O OXYRANE L 8/88C 2H 4O 1 0G 200.000 6000.000 B 44.05256 1  
 0.54887641E+01 0.12046190E-01-0.43336931E-05 0.70028311E-09-0.41949088E-13 2  
 -0.91804251E+04-0.70799605E+01 0.37590532E+01-0.94412180E-02 0.80309721E-04 3  
 -0.10080788E-06 0.40039921E-10-0.75608143E+04 0.78497475E+01-0.63304657E+04 4

75-07-0

C2OH4 ACETALDEHYDE (CH3CHO) STATWT=1. SIGMA=1. IA=2.76748 IB=6.9781  
 IC=9.03498 Ir=0.44 ROSYM=3 V(3)=412.03 cm-1 Nu=3005,2967,2917,2822,1743,1441,  
 1420,1400,1352,1113,919,867,763,509 HF298=-166.19 kJ REF=CHAO, HALL,MARSH &  
 WILHOIT JCPRD 15, (1986) p.1369 {HF298=-166.564+/-0.4 kJ REF=ATcT A} Max Lst  
 Sq Error Cp @ 6000 K 0.59%.  
 CH3CHO L 8/88C 2H 4O 1 0G 200.000 6000.000 B 44.05256 1  
 0.54041108E+01 0.11723059E-01-0.42263137E-05 0.68372451E-09-0.40984863E-13 2  
 -0.22593122E+05-0.34807917E+01 0.47294595E+01-0.31932858E-02 0.47534921E-04 3  
 -0.57458611E-07 0.21931112E-10-0.21572878E+05 0.41030159E+01-0.19987949E+05 4

Table 4 (continued)

64-19-7

C2H4O2 ETHANOIC (ACETIC) ACID STATWT=1 SIGMA=1 IA=7.40342 IB=8.85376  
 IC=15.7599 Brot (CH3)=5.6488 ROSYM=3 V(3)=168.23 cm-1 Brot (OH)=21.255 ROSYM=1  
 V(1)=2011. V(2)=3123. V(3)=192.4 cm-1 NU=3583,3051,2944,1788,1430,1382,1264,  
 1182,989,847,657,581,2996,1430,1048,642,(565,75 TORSION) HF298=-432.25 kJ.  
 REF=CHAO & ZWOLINSKI JPCRD 7, (1978),363. {HF298=-432.216+/-1.5 kJ REF=ATcT A}  
 Max Lst Sq Error Cp @ 1300 K 0.87%. HF298(liq)=-484.216+/-0.17 kJ REF=ATcT A  
 CH3COOH g 6/00C 2.H 4.O 2. 0.G 200.000 6000.000 B 60.05196 1  
 7.67084601E+00 1.35152602E-02-5.25874333E-06 8.93184479E-10-5.53180543E-14 2  
 -5.57560970E+04-1.54677315E+01 2.78950201E+00 9.99941719E-03 3.42572245E-05 3  
 -5.09031329E-08 2.06222185E-11-5.34752488E+04 1.41053123E+01-5.19873137E+04 4

79-14-1

C2H4O3 Glycolyc acid HO-CH2-COOH SIGMA=1 STATWT=1 A0=0.356783 B0=0.135128  
 C0=0.099891 NU=3561(2),2928,2919,1774,1452,1439,1332,1265,1231,1143,1090,1019,  
 854,642,621,495,468,281,270 Ir(COOH)=1.9292 ROSYM=1 HF298=-583.0+/-10 kJ  
 HF0=-567.9 kJ REF=Dorofeeva JPCRD 30 (2001),475 Calculated from original tables  
 Max Lst Sq Error Cp @ 200 K 0.44&  
 C2H4O3 Glycolic T 8/03C 2.H 4.O 3. 0.G 200.000 6000.000 B 76.05136 1  
 1.27662941E+01 1.02143437E-02-3.63547001E-06 5.83491588E-10-3.47179974E-14 2  
 -7.53528536E+04-3.96511752E+01 2.80443702E+00 2.10851644E-02 3.35863233E-05 3  
 -7.02669107E-08 3.26849274E-11-7.20649998E+04 1.51180675E+01-7.01183834E+04 4

14523-98-9

C2H4O4 METHANOIC (FORMIC) ACID (HCOOH)2 DIMER STATWT=1 SIGMA=2 IA=13.615  
 IB=37.724 IC=51.340 NU=3200,2956,1672,1395,1350,1204,675,232,215,1063,677,519,  
 1073,917,164,68,3110,2957,1754,1450,1365,1218,697,248 REF=CHAO & ZWOLINSKI  
 HF298=-820.94 KJ.  
 (FORMIC ACID)2 L 4/85C 2.H 4.O 4. 0.G 300.000 5000.000 B 92.05120 1  
 0.12207371E 02 0.13688851E-01-0.46840369E-05 0.70511663E-09-0.38369285E-13 2  
 -0.10395938E 06-0.35709808E 02 0.37692385E 01 0.27224716E-01 0.17238053E-05 3  
 -0.20776724E-07 0.99379949E-11-0.10104988E 06 0.10505494E 02-0.98737314E 05 4

2025-56-1

C2H5 ETHYL RAD. STATWT=2 SIGMA=1 IA=0.8005 IB=3.7134 IC=3.9931 IR=0.1846  
 ROSYM=3. V3=53 cm-1 NU=3112,3033,2987,2920,2842,1440(3),1366,1175,  
 1138,975,784,540, HF298=28.36 Kcal. REF= Chen, Rauk & Tschuikow-Roux (1990)  
 Max Lst Sq Error Cp & 6000 K 0.58%  
 C2H5 g 7/00C 2.H 5. 0. 0.G 200.000 6000.000 B 29.06110 1  
 4.28800015E+00 1.24337439E-02-4.41384130E-06 7.06527536E-10-4.20342270E-14 2  
 1.20564209E+04 8.45299829E-01 4.30642051E+00-4.18635208E-03 4.97137768E-05 3  
 -5.99121792E-08 2.30507301E-111.28416330E+04 4.70738797E+00 1.42712246E+04 4

74-96-4

C2H5Br ETHYL-BROMIDE SIGMA+1 STATWT=1 IA=2.8052 IB=22.5748 IC=24.3415  
 Ir=0.5218 ROSYM=3 V(3)=1361.6 cm-1 REF=Burcat G3B3 Nu=3018,2982(2),2937,  
 2880,1451(3),1386,1252,1248,1061,964(2),770,583,290 REF=Shimanouchi  
 HF298=-61.60+/-1.01 kJ REF=ATCT A {HF298=-61.9 kJ HF0=-39.95 kJ REF=CRC 2001}  
 Max Lst Sq Error Cp @200 K & 6000 K 0.54%.  
 C2H5Br ATcT/AC 2.H 5.BR 1. 0.G 200.000 6000.000 B 108.96510 1  
 6.95002116E+00 1.28709161E-02-4.60446763E-06 7.41067324E-10-4.42632344E-14 2  
 -1.06394105E+04-1.00517817E+01 3.62900361E+00 6.37387681E-03 3.97846545E-05 3  
 -5.78493445E-08 2.39750833E-11-9.02251371E+03 1.07167737E+01-7.40873485E+03 4



Table 4 (continued)

75-00-3

C2H5CL CHLOROETHANE SIGMA=1 STATWT=1 IA=2.6708 IB=15.6384 IC=17.2795  
 Ir=0.5123 ROSYM=3 V3=1341 cm-1 REF=Burcat G3B3 Nu=3014,2986,2967,2946,2881,  
 1463,1448(2),1385,1289,1251,1081,974(2),786,677,336 REF=Shimanouchi  
 HF298=-106.827+/-0.41 kJ HF0=-92.253 kJ REF=ATcT A {HF298=-112.1+/-0.7 kJ  
 REF=Manion JPCRD 31,(2002),123.} Max Lst Sq Error Cp @ 200 K & 6000 K 0.58%  
 C2H5CL ATcT/AC 2.H 5.CL 1. 0.G 200.000 6000.000 B 64.51380 1  
 6.78002126E+00 1.30428275E-02-4.67112679E-06 7.52363217E-10-4.49618504E-14 2  
 -1.60514095E+04-1.05370548E+01 3.57157429E+00 5.21386910E-03 4.33394889E-05 3  
 -6.16364154E-08 2.53706065E-11-1.44179409E+04 9.89212969E+00-1.28482617E+04 4

353-36-6

C2H5F ETHYL-FLUORIDE SIGMA=1 IA=2.3264 IB=8.9839 IC=10.2529 Ir=0.5138  
 ROSYM=3 V(3)=1196.2 cm-1 REF=Burcat G3B3 calc NU=415,810,880,1048(2),1108,  
 1277,1365,1395,1449(2),1479,2915,2941,3003(3) REF=Shimanouchi HF298=-275.21+/-  
 4.91 kJ REF=ATcT A {HF298=-261.5 kJ HF0=-246.7 kJ REF=Zachariah,  
 Westmoreland, Burgess, Tsang & Melius JPC 100,(1996),8737-8747} Max Lst Sq  
 Error Cp @ 6000 K 0.58%.  
 C2H5F ATcT/AC 2.H 5.F 1. 0.G 200.000 6000.000 B 48.05950 1  
 6.18081698E+00 1.35890229E-02-4.87040213E-06 7.84862029E-10-4.69209214E-14 2  
 -3.61552597E+04-7.96594699E+00 4.00577312E+00-3.11043983E-04 5.57188865E-05 3  
 -7.28404563E-08 2.90642195E-11-3.46425104E+04 7.92813391E+00-3.30999662E+04 4

75-03-6

C2H5I ETHYL-IODIDE SIGMA=1 STATWT=1 IA=3.01101 IB=24.4525 IC=26.4039  
 Ir=0.5225 ROSYM=3 REF=Burcat PM3 calc V(3)=1126.2 cm-1 REF=Kasuya J. Phys.  
 Soc Jap. 15,(1960),296. Nu=3024,2924,2979,2929,2884,1454,1444,1393,1378,1218,  
 1077,992,962(2),741,525,510,262 REF=IR Webbook; V17 from Sheppard JCP 17,(1949),  
 79-83. HF298=-7.047+/-0.56 kJ REF=ATcT A HF0=+8.25 kJ {HF298=-8.37 kJ  
 REF=Stull Westrum Sinke 1969} Max Lst Sq Error Cp @ 6000 K 0.51%.  
 C2H5I ATcT/AC 2.H 5.I 1. 0.G 200.000 6000.000 B 155.96557 1  
 7.97461860E+00 1.28549646E-02-4.59993101E-06 7.40450718E-10-4.42307467E-14 2  
 -4.37826965E+03-1.45972741E+01 2.63041302E+00 1.89595239E-02 1.17450857E-05 3  
 -3.10554440E-08 1.46462936E-11-2.52381380E+03 1.49681231E+01-8.47554456E+02 4

79-24-3

C2H5NO2 Nitro-Ethane STATWT = 1 IA = 7.4804 IB = 19.8289 IC = 26.2826  
 Ir(NO2) = 5.97 ROSYM = 2 V(2) = 0.08 kcal/mole Ir(CH3) = 0.51666 ROSYM = 3  
 V(3) = 3.5 kcal/mole NU=3003,(2961),2956,(2929),2754,1582,1561,(1465),1460,  
 (1447),1400,1386,1252,1141,1117,996,881,774,(639,591,501,286). HF298=-24.8 kcal  
 REF = Melius Database 1988 D74B Max Lst Sq Error Cp @ 1300 K 0.64%  
 NITROETHANE T04/98C 2.H 5.N 1.O 2.G 200.000 6000.000 B 75.06724 1  
 9.21849299E+00 1.62001532E-02-5.98159944E-06 9.81277173E-10-5.93455530E-14 2  
 -1.68676292E+04-2.07232926E+01 3.37137598E+00 1.37914267E-02 3.84687528E-05 3  
 -6.02380553E-08 2.49654782E-11-1.43330647E+04 1.40009494E+01-1.24822894E+04 4

871-31-8

C2H5N3 Ethyl Azide SIGMA=1 STATWT=1 IA=6.1562 IB=25.6515 IC=29.3530  
 Ir(CH3)=0.52082 ROSYM=3 V(3)=5533 cm-1 Ir(N3)=4.17776 ROSYM=2 V(3)=3186 cm-1  
 Nu=3143,3132,3117,3055,3043,2257,1537,1522,1520,1438,1400,1345,1301,1172,1105,  
 1005,856,808,663,576,400,282 HF298=63.784 kJ HF0=68.689 kJ REF=Burcat G3B3  
 calc {HF298=64.5 kcal REF=G2 calc Rogers & McLafferty JCP 103(18),(1995),8302}  
 Max Lst Sq Error Cp @ 6000 K 0.69%  
 C2H5N3 EthylAzyd A12/04C 2.H 5.N 3. 0.G 200.000 6000.000 B 71.08132 1  
 8.45447539E+00 1.82737204E-02-6.90153724E-06 1.13973210E-09-6.90183206E-14 2  
 2.79139524E+04-1.89068556E+01 3.12866430E+00 1.66008875E-02 3.04096708E-05 3  
 -4.97574008E-08 2.05155505E-11 3.02464801E+04 1.27193417E+01 3.20971718E+04 4

Table 4 (continued)

625-58-1

C2H5ONO2 Ethyl Nitrate STATWT = 1 IA = 9.9190168 IB = 32.356995 IC = 36.4527  
 Ir(NO2) = 5.96 ROSYM = 2 V(2) = 9.1 kcal/mole Ir(CH3) = 0.5166 ROSYM = 3  
 V(3) = 3.5 kcal NU = 3003,2959,2946,2933,2877,1703,1481,1468,1455,1427,  
 1403,1355,1296,1172,1086,1066,968,878,815,790,692,589,396,342,207.

REF = Melius Database 1988 P73BN HF298 = -37.04 kcal REF = Gray, Pratt  
 & Larkin J. Chem. Soc (1956), 210 Max Lst Sq Error Cp @ 1300 K 0.65%

ETHYL-NITRATE T05/98C 2.H 5.N 1.O 3.G 200.000 6000.000 B 91.06664 1  
 1.21360953E+01 1.70091385E-02-6.43739515E-06 1.07219880E-09-6.54950920E-14 2  
 -2.41902070E+04-3.71640527E+01 3.75721604E+00 1.93623098E-02 3.87534117E-05 3  
 -6.64089530E-08 2.82505579E-11-2.08444383E+04 1.11813240E+01-1.86391453E+04 4

2154-50-9

C2H5O ETHYL-OXIDE RAD (CH3CH2O) SIGMA=1 ROSYM=3 STATWT=2 IA=2.1281  
 IB=8.8117 IC=9.9060 IR=0.4303 V(3)=737.5 cm-1 NU=3015,3004,2937,2824,  
 2790,1468,1458,1378,1360,1321,1206,1064,1046,872,856,475,406 T0=355 IA=2.3996  
 IB=8.1338 IC=9.4591 IR=0.4375 V(3)=1029.5 cm-1 ROSYM=3 NU=3040,3028,2951,  
 2866,2850,1514,1471,1445,1356,1268,1216,1107,934,912,874,577,369, (249 torrision)  
 HF298=-13.6+/-4.0 kJ HF0=-0.2+/-4.0 kJ REF=DeTuri & Ervin JPC 103 (1999), 6911  
 for HF298 and G3MP2B3 calculations for the vibrations and moments of inertia.  
 Ruscic et al JPCRD 2003. MAX LST SQ ERROR @ 6000 K 0.61 %.

C2H5O\* RADICAL IU2/03C 2.H 5.O 1. 0.G 200.000 6000.000 B 45.06050 1  
 0.66889982E+01 0.13125676E-01-0.47038840E-05 0.75858552E-09-0.45413306E-13 2  
 -0.47457832E+04-0.96983755E+01 0.43074268E+01 0.64147205E-02 0.31139714E-04 3  
 -0.43314083E-07 0.17276184E-10-0.34027524E+04 0.59025837E+01-0.16357022E+04 4

4422-54-2

C2H5O (CH2CH2OH) RADICAL SIGMA=1 STATWT=2 IA=2.1001 IB=8.6720 IC=10.0014  
 REF=Chem3D IR(CH2)=0.79 IR(OH)=.1363 ROSYM(OH)=2  
 V(2)=201 cal, ROSYM(CH2)=2 V(2)=3000. cal. REF= Burcat, Miller & Gardiner  
 NU=3705,3093,2985,2855,2811,15001,1458,1409,1254,1223,1102,1042,951,853,433,376,  
 273,155 REF=Yamada, Bozzelli, Lay JPC A 103 (1999), 7646 Vib=scaled x 0.9;  
 HF298=5.70+/-0.85 kcal REF=Bozzelli JCP 105, (2001), 9543 MAX LST SQ ERROR  
 CP @ 6000 K 0.48 %

CH2CH2OH Radical T12/01C 2.H 5.O 1. 0.G 200.000 6000.000 C 45.06110 1  
 7.02824536E+00 1.20037746E-02-4.21306455E-06 6.69471213E-10-3.96371893E-14 2  
 -5.92493321E+03-9.40355948E+00 4.47893092E+00 7.59782301E-03 2.81794908E-05 3  
 -4.26953487E-08 1.78878934E-11-4.71446256E+03 6.38921206E+00-2.86833500E+03 4

2348-46-1

C2H5O (CH3CHOH) RADICAL SIGMA=1 STATWT=2 IA=1.8971 IB=8.9667  
 IC=10.2405 IR(CH3)=.47087 IR(OH)=.14477 ROSYM(CH3)=3 V(3)=1158. cm-1  
 ROSYM(OH)=1 V(3)=70.3 cm-1 NU=3734,3203,3164,3027,2956,1519,1459,1425,1327,  
 1213,1072,1037,923,612,407. HF298=-54.03+/-4.0 kJ REF=Janoschek & Rossi  
 Int.J. Chem. Kinet 36 (2004), 661 {HF298=-13.34+/-0.85 kcal REF=Bozzelli et al  
 JCP 105, (2001), 9543; HF298=-5.0 KCAL REF= Benson.} Max LST SQ ERROR CP @  
 6000 K 0.48%

CH3\*CHOH RADICAL T10/04C 2.H 5.O 1. 0.G 200.000 6000.000 B 45.06050 1  
 6.35842302E+00 1.24356276E-02-4.33096839E-06 6.84530381E-10-4.03713238E-14 2  
 -9.37900432E+03-6.05106112E+00 4.22283250E+00 5.12174798E-03 3.48386522E-05 3  
 -4.91943637E-08 2.01183723E-11-8.20503939E+03 8.01675700E+00-6.49827831E+03 4

Table 4 (continued)

16520-04-0

C2H5O CH2-O-CH3 RAD SIGMA=1 STATWT=2. IA=1.7787 IB=7.8857 IC=9.0727  
 IR(CH2)=0.30289 V(3)=700 cm-1 ROSYM=2 IR(CH3)=0.47197 V(3)=951 cm-1  
 ROSYM=3 NU=3262,3155,3112,3079,3020,1530,1521,1515,1479,1301,1264,1183,1151,  
 976,678,431 HF298=0.98 kJ HF0=14.08 kJ REF=Janoshcek Rossi 36 (2004),  
 {HF298=-2 kcal REF=Benson; HF298=-2.8+/-1.2 kcal REF=MacMillen Golden 1982;  
 HF298=-1.2 kcal REF=NIST 94} MAX LST SQ ERROR Cp @ 6000 K 0.52 %.  
 C2H5O CH3-O-CH2 A10/04C 2.H 5.O 1. 0.G 200.000 6000.000 B 45.06050 1  
 5.94067593E+00 1.29906358E-02-4.56921036E-06 7.26888932E-10-4.30599587E-14 2  
 -2.58503562E+03-4.52841964E+00 4.53195381E+00 7.81884271E-03 1.94968539E-05 3  
 -2.74538336E-08 1.06521135E-11-1.70629244E+03 5.06122980E+00 1.15460803E+02 4

81475-21-0

C2H5O2Cl Alfa-CHLORO-PEROXYETHANE CH3CHClO-OH SIGMA=3 IA=39.142 IB=24.814  
 IC=16.91 IR(C-C)=0.511373 IR(C-O)=4.14245 IR(O-O)=0.144446 V(3)(C-C)=1490.  
 cm-1 V(3)(C-O)=1479.46 cm-1 V(3)(O-O)=2427.3 cm-1 NU=3652,3019,2989,2977,2909,  
 1469,1464,1428,1416,1359,1300,1167,1122,1068,1009,890,632,518,430,316,305  
 HF298=-50.9 KCAL REF=Lay et al JPC 100, (1996), 8240 Max Lst Sq Error Cp @ 6000 K  
 0.6%  
 C2H5O2CL T01/97C 2.H 5.O 2.CL 1.G 200.000 6000.000 B 96.51320 1  
 1.15961106E+01 1.46988166E-02-5.56315884E-06 9.24997440E-10-5.64231971E-14 2  
 -3.06724523E+04-3.20337220E+01 3.19878206E+00 2.50806853E-02 1.51506919E-05 3  
 -4.08074392E-08 1.89776224E-11-2.77443750E+04 1.43864750E+01-2.56137283E+04 4

3170-61-4

C2H5OO PEROXYETHYL RADICAL STATWT=2 IA=2.4505 IB=18.5705 IC=19.984  
 NU=2955,2936,2934,2901,2874,1493,1467,1454,1410,1371,1259,1152,1145,1129,1006,  
 860,786,491,300,231,91.9 REF=Melius MP4 A40 1988 HF298=-6.86 kcal REF=  
 Atkinson et. al, JPCRD 28 (1999), 191 {Hf298= -2.32 kcal REF=Melius 1988}  
 {HF298=-4. kcal REF=NIST 1994 estimate} Max Lst sq Error Cp @ 1300 K 0.58%  
 C2H5OO PEROXYETH T08/00C 2.H 5.O 2. 0.G 200.000 6000.000 C 61.06050 1  
 8.05957692E+00 1.52921019E-02-5.54442603E-06 9.00496195E-10-5.41302799E-14 2  
 -7.31028500E+03-1.59992904E+01 5.21694144E+00 1.24160003E-04 6.15529492E-05 3  
 -7.94505636E-08 3.12101317E-11-5.41455775E+03 4.22381533E+00-3.45206633E+03 4

74-84-0

C2H6 ETHANE STATWT=1. SIGMA=6. IA=1.0481 IB=IC=4.22486 Ir=.26203 ROSYM=3  
 V0=2.96 kcal NU=2954,1388,995,2896,1379,2969(2),1468(2),1190(2),2985(2),  
 1469(2),822(2) HF298=-83.863 kJ REF=CHAO WILHOIT & ZWOLINSKI JPCRD 2, (1973),  
 427 {HF298=-83.791 +/-0.20 kJ REF=ATcT A} MAX LST SQ ERROR Cp @ 6000K 0.63%.  
 C2H6 g 8/88C 2.H 6. 0. 0.G 200.000 6000.000 B 30.06904 1  
 4.04666411E+00 1.53538802E-02-5.47039485E-06 8.77826544E-10-5.23167531E-14 2  
 -1.24473499E+04-9.68698313E-01 4.29142572E+00-5.50154901E-03 5.99438458E-05 3  
 -7.08466469E-08 2.68685836E-11-1.15222056E+04 2.66678994E+00-1.00849652E+04 4

15337-44-7

(CH3)2N DIMETHYL AZIDE Dimethyl-Amidogen RADICAL SIGMA=2 STATWT=2 IA=2.1047  
 IB=8.6639 IC=9.7229 (Ir=0.48229 ROSYM=3 V3=1253 cm-1)x2 Nu=3118(2),3006,  
 2998,2968,2957,1522,1518,1501,1493,1444,1420,1222,1219,1034,1025,938,919,433  
 HF298=159.854 kJ. HF0=177.58 kJ Max Lst Sq Error Cp @ 6000 K 0.55%.  
 CH3-N\*-CH3 A09/04C 2.H 6.N 1. 0.G 200.000 6000.000 B 44.07578 1  
 6.51948001E+00 1.52842778E-02-5.42514086E-06 8.68466302E-10-5.16752360E-14 2  
 1.60207871E+04-1.03264216E+01 4.35206979E+00 2.20630039E-03 5.25356947E-05 3  
 -6.99538040E-08 2.80551471E-11 1.74911105E+04 5.32379524E+00 1.92258959E+04 4

Table 4 (continued)

31277-24-4

C2H6N Methyl-Methylen-Amine Radical \*CH2-NH-CH3 SIGMA=1 STATWT=2 Ia=1.9758  
 Ib=8.6300 Ic=9.0053 Ir(CH3)=0.46839 ROSYM=3 V(3)=1253. cm-1 Ir(CH2)=0.30207  
 ROSYM=2 V(3)=1253. cm-1 Nu=3550,3249,3143,3128,3084,2993,1556,1525,1513,1493,  
 1467,1304,1261,1149,1053,973,722,675,392 HF298=156.58 kJ HF0=174.070 kJ  
 REF=Janoschek & Rossi Int. J. Chem Kin. 36, (2004), Max Lst Sq Error Cp @  
 6000 K 0.48%

CH2-NH-CH3	A09/04C	2.H	6.N	1.	0.G	200.000	6000.000	B	44.07578	1
6.97606586E+00	1.44632740E-02	-5.03598536E-06	7.95670852E-10	-4.69087405E-14						2
1.56142819E+04	-1.14299775E+01	3.14378173E+00	1.40061918E-02	2.35060038E-05						3
-4.17414861E-08	1.82376254E-11	1.71384932E+04	1.08365098E+01	1.88321380E+04						4

4143-41-3

C2H6N2 AZOMETHANE (CH3NNCH3) STATWT=1 SIGMA=2 IA=2.063 IB=19.082 IC=20.029  
 IR=0.425 V0=1700. ROSYM=3 NU=2989,2926,1583,1437,1381,1179,919,591,2977,  
 1416,1027,2981,1440,1111,312,2988,2925,1447,1384,1112,1008,353, (2148222 TORSION)  
 HF298=35.54 kcal. REF=PAMIDIMUKKALA, ROGERS & SKINNER MAX LST SQ ERROR CP @  
 1300. 0.9%.

C2H6N2	T 8/81C	2.H	6.N	2.	0.G	300.000	5000.000	B	58.08280	1
0.81902246E 01	0.15981115E-01	-0.53652748E-05	0.79098639E-09	-0.41925359E-13						2
0.13938773E 05	-0.18192831E 02	0.34860029E 01	0.18514410E-01	0.86240079E-05						3
-0.17172741E-07	0.61034997E-11	0.15975109E 05	0.92264036E 01	0.17884533E 05						4

4164-28-7

C2H6N2O2 N-methyl N-nitromethanamine (CH3)2N-NO2 SIGMA=2 IAIBIC=11752E-117  
 IR(CH3)=0.59 IR(NO2)=3.94 ROSYM(CH3)=3 ROSYM(NO2)=2 V3(CH3)=1050 cm-1  
 V2(NO2)=2800 cm-1 NU=3033(2),2948(2),2993(2),1528,1462,1456,1454,1450,1441,  
 1411,1304,1292,1248,1144,1110,1050,1023,838,762,626,619,427,350,225 HF298=-4.8  
 kJ REF=Dorofeeva & Tolmach Thermochim Acta 240, (1994), 47-66 Max Lst Sq Error  
 Cp @ 1300 K 0.60 %.

(CH3)2N-NO2	T10/99C	2.H	6.N	2.O	2.G	200.000	6000.000	B	90.08192	1
1.24703937E+01	1.86034893E-02	-6.89301702E-06	1.13154966E-09	-6.84339128E-14						2
-6.24684007E+03	-3.95039089E+01	4.22510053E+00	2.24381715E-02	3.20605902E-05						3
-5.84889497E-08	2.50090693E-11	-3.01379947E+03	7.74519704E+00	-5.77304014E+02						4

64-17-5

C2H5OH liquid Ethanol (L) DATA FROM TRC 12/84 HF298=-277.51 kJ {hf298=-277.007  
 +/-0.25 kJ REF=ATcT A}

C2H5OH(L)	P12/84C	2.H	6.O	1.	0.C	159.000	390.000	B	46.06844	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00						2
0.00000000E+00	0.00000000E+00	7.56212501E+00	6.05917882E-02	-4.59385998E-04						3
1.40542149E-06	-1.08065385E-09	-3.65331092E+04	-3.17590773E+01	-3.33765910E+04						4

Table 4 (continued)

64-17-5

C2H6O ETHANOL (C2H5OH) STATWT=1. SIGMA=3 SIGMA BARRIER CH3=3. ROSYM OH=1  
 This is an equilibrium mixture of one trans and two gauche isomers, therefore sigma was set artificially to 3. The two gauche isomers are equal. The trans values are: IAIBIC=218.459 Brot(CH3)=6.4144 cm-1 V(3)CH3=1166. Brot(OH)=21.07 cm-1 V(OH) (1)=57 (2)=8.025 (3)=395. NU=3659,2985,2939,2900,1460,1430,1395,1320,1245,1055,1026,883,422,2887(2),1460,1270,1117,801 The cis values are: IAIBIC=233.455E-117 Brot(CH3)=6.416 cm-1 Brot(OH)=20.94 cm-1 V(3) CH3=1331 V(OH) as for trans NU=3675,2985,2939,2900,1460(2),1430,1395,1320,1245,1055,1026,887,596,2887(2)1270,1070,801 HF298=-234.95 KJ REF=CHAO, HALL, MARSH & WILHOIT JPCRD 15 (1986),1369. {HF298=-234.607+/-0.28 kJ REF=ATcT A}  
 C2H5OH L 8/88C 2H 6O 1 OG 200.000 6000.000 B 46.06904 1  
 0.65624365E+01 0.15204222E-01-0.53896795E-05 0.86225011E-09-0.51289787E-13 2  
 -0.31525621E+05-0.94730202E+01 0.48586957E+01-0.37401726E-02 0.69555378E-04 3  
 -0.88654796E-07 0.35168835E-10-0.29996132E+05 0.48018545E+01-0.28257829E+05 4

115-10-6

C2H6O DIMETHYL-ETHER SIGMA=2 IAIBIC=170.493 IR=0.4291 ROSYM=3  
 V(3)=903.4 cal Nu=2999(2),2935,2920,2820(2),1485,1467,1463,1459,1449,1432,1250,1179,1178,1148,1104,931,424 HF298=-184.05 KJ REF=CHAO, HALL, MARSH & WILHOIT JPCRD 15, (1986),1369 HF298=-183.935+/-0.46 kJ REF=ATcT A}  
 CH3OCH3 L 9/88C 2H 6O 1 OG 200.000 6000.000 B 46.06904 1  
 0.56483880E+01 0.16338220E-01-0.58680268E-05 0.94683462E-09-0.56650169E-13 2  
 -0.25100722E+05-0.59623267E+01 0.53055789E+01-0.21421160E-02 0.53085949E-04 3  
 -0.62313044E-07 0.23072397E-10-0.23979910E+05 0.71342649E+00-0.22136501E+05 4

3031-74-1

C2H6O2 PEROXYETHANE C2H5O-OH SIGMA=1 STATWT=1 IA=21.607 IB=20.135 IC=2.7509  
 IR(CH3)=0.49484 ROSYM=3 V(3)(CH3)=1143.7 cm-1 IR(C2H5)=2.859 ROSYM=1  
 V(3)(C2O5)=1479.46 cm-1 IR(OH)=0.1428 ROSYM=1 V(3)(OH)=2427.3 cm-1 NU=3661,2966,2955,2936,2898,2892,1484,1481,1466,1423,1405,1383,1263,1174,1153,1087,1002,868,804,481,293 HF298=-41.5 Kcal REF=Lay et al JPC 100,(1996),8240 Max Lst Sq Error Cp @ 6000 K 0.6%  
 C2H6O2 T10/96C 2.H 6.O 2. O.G 200.000 6000.000 B 62.06844 1  
 9.99511555E+00 1.47311626E-02-5.30621235E-06 8.58442516E-10-5.14814807E-14 2  
 -2.53850722E+04-2.53504050E+01 4.37310002E+00 1.04422436E-02 4.63854723E-05 3  
 -7.02772770E-08 2.93034879E-11-2.29362227E+04 8.30134323E+00-2.08834916E+04 4

690-02-8

C2H6O2 Dimethyl Peroxide CH3-O-O-CH3 SIGMA=2 STATWT=1 IAIBIC=1123.E-117  
 (Ir(CH3)=0.4910 ROSYM=3 V(3)=900 cm-1)x2 Ir(CH3O-)=1.5928 ROSYM=1 V(0)=1341.3  
 V(1)=2081 V(2)=1052.2 V(3)=225.5 cm-1 NU=2945,2917,2900,1487,1474,1433(2),1198,1165,1020,786,448,3000,2965,2818,1483,1430,1119,1112,1032,376 HF298=-125.5 +/-5.0 kJ HF0=-106.5 kJ REF=Dorofeeva et al JPCRD 30,(2001),475 Max Lst Sq Error Cp @ 2500 K 0.53% Calculated from original Tables + NASA extesion.  
 C2H6O2 T 8/03C 2.H 6.O 2. O.G 200.000 6000.000 B 62.06784 1  
 7.59782714E+00 1.74427831E-02-6.37185354E-06 1.03573213E-09-6.20934305E-14 2  
 -1.86722111E+04-1.25718099E+01 5.18445635E+00 7.41530799E-03 4.06423876E-05 3  
 -5.56242513E-08 2.20244947E-11-1.71688382E+04 3.98453355E+00-1.50339587E+04 4

Table 4 (continued)

75-08-1

C2H5SH ETHANETHIOL DATA FROM STULL WESTRUM & SINKE 1969, EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS. HF298=-11.02 KCAL Max Lst Sq Error H-Href @ 300 K \*6.7%\*.

C2H6S	T 4/93C	2H	6S	1	OG	298.150	5000.000	B	62.13564	1
0.64687045E+01	0.16391622E-01	-0.60377275E-05	0.10524727E-08	-0.70286890E-13						2
-0.86436726E+04	-0.69816273E+01	0.21847425E+01	0.24139946E-01	-0.54359062E-05						3
-0.71826248E-08	0.40986272E-11	-0.72094881E+04	0.16264503E+02	-0.55454477E+04						4

75-18-3

C2H6S DIMETHYL SULFIDE CH<sub>3</sub>-S-CH<sub>3</sub> DATA FROM STULL WESTRUM & SINKE EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS. HF298=-8.97 KCAL Max Lst Sq Error H-Href @ 300 K \*6.4%\*

C2H6S (CH <sub>3</sub> SCH <sub>3</sub> )	T 4/93C	2H	6S	1	OG	298.150	5000.000	B	62.13564	1
0.61189311E+01	0.16882055E-01	-0.63478415E-05	0.11172322E-08	-0.74890322E-13						2
-0.74615078E+04	-0.61902955E+01	0.19139966E+01	0.29420442E-01	-0.24128528E-04						3
0.15495718E-07	-0.50061422E-11	-0.62072425E+04	0.15648303E+02	-0.45138535E+04						4

624-92-0

C2H6S<sub>2</sub> DIMETHYL DISULFIDE CH<sub>3</sub>-S-S-CH<sub>3</sub> DATA FROM STULL WESTRUM & SINKE EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS. HF298=-5.77 KCAL Max Lst Sq Error H-Href @ 300 K \*7.8%\*

C2H6S <sub>2</sub>	T 4/93C	2H	6S	2	OG	298.150	5000.000	B	94.20164	1
0.91856110E+01	0.17160184E-01	-0.66808919E-05	0.12071229E-08	-0.82458844E-13						2
-0.69404925E+04	-0.17999496E+02	0.51094624E+01	0.20928434E-01	0.43660805E-05						3
-0.17144491E-07	0.75300808E-11	-0.53653977E+04	0.50798739E+01	-0.29035602E+04						4

124-40-3

C2H<sub>7</sub>N DIMETHYLAMINE CH<sub>3</sub>-NH-CH<sub>3</sub> SIGMA=2 STATWT=1 IA=2.4308 IB=9.0358 IC=10.2300 (IR=0.48178 ROSYM=3 V(3)=1253. cm<sup>-1</sup>)x2 Nu=3494,3117(2),3069(2),2947,2939,1548,1543,1526,1513,1497(2),1467,1284,1203,1183,1112,1045,955,792,387 HF298=-15.259 kJ HF0=6.501 kJ REF=Burcat G3B3 calc. {HF298=-19+/-2 kJ REF=Cox & Pilcher 1970; HF298=-18.4+/-0.5 kJ REF=Pedley & Reelance 1977; HF298=-20.92 kJ REF=NIST 94; V(3) see East & Radom JCP106,(1997),6655} Max Lst Sq Error Cp @ 6000 K 0.57%.

CH <sub>3</sub> -NH-CH <sub>3</sub>	A09/04C	2.H	7.N	1.	O.G	200.000	6000.000	B	45.08372	1
6.04266054E+00	1.81505461E-02	-6.40296907E-06	1.02080428E-09	-6.05674188E-14						2
-5.07188602E+03	-8.95081700E+00	4.84262853E+00	-2.23650748E-03	6.82702875E-05						3
-8.54283982E-08	3.33024641E-11	-3.62971842E+03	2.86477868E+00	-1.83523118E+03						4

40613-93-2

(CH<sub>3</sub>)<sub>2</sub>N-NH\* UNSYMETRICAL DIMETHYL HYDRAZINE RADICAL SIGMA=2 STATWT=2 Ia=8.5287 Ib=9.4466 Ic=16.6828 (Ir(CH<sub>3</sub>)=0.50137 V(3)=1049 cm<sup>-1</sup> ROSYM=3)x2 Ir(NH)=0.162277 ROSYM=2 V(3)=3778 cm<sup>-1</sup> Nu=3371,3170,3130,3099,3089,3004,2991,1545,1530,1517,1504,1490,1478,1456,1376,1211,1173,1136,1114,1058,840,548,492,416 HF298=207.685 kJ HF0=232.276 kJ REF=G3B3 calc. {HF298=40.2+/-2. kcal REF=Bozzelli & Ritter} Max Lst Sq Error Cp @ 6000 K 0.64%.

(CH <sub>3</sub> ) <sub>2</sub> N-NH*	A10/04C	2.H	7.N	2.	O.G	200.000	6000.000	B	59.09046	1
7.94121637E+00	1.96086909E-02	-7.11650271E-06	1.15466458E-09	-6.93050294E-14						2
2.09691279E+04	-1.71912552E+01	3.09064932E+00	1.73629496E-02	3.01166251E-05						3
-4.98285239E-08	2.07770639E-11	2.31080463E+04	1.17272562E+01	2.49786689E+04						4

Table 4 (continued)

540-73-8

CH<sub>3</sub>NH-NHCH<sub>3</sub> SYMETRICAL DIMETHYL HYDRAZINE SIGMA=4 IA=4.593949 IB=17.1057  
 IC=18.565859 NU=3378,3294,2948,2936,2902,2900,2827,2799,1508.5,1491,1474,1471,  
 1465,1457,1432,1421,1222.5,1190,1157,1119,1113,1011,900.5,863,757,442,404  
 N-CH<sub>3</sub> Rotation IR=0.488 Potential Barrier V(3)=1049 cm<sup>-1</sup> ROSYM=3 N-N Rotation  
 IR=1.53152 Potential Barrier V(2)=3778 cm<sup>-1</sup> ROSYM=2 REF=C. Melius BAC/MP4  
 Calculations, Private Communication HF298=22.584+/-1.8 KCAL Max Lst Sq Error  
 Cp @ 1300 K 0.65%

C2H8N2 SYM	T 7/93C	2H	8N	2	OG	200.000	6000.000	B	60.09900	1
	0.80414886E+01	0.21261224E-01	-0.77211118E-05	0.12549260E-08	-0.75477198E-13					2
	0.70952651E+04	-0.19466398E+02	0.52268579E+01	0.75034124E-03	0.75377281E-04					3
	-0.95913660E-07	0.37320229E-10	0.92788780E+04	0.19786705E+01	0.11364645E+05					4

57-14-7

(CH<sub>3</sub>)<sub>2</sub>N-NH<sub>2</sub> UNSYMETRICAL DIMETHYL HYDRAZINE SIGMA=18. STATWT=1 IAIBIC=14.95E-115  
 NU=3338,3315,2980(2),2961(2),2816,2777,1587,1464(2),1449(2),1402(2),1319,1246,  
 1215,1144,1060,1032,966,908,808,459,441,411 IR(CH<sub>3</sub>)=0.503 IR(NH<sub>2</sub>)=0.303 ROT  
 INT BARRIER V3(CH<sub>3</sub>)=4.69 KCAL V3(NH<sub>2</sub>)=3. KCAL REF=J.R. Durig & W.C. Harris J.  
 CHEM. Phys. 51 (1969), 4457. MAX LST SQ ERROR Cp @ 6000 K 0.30% HF298=53.33 KJ  
 C2H8N2 UNSYM T09/91C 2H 8N 2 OG 200.000 6000.000 B 60.09900 1  
 0.95884921E+01 0.20043079E-01 -0.71185025E-05 0.11401487E-08 -0.67870741E-13 2  
 0.18116417E+04 -0.25995709E+02 0.30395710E+01 0.22043065E-01 0.30487429E-04 3  
 -0.57055204E-07 0.25070487E-10 0.43464264E+04 0.11553546E+02 0.64008583E+04 4

4120-02-9

CCN RADICAL SIGMA=1 STATWT=2 B0=0.398 NU=1923,324(2),1051  
 T0=40.34 SIGMA=1 STATWT=2 B0=0.398 Nu=1923,324(2),1051  
 T0=21259.20 SIGMA=1 STATWT=4 B0=0.414 Nu=1771,451(2),1242  
 T0=22413.25 SIGMA=1 STATWT=2 B0=0.405 Nu=1771,445(2),1242  
 T0=26661.73 SIGMA=1 STATWT=2 B0=0.413 Nu=1859,470(2),1257 REF=Jacox 98  
 HF298=679.07+/-6.23 kJ REF=ATcT A {HF298=604.85+/-20 kJ REF=Gurvich 91;  
 HF298=584.51 REF=JANAF 66} Max Lst Sq Error Cp @ 1300 K 0.34%.

CCN Radical	ATcT/AC	2.N	1.	0.	0.G	200.000	6000.000	B	38.02814	1
	5.51786423E+00	1.95500288E-03	-7.53385165E-07	1.27744269E-10	-7.82860791E-15					2
	7.97839404E+04	-3.83516102E+00	3.40722586E+00	9.44213617E-03	-1.30137091E-05					3
	1.06894447E-08	-3.68570001E-12	8.03329359E+04	6.78654202E+00	8.16728827E+04					4

53590-27-5

CNC RADICAL SIGMA=2 STATWT=2 IB=6.173 NU=1100,157.4,1453,275.9  
 T0=26.41 SIGMA=2 STATWT=2 IB=6.173 NU=1100,270.4,1453,484.6 REF=Gurvich 91  
 HF298=675.85+/-5.89 kJ REF=ATcT A {HF298=654.94+/-40 kJ REF=Gurvich 91;  
 HF298=472.79 kJ REF=JANAF 70} Max Lst Sq Error Cp @ 1300 K 0.30%.

CNC Radical	ATcT/AC	2.N	1.	0.	0.G	200.000	6000.000	B	38.02814	1
	5.93219820E+00	1.57955995E-03	-6.12495852E-07	1.03897382E-10	-6.43334740E-15					2
	7.92421706E+04	-6.60234593E+00	3.98662721E+00	5.23128299E-03	-6.00388565E-07					3
	-3.37882585E-09	1.75803055E-12	7.98756324E+04	3.89919746E+00	8.12856079E+04					4

160727-65-1

C2NO CYANOXOMETHYL Radical OC\*CN T0=0 STATWT=2 SYMNO=1 IAIBIC=183 E-117  
 NU=2249,1703,909,488,174,233 T0=15500. [above values repeated]. HF298=210.0  
 +/-10.0 kJ HF0=207.2+/-10.0 kJ REF=Dorofeeva et al JPCRD 30 (2001),475.  
 Max Lst Sq Error Cp @ 1300 K 0.40%.

C2NO OC*CN RAD	g /01C	2.N	1.0	1.	0.G	200.000	6000.000	B	54.02754	1
	6.73206516E+00	3.16535587E-03	-1.21983158E-06	2.11386461E-10	-1.32957980E-14					2
	2.29243121E+04	-6.22708465E+00	4.17831827E+00	1.30289906E-02	-1.93104852E-05					3
	1.71821589E-08	-6.20330248E-12	2.35717677E+04	6.48584348E+00	2.52570506E+04					4

Table 4 (continued)

460-19-5

C2N2 Dicyanogen NC-CN Calculated from original Gurvich 79 tables

HF298=309.28+/-1.03 kJ REF=ATcT A {HF298=309.1+/-0.8 kJ REF=Gurvich 79}

Max Lst Sq Error Cp @ 1300 K 0.40%

C2N2 Dicyanogen	ATcT/AC	2.N	2.	0.	0.G	200.000	6000.000	A	52.03488	1
6.70549520E+00	3.64271185E-03	-1.30939702E-06	2.16421413E-10	-1.31193815E-14						2
3.48824335E+04	-1.04803146E+01	2.32928126E+00	2.61540993E-02	-4.90009889E-05						3
4.61923035E-08	-1.64325831E-11	3.56900732E+04	9.86348075E+00	3.71976220E+04						4

88466-66-4

C2(NO2)2 DiNitroAcetylene NO2-CC-NO2 SIGMA=2 STATWT=1 IA=12.8841 IB=95.4463

IC=95.4591 Ir=3.2220 ROSYM=2 [V(3)=1753 cm-1 (5.04 kcal) REF=Burcat JPCRD, 28

(1999), 63-130] One Rotor Only. Nu=2334, 1644(2), 1380, 1378, 1072, 867, 748(2), 697,

602(2), 366, 272(2), 101(2) HF298=349.05 kJ HF0=356.25 kJ REF=Burcat G3B3 calc

{HF298=152 kJ est REF=THERGAS} Max Lst Sq Error Cp @ 1300 K 0.42%

C2(NO2)2	A	1/05C	2.N	2.O	4.	0.G	200.000	6000.000	B	116.03248	1
1.49179250E+01	6.67809195E-03	-2.60703718E-06	4.39898434E-10	-2.70718721E-14							2
3.63490468E+04	-4.64070026E+01	3.67763481E+00	3.74702265E-02	-3.06683850E-05							3
7.87653935E-09	1.04579070E-12	3.94733196E+04	1.17296150E+01	4.19803471E+04							4

13223-78-4

C2(NO2)4 TetraNitroEthylene SIGMA=4 STATWT=1 IA=87.6957 IB=115.3279

IC=177.3303 (Ir=5.84 ROSYM=2 V3=1763 cm-1)x4 Nu=1713, 1707, 1696, 1684, 1672,

1410, 1392, 1355, 1346, 1138, 987, 953, 866, 805, 802, 769, 755, 726, 678, 608, 550, 541, 424,

406, 346, 250, 242, 208, 188.6, 157, 153.4, 109.5 \*\*\* HF298=N/A \*\*\* {HF298=20.58 kcal

REF=MOPAC 2000 PM3} Max Lst Sq Error Cp @ 1300 K 0.47%.

C2(NO2)4 NO HF	A	6/05C	2.N	4.O	8.	0.G	200.000	6000.000	B	208.04356	1
2.93745614E+01	9.52232507E-03	-4.15475512E-06	7.43640117E-10	-4.73972776E-14							2
-1.11737134E+04	-1.18329714E+02	5.73270594E+00	6.71446931E-02	-3.79861174E-05							3
-1.32109381E-08	1.37580306E-11	-4.33836220E+03	5.47592016E+00	N/A							4

918-37-6

C2N6O12 HEXANITROETHANE C2(NO2)6 SIGMA=6 IAIBIC=6364500.E-117 (IR(NO2)=59.6)x6

IR(C(NO2)3)=684 V(2)-NO2=2800 cm-1 V(3)-C(NO2)3=1000 cm-1 NU=1627, 1353,

1143, 858, 375, 335, 113, 1630(2), 1268(2), 1003(2), 665(2), 391(4), 238(2), 103(2), 1621,

1333, 888, 582, 376, 240, 1639(2), 1285(2), 820(2), 633(2), 383(2), 347(2), 155(2), 92(2),

642, 774 REF= Olga Dorofeeva Unpublished Results 1999 HF298=179.+/-5.9 kJ

REF= Pepekin Miroshichenko, Lebedev, Aspin Rus J. Phys. Chem. Eng. Trans. 42,

(1968), 1583-1584 Max Lst Sq Error Cp @ 1200 K 0.58%

Hexanitroethane	T11/99C	2.N	6.O	12.	0.G	200.000	6000.000	C	300.05524	1
4.21870612E+01	1.23800129E-02	-5.52306964E-06	1.00910711E-09	-6.53407906E-14						2
5.66970453E+03	-1.69918944E+02	1.06751275E+01	1.00230936E-01	-1.00773651E-04						3
5.18003948E-08	-1.19450365E-11	1.46844877E+04	-6.42835467E+00	2.15286289E+04						4

12071-23-7

C2O SIGMA=1 STATWT=3 B0=0.385 NU=1971, 379.53(2), 1063

T0=5310. SIGMA=1 STATWT=2 B0=0.385 NU=1950, 379.53(2), 1063

T0=8190. SIGMA=1 STATWT=1 B0=0.385 NU=2010, 379.53(2), 1063

T0=11651. SIGMA=1 STATWT=6 B0=0.407 Nu=2046, 594.75(2), 1284 REF=Jacox 98

HF298=291.04+/-12 kJ HF0=287.0 kJ REF=Gurvich 91 {HF298=286.6 kJ REF=JANAF}

Max Lst Sq Error Cp @ 1200 K 0.23%.

C2O	g	8/00C	2.O	1.	0.	0.G	200.000	6000.000	B	40.02080	1
5.42468378E+00	1.85393945E-03	-5.17932956E-07	6.77646230E-11	-3.53315237E-15							2
3.31537194E+04	-3.69608405E+00	2.86278214E+00	1.19701204E-02	-1.80851222E-05							3
1.52777730E-08	-5.20063163E-12	3.37501779E+04	8.89759099E+00	3.50037063E+04							4



Table 4 (continued)

83917-77-5

C2S2 Dicarbon Disulfide S=C=C=S From original TRC(6/01) data to 2000 extrapolated using Wilhoit's polynomials to 6000. HF298=376.66 kJ HF0=373.8 kJ

Max Lst Sq Error Cp @ 5500 K 0.40%

C2S2	g 6/01C	2.S	2.	0.	0.G	200.000	6000.000	D	88.15340	1
	7.55839728E+00	3.57346918E-03	-1.44439554E-06	2.47666128E-10	-1.53533628E-14					2
	4.26904697E+04	-1.15835580E+01	2.93494482E+00	2.52355574E-02	-4.45369876E-05					3
	4.04727658E-08	-1.41864967E-11	4.36250292E+04	1.03727472E+01	4.53015271E+04					4

12075-35-3

C3 CALCULATED FROM TSIV TABLES 1979 HF298=839.96 kJ HF0=831. kJ Max Lst Sq Error Cp @ 6000 K 0.66%.

C3	RUS 79C	3	0	0	0G	200.000	6000.000	B	36.03210	1
	0.48035776E+01	0.21451125E-02	-0.10729208E-05	0.26073528E-09	-0.20163197E-13					2
	0.99396542E+05	0.38936985E+00	0.54328396E+01	-0.44675438E-02	0.14932148E-04					3
	-0.14795314E-07	0.50142111E-11	0.99495722E+05	-0.15872071E+01	0.10102201E+06					4

6111-63-3

C3D4 CYCLOPROPENE-D4 STATWT=1. SIGMA=2. IA=3.861 IB=4.9423 IC=7.826

NU=2435,2142,1548,1147,1023,639,749,640,2313,885,863(2),637,2262,424

REF=BURCAT(1982) MAX LST SQ ERROR CP @ 1300 K 0.79 % .HF298=63.0 KCAL

C3D4	T 2/82C	3D	4	0	0G	300.000	5000.000	B	44.0894	1
	0.89251080E+01	0.92740692E-02	-0.33307069E-05	0.52548144E-09	-0.30162352E-13					2
	0.27717801E+05	-0.24771932E+02	0.87993717E+00	0.25426447E-01	-0.47690091E-05					3
	-0.14818401E-07	0.86449008E-11	0.30267191E+05	0.18314783E+02	0.31592361E+05					4

1517-52-8

C3D6 CYCLOPROPANE-D6 STATWT=1. SIGMA=6 IA=IB=6.0672 IC=8.75747 NU=2236,1274,956,800,870,2336,614,2211(2),1072(2),855(2),717(2),2329(2),940(2),528(2)

REF=DUNCAN &amp; BURNS MAX LST SQ ERROR @ 1300 K 0.85 % . HF298=32.85 KJ. REF= C3H6

C3D6	T12/81C	3D	6	0	0G	300.000	5000.000	B	48.1176	1
	0.10402956E+02	0.12471735E-01	-0.44642438E-05	0.70182371E-09	-0.40115975E-13					2
	-0.77593262E+03	-0.35093755E+02	-0.79611647E+00	0.35631880E-01	-0.75448597E-05					3
	-0.20582778E-07	0.12364153E-10	0.27102590E+04	0.24640681E+02	0.39509243E+04					4

144087-36-5

C3F Radical SIGMA=1 STATWT=2 IA=0.4623 IB=18.3231 IC=18.7854 Nu=1989,1481,984,528,207.6,201.3 HF298=564.96+/-8. kJ HF0=559.052 kJ REF=Burcat G3B3 calc {HF298=565.68 kJ HF0=559.32 kJ REF=Bauschlicher & Ricca JPC A 104,(2000),4581.} Max Lst Sq Error Cp @ 1300 K 0.39%.

C3F Radical	CC A 7/05C	3.F	1.	0.	0.G	200.000	6000.000	B	55.03050	1
	7.03171830E+00	2.90941364E-03	-1.10990795E-06	1.86328934E-10	-1.14568532E-14					2
	6.54694442E+04	-8.15279504E+00	4.38610072E+00	1.00099976E-02	-9.11997924E-06					3
	5.33167678E-09	-1.60169978E-12	6.62665052E+04	5.70938026E+00	6.79483400E+04					4

268566-74-1

C3F3 PerfluoroPropargyl Radical FC=C=CF2 SIGMA=1 STATWT=2 IA=7.8325

IB=50.2709 IC=57.3421 Nu=2046,1588,1305,1110,792,563,519,488,400,338,161,105

HF298=-32.13 kcal REF Burcat B3LYP calc {HF298=-31.94 kcal HF0=-32.32 kcal

REF=Bauschlicher Ricca JPC A 104 (2000),4581} Max Lst Sq Error Cp @ 1300 K 0.43%.

C3F3	A12/04C	3.F	3.	0.	0.G	200.000	6000.000	B	93.02731	1
	1.12378484E+01	4.72022510E-03	-1.81319626E-06	3.05774873E-10	-1.88599788E-14					2
	-2.02557682E+04	-2.73469146E+01	2.76396544E+00	3.57836163E-02	-5.06266174E-05					3
	3.86565828E-08	-1.21457550E-11	-1.82047635E+04	1.47800354E+01	-1.61668418E+04					4

Table 4 (continued)

207602-05-9

C3F3 PerfluoroPropynyl radical CF<sub>3</sub>CC\* SIGMA=3 STATWT=2 IA=14.9388 IB=27.3321  
 IC=27.3330 Nu=2284,1246,1202(2),814,569(2),537,408(2),120.5(2) HF298=-18.90  
 kcal HF0=-79.61 kcal REF=Burcat G3B3 calc. {HF298=-108.49 HF0=-108.16+/-4.4  
 kJ REF=Zhang JOC 63, (1998), 3591 CBS-4 method} Max Lst Sq Error Cp @ 1300 0.39%  
 C3F3 PerfluoroP A 3/05C 3.F 3. 0. 0.G 200.000 6000.000 B 93.02731 1  
 1.13343476E+01 4.59574371E-03-1.75919317E-06 2.96031787E-10-1.82334031E-14 2  
 -1.36485761E+04-2.95107171E+01 2.43391095E+00 3.54454173E-02-4.51718459E-05 3  
 2.97572187E-08-8.01600457E-12-1.14678345E+04 1.50070211E+01-9.51079498E+03 4

461-68-7

C3F4 PerfluoroAllene F<sub>2</sub>C=C=CF<sub>2</sub> SIGMA=2 STATWT=1 IA=14.7610 IB=67.9178  
 IC=67.9238 Nu=2151,1600,1279(2),1058,736,628(2),573,551(2),389,152,90(2)  
 HF298=-553.71 kJ HF0=-551.95 kJ REF=Burcat G3B3 calc {HF298=-132.34 kcal  
 REF=Bauschlicher & Ricca JPC A 104 (2000), 4581} Max Lst Sq Error Cp @ 1300 K  
 0.42%  
 C3F4 PerfluoroA A12/04C 3.F 4. 0. 0.G 200.000 6000.000 B 112.02571 1  
 1.31232153E+01 5.83382768E-03-2.24315688E-06 3.78529136E-10-2.33580739E-14 2  
 -7.14789913E+04-3.76087467E+01 2.39178498E+00 4.14799223E-02-4.99529342E-05 3  
 3.11694452E-08-8.01916112E-12-6.87659176E+04 1.64654537E+01-6.65926743E+04 4

116-15-4

C3F6 HEXAFLUORO PROPENE IA=33.2512 IB=67.0866 IC=85.5099 IR=9.6027 ROSYM=3  
 [V(3)=1595 cm<sup>-1</sup> REF=Ruscic & Burcat as in C2F6] NU=1851,1415,1356,1238,1231,  
 1201,1047,765,651,637,597,550,505,456,368,359,251,237,180,120 HF298=-1157.05 kJ  
 HF0=-1150.95 kJ REF=Burcat G3B3 calc {HF298=-1151.7 kJ REF=Papina Kolesov  
 Golovanova Russ JPC 61, (1987), 1168 Exp spectra=NIELSEN CLAASSEN & SMITH JCP, 20,  
 (1952), 1916; HF298=-268.9 KCAL REF=NIST 94} Max Lst Sq Error Cp @ 1300 K 0.40%.  
 C3F6 CF<sub>2</sub>=CF-CF<sub>3</sub> A11/04C 3.F 6. 0. 0.G 200.000 6000.000 B 150.02252 1  
 1.87296098E+01 5.74055067E-03-2.31302367E-06 4.01017749E-10-2.51741915E-14 2  
 -1.46123551E+05-6.59853551E+01 2.35781302E+00 5.80498289E-02-6.67557556E-05 3  
 3.68109988E-08-7.92990472E-12-1.41947032E+05 1.68586208E+01-1.39184698E+05 4

3248-60-0

C3F7 RADICAL CF<sub>3</sub>CF\*CF<sub>3</sub> SIGMA=18 STATWT=2 IA=38.9352 IB=80.40703 IC=91.12589  
 NU=1393,1370,1290,1243,1238,1204,1182,969,769,687,684,598,534,522,492,443,335,  
 311,286.5,241,167,132,50.3,16.8 HF298=-321.91 kcal REF=Melius database 1987  
 AB1W {HF298=-332.41 kcal REF=Bauschlicher & Ricca JPC A 104, (2000), 4581-85}  
 Max Lst Sq Error Cp @ 1300 K 0.40%  
 C3F7 CF<sub>3</sub>CF\*CF<sub>3</sub> M T12/99C 3.F 7. 0. 0.G 200.000 6000.000 C 169.02092 1  
 2.05301132E+01 7.60062764E-03-2.96491015E-06 5.04882378E-10-3.13452721E-14 2  
 -1.69702083E+05-7.19281430E+01 3.14241614E+00 6.03443070E-02-6.17598017E-05 3  
 2.79379580E-08-4.02551172E-12-1.65147364E+05 1.66897624E+01-1.62020670E+05 4

76-19-7

C3F8 OCTAFLUOROPROPANE (FC-218) SIGMA=18 CALCULATED AND EXTRAPOLATED USING  
 BOZZELLI & RITTER'S PROGRAM. HF298=-1760.12 KJ. REF=DOMALSKI & HEARING JPCRD  
 22 (1993), p. 1065.  
 C3F8 FC-218 T 1/94C 3F 8 0 0G 298.150 5000.000 D 188.02023 1  
 0.23380508E+02 0.71509045E-02-0.30004329E-05 0.55566723E-09-0.37865981E-13 2  
 -0.22034342E+06-0.89673706E+02 0.16732611E+01 0.72542284E-01-0.70291850E-04 3  
 0.25054365E-07-0.94876882E-12-0.21484389E+06 0.20590469E+02-0.21169268E+06 4

Table 4 (continued)

53590-28-6

C3H RAD CC-CH T0=0 STATWT=2. SIGMA=1. IA=0.0353 IB=7.5023 IC=7.5376  
 Nu=3238,1825,1167,467,[72.5,275.5] T0=19187 STATWT=2 IA=0.0353 IB=7.5023  
 IC=7.5376 Nu=2800,1836,1091,881,460(2) T0=20538. STATWT=2 IA=0.0353 IB=7.5023  
 IC=7.5376 Nu=2800,1836,1091,784,493(2) HF298=171.94+/-1.9 kcal HF0=170.67  
 kcal REF=Burcat G3B3 calc; Vibrations from Jacox (Webbook 2005) and G3B3 calc[]  
 {HF0=127.1 kcal REF=Duff & Bauer Los Alamos Rep 2556 1961; SPANGENBERG &  
 BORGER Z.Phys. Chem (Leipzig) 255,(1974),1; HF298=163.5 kcal REF=Estimated  
 from C2H C4H and C6H by Kiefer et al Comb. Sci Technol 82,(1992),101 \*\*\* Note  
 Duff & Bauer expect SIGMA=4 and Spangenberg gives SIGMA=3 for HCC-C linear  
 configuration} MAX LST SQ ERROR Cp @ 1300K 0.3%.  
 C3H Radical HCCC A 7/05C 3.H 1. 0. 0.G 200.000 6000.000 B 37.04004 1  
 6.14184491E+00 3.39661013E-03-1.21915444E-06 1.97782838E-10-1.18312807E-14 2  
 8.44225753E+04-6.44480148E+00 3.34917187E+00 1.65822626E-02-2.77115653E-05 3  
 2.51382364E-08-8.85285352E-12 8.49863168E+04 6.80362439E+00 8.65225703E+04 4

431-89-0

C3HF7 2-HEPTAFLUORO-PROPANE CF3-CHF-CF3 (FC-227ea) SIGMA=2 STATWT=1 IA=38.9667  
 IB=78.08525 IC=88.49144 NU=2966,1428,1392,1324,1296,1280,1242,1224,1150,1131,  
 896,853,725,669,593,535,519,502,442,335,314,283,232,214,152,89.7.26.9  
 HF298=-374.00 KJ REF=Melius Database 1987 AB1V {HF298=-374.47 kcal REF=Zhang  
 JOC 63,(1998),3590-94} Max Lst Sq Error Cp @ 1300 K 0.44%.  
 C3F7H FC227EA T12/99C 3.H 1.F 7. 0.G 200.000 6000.000 C 170.02886 1  
 2.03195617E+01 1.04618873E-02-3.99351610E-06 6.70976809E-10-4.12886922E-14 2  
 -1.96070480E+05-7.39087817E+01 3.19381844E+00 5.64358210E-02-4.24435538E-05 3  
 6.01422805E-09 4.21730731E-12-1.91302556E+05 1.47970140E+01-1.88203033E+05 4

1070-71-9

C3HN CYANO-ACETYLENE HCC-CN SIGMA=1 STATWT=1 IB=18.4925 Nu=3489,2385,2186,  
 911,651(2),573.5(2),260(2) HF298=368.414 kJ HF0=367.225 kJ REF=Burcat G3B3  
 calc {HF298=84.6 kcal REF=ESTIMATED BY MACKIE & COLKET 22nd COMBUST SYMP 1990;  
 HF298=84.0 kcal REF=Knight Freeman McEwan Int.J Mass. Spect.Ion Phys. 67,(1985),  
 317; HF298=90.7 kcal NIST 94} Max Lst Sq Error Cp @ 1300 K 0.34%  
 C3HN Cyano-Acety A 2/05C 3.H 1.N 1. 0.G 200.000 6000.000 B 51.04678 1  
 7.44515032E+00 5.27107604E-03-1.86735278E-06 2.98683734E-10-1.77665376E-14 2  
 4.16450237E+04-1.46187448E+01 5.87779106E-01 3.84323486E-02-6.61566501E-05 3  
 5.72555769E-08-1.89892637E-11 4.29066005E+04 1.74909167E+01 4.43097371E+04 4

16165-40-5

C3H2 CYCLOPROPENYLIDENE BI-RADICAL SINGLET SIGMA=2 STATWT=1 Ia=2.35340 Ib=2.4065  
 Ic=4.8941 Nu=788,887,[898,979],1063,1277,[1588,3080,3114] REF=Webbook NIST2000  
 +[] Vereecken, et al JCP 108,(1998),1068 HF298=114 kcal REF= Kiefer et.al.  
 J. Phys. Chem 101,(1997), 4057 {HF298=121.63+/-6.3 kcal REF=Melius 1988 P60V}  
 {HF298=136 kcal REF=PM3 RHF calculation} Max Lst Sq Error Cp @ 200 K 0.82%  
 C3H2(1) Cyclo T12/00C 3.H 2. 0. 0.G 200.000 6000.000 B 38.04888 1  
 5.69445684E+00 6.53821901E-03-2.35907266E-06 3.82037384E-10-2.29227460E-14 2  
 5.49264274E+04-6.96163733E+00 3.18167129E+00-3.37611741E-04 3.95343765E-05 3  
 -5.49792422E-08 2.28335240E-11 5.61816758E+04 9.06482468E+00 5.73666999E+04 4

Table 4 (continued)

117992-80-0

C3H2 (3) RAD PROPADIENYLIDENE H2C\*-CC\*. TRIPLET SIGMA=1 STATWT=2 Ia=0.2852  
 Ib=7.9457 Ic=8.23089 REF=Melius A69E Nu=3116,3030,1409,1320,956,913,615,437,  
 344 HF298=155.6 kcal REF=Kiefer et.al. JPC 101, (1997), 4057 Singlete = 127.5  
 Kcal + Vereecken et al, JCP 108, (1998), 1068 avg addition for triplet  
 {HF298=160.7 kcal.REF=Melius Database 1988 A69D} Max Lst Sq Error Cp @ 6000 K  
 0.47%

C3H2 H2C*-CC*	T12/00C	3.H	2.	0.	0.G	200.000	6000.000	B	38.04888	1
6.67324762E+00	5.57728845E-03	-1.99180164E-06	3.20289156E-10	-1.91216272E-14						2
7.57571184E+04	-9.72894405E+00	2.43417332E+00	1.73013063E-02	-1.18294047E-05						3
1.02756396E-09	1.62626314E-12	7.69074892E+04	1.21012230E+01	7.83005132E+04						4

67152-18-5

C3H2(3) RAD \*HC=C=CH\* PROP-2-VINYLLIDENE TRIPLET SIGMA=2 STATWT=2 Ia=0.075  
 Ib=8.2828 Ic=8.3057 {HF298=129.39 kcal} REF=Melius 1988 A69K  
 Nu=[3318],3265,1621,[1238,434],401,[337],246,[209] REF=Webbook NIST2000  
 +[]Vereecken, et al JCP 108, (1998), 1068 HF298=180.5 kcal REF=Kiefer et. al.  
 JPC 101, (1997), 4057 2-propargyl=87.71 kcal +92.8 kcal Vereecken et.al  
 Max Lst Sq Error Cp @ 6000 K 0.38%

C3H2 HC*=C=C*H (3)S 4/01C	3.H	2.	0.	0.G	200.000	6000.000	B	38.04888	1
7.47247827E+00	4.57765160E-03	-1.56482125E-06	2.43991965E-10	-1.42462924E-14					2
8.83321441E+04	-1.27113314E+01	3.74356467E+00	2.51955211E-02	-4.62608277E-05					3
4.34360520E-08	-1.53992558E-11	8.89297787E+04	4.22612394E+00	9.08356403E+04					4

2008-19-7

C3H2(1) RAD HCC-CH\*\* PROP-2-VINYLLIDENE SINGLET SIGMA=1 STATWT=1 Ia=0.15205  
 Ib=8.0709 Ic=8.22298 {HF298=141.43+/-2.67 kcal} REF=Melius Database 1988 A69G  
 Nu=3120,3115,1769,1195,936,784,436,319,285 HF298=195.5+/-10 kcal REF=Vereecken,  
 et al JCP 108, (1998), 1068 15 kcal above triplet Max Lst Sq Error Cp @ 6000 K  
 0.36%

C3H2 HCC-CH** (1) S 4/01C	3.H	2.	0.	0.G	200.000	6000.000	B	38.04888	1
6.74647935E+00	5.43300689E-03	-1.92072371E-06	3.06675624E-10	-1.82157001E-14					2
9.59157420E+04	-1.02270830E+01	2.87526884E+00	1.99235624E-02	-2.41971222E-05					3
1.66378231E-08	-4.69230977E-12	9.68191728E+04	8.88674315E+00	9.83788582E+04					4

207602-02-6

C3H2F3 1,1,1-Trifluoro-2-propylene-3-yl CF3-CH=CH\* SIGMA=1 STATWT=2  
 IA=15.3778 IB=27.8501 IC=28.3454 Ir=2.398804 ROSYM=3 V(3)=1133 cm-1  
 Nu=3285,3106,1711,1306,1296,1188,1175,903,854,780,718,619,541,520,430,330,251  
 HF298=-376.895 kJ HF0=-369.47 kJ REF=Burcat.G3B3 calculat. {HF298=90.96 kcal  
 REF=Liu et al J. Org. Chem 63, (1998), 3590}. Max Lst Sq Error Cp @ 6000 K 0.36%  
 C3H2F3 CF3-CH=C A10/04C 3.H 2.F 3. 0.G 200.000 6000.000 B 95.04319 1  
 1.27774168E+01 7.93163451E-03 -2.88750413E-06 4.67651599E-10 -2.80481227E-14 2  
 -5.02306417E+04 -3.79660841E+01 6.81987133E-01 4.69264463E-02 -4.86400872E-05 3  
 2.20469507E-08 -2.75414626E-12 -4.72313621E+04 2.29560885E+01 -4.53297573E+04 4

207602-03-7

C3H2F3 TrifluoroAllyl Radical CF3-C\*=CH2 SIGMA=3 STATWT=2 IA=15.1017  
 IB=29.4580 IC=29.6337 Ir=2.055274 ROSYM=3 V(3)=1133. cm-1 Nu=3203,3103,  
 1777,1437,1239,1203,1174,1016,932,805,636,595,545,479,415,324,198  
 HF298=-89.613+/-1.9 kcal HF0=-87.91 kcal REF=Burcat G3B3 calc {HF298=-90.22  
 kcal REF=Liu et al J. Org. Chem 63, (1998), 3590}. Max Lst Sq Error Cp @ 1300 K  
 0.38%

C3H2F3 CF3C*=CH2 A10/04C	3.H	2.F	3.	0.G	200.000	6000.000	B	95.04319	1
1.25859962E+01	8.12317961E-03	-2.95982852E-06	4.80631726E-10	-2.89086264E-14					2
-4.99277916E+04	-3.65971752E+01	1.34293581E+00	4.37082126E-02	-4.41291023E-05					3
1.98066011E-08	-2.52757681E-12	-4.70859152E+04	2.02494155E+01	-4.50947551E+04					4

Table 4 (continued)

203455-97-4

C3H2N CYANO-ETHYLENE RADICAL HC\*=CH-CN SIGMA=1 STATWT=2 IA=1.2735 IB=16.6759  
 IC=17.9494 Ir=0.0028296 V(3)=0. ROSYM=1 Nu=3280,3087,2352,1661,1274,1018,835,  
 801,701,557,374 HF298=442.855 kJ HF0=445.486 kJ REF=Burcat G3B3 calc  
 {HF298=97. kcal REF= MACKIE & COLKET 22nd COMBUST SYMP. 1990} Max Lst Sq Error  
 Cp @ 6000 0.43%

C3H2N CH=CHCN	A12/04C	3.H	2.N	1.	0.G	200.000	6000.000	B	52.05472	1
6.99670220E+00	7.50618110E-03	-2.68300369E-06	4.31684490E-10	-2.57821318E-14						2
5.04796219E+04	-1.01552187E+01	2.15324611E+00	2.06638717E-02	-1.33975241E-05						3
7.77214839E-10	2.02897347E-12	5.18184058E+04	1.48728946E+01	5.32629680E+04						4

2932-78-7

C3H3 RAD STATWT=2. SIGMA=2. IA=.29055 IB=8.8826 IC=9.16487 NU=3264,3081,  
 2990,1912,1390,1007,930,607,585,449,364,331 REF=Kumaran et.al. Israel J. Chem,  
 36, (1996),223 HF298=346. kJ REF=TSANG, Int. J. Chem. Kinet 10 (1978),687  
 Max Lst Sq Error Cp @ 6000 K 0.39%

C3H3 PROPARGYL	T 5/97C	3.H	3.	0.	0.G	200.000	6000.000	B	39.05682	1
7.14221880E+00	7.61902005E-03	-2.67459950E-06	4.24914801E-10	-2.51475415E-14						2
3.89087427E+04	-1.25848435E+01	1.35110927E+00	3.27411223E-02	-4.73827135E-05						3
3.76309808E-08	-1.18540923E-11	4.01057783E+04	1.52058924E+01	4.16139977E+04						4

7747-84-4

C3H3Cl 1-CHLORO,1-PROPYNE Cl-CC-CH3 SIGMA=3 STATWT=1 Ia=0.5250 Ib=Ic=37.9661  
 No Internal Rotation Nu=3106.7(2),3044,2361,1507(2),1445,1102,1070(2),585,  
 336(2),191(2) HF298=184.7 kJ HF0=189.55 kJ S298=283.82 J REF=Burcat G3B3  
 calc {S298=283.96 J REF=STULL WESTRUM & SINKE 1969; HF298=35.2 KCAL REF=NIST 94}  
 Max Lst Sq Error Cp @ 1300 K 0.49%

C3H3Cl 1 Chloro	A01/05C	3.H	3.CL	1.	0.G	200.000	6000.000	B	74.50862	1
7.44950828E+00	1.02120055E-02	-3.65216636E-06	5.87697151E-10	-3.50986872E-14						2
1.91733144E+04	-1.20833043E+01	4.62329724E+00	1.34961392E-02	1.78124553E-06						3
-9.69193752E-09	4.35320141E-12	2.02385699E+04	3.76810011E+00	2.22155061E+04						4

624-65-7

C3H3Cl 3-CHLORO,1-PROPYNE H-CC-CH2Cl SIGMA=1 IA=3.42022 IB=27.5776  
 IC=30.49975 NU=3339,3048,2990,2051,1442,1283,1174,937,898,727,553,533,407,229,  
 151 HF0=40.10 KCAL REF=Kumaran et.al. ISRAEL J. Chem 36, (1996),223 Max Lst  
 Sq Error Cp @ 6000 K 0.43%

C3H3Cl CH2Cl-CCH	T 5/97C	3.H	3.CL	1.	0.G	200.000	6000.000	B	74.50952	1
8.60964894E+00	9.12088266E-03	-3.24810521E-06	5.21296691E-10	-3.10793797E-14						2
1.61738376E+04	-1.69659939E+01	2.49757092E+00	2.75585732E-02	-2.33670745E-05						3
8.99167349E-09	-7.08099389E-13	1.77912033E+04	1.42223355E+01	1.95717345E+04						4

17336-56-0

C3H3Cl 3-CHLOROCYCLOPROPENE SIGMA=1 IA=3.9183 IB=21.13565 IC=22.3311  
 NU=3201,3161,3061,1602,1289,1164,1036,1025,916,854,804,708,572,348,344  
 HF0=53.88 kcal REF=Kumaran et.al. ISRAEL J. Chem 36, (1996),223 Max Lst Sq  
 Error Cp @ 200 K 0.54%

3-C3H3Cl CY	T 5/97C	3.H	3.CL	1.	0.G	200.000	6000.000	B	74.50952	1
8.70661016E+00	9.10661478E-03	-3.26153884E-06	5.25606764E-10	-3.14309766E-14						2
2.26426992E+04	-1.98513212E+01	1.38549419E+00	2.36867059E-02	4.57822305E-07						3
-2.34745441E-08	1.29903835E-11	2.48296574E+04	1.90259812E+01	2.62593301E+04						4

Table 4 (continued)

3223-70-9

C3H3Cl CHLOROALLENE CHCl=C=CH2 SIGMA=1 IA=2.57347 IB=29.7692 IC=31.7616  
 NU=3130,3111,3041,1954,1428,1260,1085,985,858,833,766,550,490,294,175 HF0=39.86  
 kcal REF=Kumaran et.al. ISRAEL J Chem 36,(1996),223 Max Lst Sq Error Cp @  
 6000 K 0.48%

C3H3Cl CHCl=C=CH2 T 5/97C 3.H 3.CL 1. 0.G 200.000 6000.000 B 74.50952	1
8.48868205E+00 9.30781907E-03-3.33392517E-06 5.37178372E-10-3.21149115E-14	2
1.58981402E+04-1.72834335E+01 2.17876528E+00 2.46488928E-02-1.08872907E-05	3
-6.58963705E-09 5.61690902E-12 1.77072077E+04 1.57028855E+01 1.93458135E+04	4

38784-58-6

C3H3F2 1,1 DifluoroAllyl Rad CF2\*-CH=CH2 SIGMA=1 STATWT=2 Ia=8.2253  
 Ib=20.9713 Ic=29.1966 Ir=2.49336 ROSYM=2 (V(3)=4442. cm-1 REF=Nicolaides  
 Borden JACS 114,(1992),8682) Nu=3202,3102,1778,1436,1239,1203,1174,1015,932,  
 804,636,595,545,479,415,322,195 HF298=-224.44 HF0=-216.93 kJ REF=Burcat  
 G3B3 calc Max Lst Sq Error Cp @ 6000 K 0.5%

C3H3F2 *CF2CH=CH2 A10/04C 3.H 3.F 2. 0.G 200.000 6000.000 B 77.05273	1
1.20299701E+01 9.70691401E-03-3.73228917E-06 6.22509253E-10-3.79752625E-14	2
-3.17722163E+04-3.50037599E+01 1.41349839E+00 4.11613237E-02-3.70006458E-05	3
1.39241732E-08-9.09220613E-13-2.89446642E+04 1.92959205E+01-2.69935484E+04	4

677-21-4

C3H3F3 3,3,3-TriFluoroPropene CF3-CH=CH2 SIGMA=1 STATWT=1 IA=15.6158  
 IB=28.6947 IC=29.4268 Ir=4.12557 V(3)=1133. cm-1 ROSYM=3 Nu=3270,3209,3184,  
 1746,1476,1338,1311,1204,1189,1040,1025,990,815,722,631,541,510,428,315,273  
 HF298=-631.13 +/-6. kJ HF0=-619.512 kJ REF=Burcat G3B3 calc. {exper HF298=  
 -614.2+/-6.7 kJ REF=Kolesov Martinov Skuratov Zh Fiz Khim 41, (1967),913}  
 Max Lst Sq Error Cp @ 6000 K 0.44%

C3H3F3 CF3-CH=CH2 A10/04C 3.H 3.F 3. 0.G 200.000 6000.000 B 96.05113	1
1.22166309E+01 1.11177411E-02-4.07566929E-06 6.63454514E-10-3.98729557E-14	2
-8.08780489E+04-3.63340348E+01 1.56834820E+00 3.70715693E-02-1.66534622E-05	3
-1.15669918E-08 9.46282072E-12-7.78570098E+04 1.92579065E+01-7.59072147E+04	4

659-86-9

C3H3I Propargyl-Iodide HCC-CH2I ROSYM=1 STATWT=1 IA=4.2629 IB=50.5553  
 IC=54.2860 Nu=3335,3008,2958,2130,1423,1160,1116,959,810,640(2),570,364,314,157  
 REF=Evans & Nyquist Spectrochim. Acta 19,(1963),1153 + Shimanouchi  
 HF0=66.05+/-3 kcal REF=R. Sivaramakrishnan priv com (average of 18 DFT calc)  
 {HF298=62.5 kcal REF=NIST 94} Max Lst Sq Error Cp @ 6000 K 0.42%.

C3H3I HCC-CH2I A08/05C 3.H 3.I 1. 0.G 200.000 6000.000 B 165.96039	1
8.77076155E+00 8.97879849E-03-3.19709416E-06 5.13045142E-10-3.05841243E-14	2
2.89209233E+04-1.61953422E+01 1.77065981E+00 3.23171844E-02-3.30028158E-05	3
1.72548900E-08-3.30499156E-12 3.06564929E+04 1.89621093E+01 3.23617735E+04	4

2936-44-9

C3H3I Allenyl-Iodide CH2=C=CHI ROSYM=1 STATWT=1 IA=3.2635 IB=53.3694  
 IC=56.0567 Nu=3070(2),3004,1425,1178,1076,995,854,807,625,609,485,387,154  
 REF=Nyquist, Lo, Evans Spectrochim. Acta 20,(1964),619 + Shimanouchi  
 HF0=65.04+/-3 kcal REF=R. Sivaramakrishnan priv com (average of 18 DFT calc)  
 {HF298=65.0 kcal REF=NIST 94} Max Lst Sq Error Cp @ 6000 K 0.45%.

C3H3I CH2=C=CHI A08/05C 3.H 3.I 1. 0.G 200.000 6000.000 B 165.96039	1
8.61889065E+00 9.23264155E-03-3.31619693E-06 5.35302881E-10-3.20432212E-14	2
2.82781947E+04-1.61650316E+01 1.56192699E+00 2.90621358E-02-2.07764182E-05	3
2.89078143E-09 2.30016897E-12 3.01851729E+04 2.01151502E+01 3.17658226E+04	4

Table 4 (continued)

107-13-1

C3H3N CYANO ETHYLENE (ACRYLONITRILE) H2C=CH-CN SIGMA=1 STATWT=2 IA=1.6625  
 IB=17.0159 IC=18.6784 Ir=9.9136E-04 ROSYM=1 V(3)=0. Nu=3274,3196,3184,2349,  
 1696,1463,1332,1119,1008,980,890,713,578,356 HF298=184.037 kJ HF0=190.96 kJ  
 {HF298=43.9 KCAL REF=MACKIE & COLKET 22nd COMBUSTION SYMP 1990} Max Lst Sq  
 Error Cp @ 6000 0.50%

C3H3N	CH2=CHCN	A12/04C	3.H	3.N	1.	0.G	200.000	6000.000	B	53.06266	1
6.52096861E+00	1.05028771E-02	-3.73734374E-06	5.99498117E-10	-3.57283503E-14							2
1.92525453E+04	-9.59580896E+00	3.04396646E+00	1.05333467E-02	1.96574996E-05							3
-3.42001077E-08	1.48155667E-11	2.06456740E+04	1.05816246E+01	2.21344883E+04							4

72241-20-4

C3H3O ACROLEIN RADICAL CH2=CH-C\*=O STATWT=2 SIGMA=1 IA=1.3827 IB=18.0831  
 IC=19.4658 Ir=1.45434 ROSYM=1 [V(3)=200 cm-1 est] Nu=3263,3177,3139,1904,  
 1691,1442,1302,1118,1101,1014,1044,894,639,541,307 HF298=88.53 kJ REF=Janoschek  
 Rossi Int J. Chem Kinet. 36 (2004), {HF298=17.3 kcal REF=McMillan &  
 Golden Ann Rev. Phys. Chem 33, (1982), 493.} Max Lst Sq Error Cp @ 6000 K 0.51%

C3H3O	CH2=CHC*O	A10/04C	3.H	3.O	1.	0.G	200.000	6000.000	B	55.05532	1
6.90703955E+00	1.02341927E-02	-3.65649593E-06	5.87914100E-10	-3.51359226E-14							2
7.62708561E+03	-7.29856114E+00	4.11237192E+00	5.05829116E-03	3.17832265E-05							3
-4.55489258E-08	1.86325507E-11	8.99713585E+03	1.01743843E+01	1.06476509E+04							4

210548-95-1

C3H3O Acrolein Radical \*CH2-CH=CO SIGMA=1 STATWT=2 IA=1.6435 IB=18.0834  
 IC=19.7269 Ir=0.28398 ROSYM=2 V(3)=270 cm-1 Nu=3302,3202,3177,2189,1503,  
 1401,1186,1108,931,720,643,531,377,300 HF298=93.56 kJ REF=Janoschek Rossi  
 Int. J. Chem Kinet 36 (2004), Max Lst Sq Error Cp @ 6000 K 0.43%.

C3H3O	CH2-CH=C=O	A10/04C	3.H	3.O	1.	0.G	200.000	6000.000	B	55.05532	1
7.69322269E+00	9.37928910E-03	-3.31475709E-06	5.29225760E-10	-3.14360567E-14							2
8.15590313E+03	-1.21011994E+01	3.13639619E+00	1.99890906E-02	-7.99294937E-06							3
-4.77227085E-09	3.89527783E-12	9.50725768E+03	1.18910245E+01	1.12526174E+04							4

74-99-7

H4C3 PROPYNE STATWT=1. SIGMA=3. IA=.5283 IB=IC=9.8172 NU=3334,2918,2142,  
 1382,931,3008(2),1452(2),1053(2),633(2),328(2) REF=SHIMANOUCI HF298=44.319  
 kcal REF=TRC(API #44). {HF298=185.210+/-0.69 kJ REF=ATcT A} MAX LST SQ  
 ERROR CP @ 1300K 0.59%.

H4C3	PROPYNE	T 2/90H	4C	3	0	OG	200.000	6000.000	B	40.06476	1
0.60252400E+01	0.11336542E-01	-0.40223391E-05	0.64376063E-09	-0.38299635E-13							2
0.19620942E+05	-0.86043785E+01	0.26803869E+01	0.15799651E-01	0.25070596E-05							3
-0.13657623E-07	0.66154285E-11	0.20802374E+05	0.98769351E+01	0.22302059E+05							4

463-49-0

C3H4 ALLENE STATWT=1. SIGMA=4. IA=.555 IB=IC=9.4389 NU=3015,1443,1073,  
 865,3007,1957,1398,3086(2),999(2),841(2),355(2) REF=SHIMANOUCI HF298=190.92 kJ  
 REF=TRC(1988). {HF298=190.297+/-1.kJ REF=ATcT A} MAX LST SQ ERROR Cp @  
 1300K 0.3%.

C3H4	ALLENE	L 8/89C	3H	4	0	OG	200.000	6000.000	B	40.06476	1
0.63168722E+01	0.11133728E-01	-0.39629378E-05	0.63564238E-09	-0.37875540E-13							2
0.20117495E+05	-0.10995766E+02	0.26130445E+01	0.12122575E-01	0.18539880E-04							3
-0.34525149E-07	0.15335079E-10	0.21541567E+05	0.10226139E+02	0.22962267E+05							4

Table 4 (continued)

2781-85-3

C3H4 CYCLOPROPENE STATWT=1 SIGMA=2 IA=2.792 IB=3.846 IC=6.085 NU=3152,  
 2909,1653,1483,1105,905,996,815,3116,1043,1011,769,2995,1088,569 REF=YUM &  
 EGGERS JPC 83, (1979), 501 HF298=277.1 kJ HF0=285.82 kJ REF=Dorofeeva,  
 Gurvich & Jorish JPCRD 15 (1986) 437. {HF298=277.19+/-2.46 kJ REF=ATcT A}  
 MAX LST SQ ERROR Cp @ 200 K \*\*1.02%\*\*\*.  
 C3H4, cyclo- g 5/90C 3.H 4. 0. 0.G 200.000 6000.000 B 40.06386 1  
 6.28078872E+00 1.12393798E-02-4.01957416E-06 6.46920405E-10-3.86433056E-14 2  
 3.03415080E+04-1.11420363E+01 2.24666571E+00 5.76237942E-03 4.42080338E-05 3  
 -6.62906810E-08 2.81824735E-11 3.21284389E+04 1.33451493E+01 3.33272797E+04 4

N/A

C3H4CL 3-CHLOROPROPENYL-1 (\*CH=CH-CH2CL) SIGMA=1 STATWT=2 IA=3.7226 IB=29.1756  
 IC=30.0056 Ir=2.799 ROSYM=3 [V(3)=1341. cm-1 from Burcat's CH3-CH2CL]  
 Nu=3259,3173,3144,3103,1682,1505,1318,1282,1190,1057,944,884,839,724,634,371,294  
 HF298=250.253 kJ HF0=259.680 kJ {HF298=56.3 KCAL REF=Weismann & Benson Prog  
 Energy Comb. Sci 15, (1989), 273} Max Lst Sq Error Cp @ 200 K 0.51%.  
 C3H4Cl Burcat A 1/05C 3.H 4.CL 1. 0.G 200.000 6000.000 B 75.51656 1  
 8.99997348E+00 1.08934778E-02-3.85998654E-06 6.13698724E-10-3.62944135E-14 2  
 2.63367200E+04-1.92754080E+01 2.84325299E+00 1.88013644E-02 1.44431707E-05 3  
 -3.74591048E-08 1.79821858E-11 2.83529496E+04 1.43805597E+01 3.00983952E+04 4

34853-20-8

C3H4CL 1-CHLOROALLYL (CHCL=CH-CH2\*) SIGMA=1 STATWT=2 IA=1.8366 IB=32.3206  
 IC=34.1572 Ir(CH2\*)=0.2781 ROSYM=2 V(3)=272 cm-1 est Nu=3270,3237,3180,3175,  
 1539,1471,1294,1289,1217,1019,990,809,788,662,541,432,264 HF298=137.444 kJ  
 HF0=147.12 kJ REF=Burcat G3B3 calc {HF298=25.6 KCAL. REF=Weisman & Benson  
 Prog Energy Comb. Sci 15, (1989), 273} Max Lst Sq Error Cp @ 6000 K 0.45%.  
 ClC3H4 Burcat A 2/05C 3.H 4.CL 1. 0.G 200.000 6000.000 B 75.51656 1  
 8.44848616E+00 1.13179396E-02-3.99885260E-06 6.38428093E-10-3.79250140E-14 2  
 1.29285877E+04-1.62575139E+01 3.16995308E+00 1.57436972E-02 1.85511623E-05 3  
 -3.88261489E-08 1.77294125E-11 1.47902471E+04 1.32175604E+01 1.65306675E+04 4

3264-99-1

C3H4N 2-PROPIONITRILE RADICAL CH3-CH\*CN STATWT=2 SIGMA=1 IA=2.1315 IB=18.4528  
 IC=20.0640 Ir(CH3)=0.5065 ROSYM=3 [V(3)=1087 cm-1 REF=East & Radom JCP 106,  
 (1997), 6655] Nu=3199,3149,3071,3028,2152,1519,1500,1432,1401,1153,1112,1011,  
 868,591,575,426,223 HF298=222.71 kJ HF0=232.213 kJ REF=Burcat G3B3 calc.  
 Max Lst Sq Error Cp @ 6000 K 0.49%  
 C3H4N CH3-CH\*-CN A01/05C 3.H 4.N 1. 0.G 200.000 6000.000 B 54.07060 1  
 7.65917674E+00 1.21423335E-02-4.32088899E-06 6.93007104E-10-4.12936689E-14 2  
 2.34859398E+04-1.34087027E+01 2.90886208E+00 2.10250151E-02-3.11710857E-06 3  
 -1.06743259E-08 5.98989202E-12 2.50292497E+04 1.22020513E+01 2.67852167E+04 4

288-32-4

C3H4N2 1,3-DIAZOLE, IMIDAZOLE, GLYOXALINE SYMNO=1 IA=8.4525 IB=8.7054  
 IC=17.1579 NU=3501,3103,3077,3075,1558,1487,1418,1344,1260,1123,1102,1064,1034,  
 912,892,879,862,749,655,619,478 HF298=33.69 KCAL REF=C. MELIUS DATABASE  
 BACMP22 #38 P1TZ Max Lst Sq Error Cp @ 6000 K \*\*1.04%\*\*  
 C3H4N2 1,3-DIAZOLET 9/96C 3H 4N 2 0G 200.000 6000.000 B 68.07824 1  
 0.92025957E+01 0.14142668E-01-0.51071395E-05 0.82778679E-09-0.49706044E-13 2  
 0.12518192E+05-0.26079671E+02 0.13020933E+01 0.11479286E-01 0.60444678E-04 3  
 -0.95013016E-07 0.40803163E-10 0.15689407E+05 0.20116256E+02 0.16953369E+05 4



Table 4 (continued)

97645-24-4

C3H4N4O6 1,3,3-Tri-Nitro-Azetidine SYMNO = 2 STATWT = 1 IA = 60.59091  
 IB = 147.3316 IC = 169.6545 Ir(NO2) = 5.96 ROSYM = 2 V(2) = 12.5 kcal/mole  
 3036,3021,2973,2900,1589(2),1538,1510,1428,1403,1380,1365,1340,1325,1280,  
 1216,1200,1183,1172,1113,1085,1057(2),906,865(2),843(2),816,761(2),712,662(2),  
 626(3),601,564(3),480(2),162. REF = Yu, Zhang & Bauer, (THEOCHEM)15, (1998), 5846  
 HF298 = 26.22 +/- 1. kcal REF = Wilcox, Zhang & Bauer (Theochem)538, (2001), 67-72.  
 {HF298 = 30.7 kcal REF = Politzer et al J. Molec Struct (THEOCHEM)338, (1995),  
 249.} Max Lst Sq Error Cp @ 200 K 0.98%  
 1,3,3 TRI-NITRO- S03/01C 3.H 4.N 4.O 6.G 200.000 6000.000 B 192.08812 1  
 2.22004023E+01 2.61448557E-02-1.00734632E-05 1.69575778E-09-1.04302158E-13 2  
 2.69785949E+03-9.72924159E+01-3.22895573E+00 6.02068540E-02 4.89990294E-05 3  
 -1.24714696E-07 5.86010192E-11 1.12669368E+04 4.22296092E+01 1.31943410E+04 4

107-02-8

C3H4O 2-PROPENAL, ACROLEIN, ACRYLALDEHYDE CH2=CH-CHO SIGMA=1 STATWT=1  
 IA=1.7491 IB=18.1314 IC=19.8805 Ir=1.61967 ROSYM=1 (V(3)=200 cm-1 est.)  
 REF=Burcat G3B3 Nu=3103,3028,3000,2800,1724,1625,1420,1360,1275,1158,912,564,  
 327,993,980,959,593,157 REF=Shimanuchi, HF298=-68.065 kJ HF0=-57.913 kJ  
 {HF298=-17.8 +/- 0.3 kcal REF=NIST 94} Max Lst Sq Error Cp @ 6000 K 0.57%  
 C3H4O CH2=CH-CHO A10/04C 3.H 4.O 1. 0.G 200.000 6000.000 B 56.06326 1  
 7.31820729E+00 1.27398510E-02-4.60112009E-06 7.44735077E-10-4.46993049E-14 2  
 -1.16137229E+04-1.11884734E+01 3.98487241E+00 3.40751550E-03 4.81227535E-05 3  
 -6.61399005E-08 2.67817331E-11-9.83297241E+03 1.03960574E+01-8.18632872E+03 4

79-10-7

C3H4O2 Acrylic Acid CH2=CH-C(O)-OH SIGMA=1 STATWT=1 IA=7.6170 IB=19.8062  
 IC=27.4232 Ir(-C(O)-OH)=2.4506 ROSYM=1 [V(3)=2575 cm-1 REF=Baaden, Granger &  
 Strich Molec. Phys. 98, (200), 329-342] Ir(OH)=0.14576 ROSYM=1 V(3)=1100 cm-1  
 est. Nu=3692,3268,3213,3178,1715,1464,1380,1306,1180,1084,1031,1001,846,  
 824,666,622,492,487 HF298=-326.051 kJ HF0=-312.517 kJ REF=Burcat G3B3 calc  
 Max Lst Sq Error Cp @ 6000 K 0.47%.  
 C3H4O2 CH2=CH-C A01/05C 3.H 4.O 2. 0.G 200.000 6000.000 B 72.06266 1  
 1.04962923E+01 1.20559957E-02-4.34149310E-06 6.99425892E-10-4.18003976E-14 2  
 -4.37332461E+04-2.75425657E+01 1.24227207E+00 3.00698605E-02-1.48206586E-06 3  
 -2.42738150E-08 1.33121686E-11-4.08667843E+04 2.19242842E+01-3.92146683E+04 4

1981-80-2

C3H5 ALLYL RAD SYMMETRIC STABILIZED BY RESONANCE CH2-C\*H-CH2 STATWT=2 SIGMA=2  
 IA=1.52057 IB=8.20036 IC=9.70572 REF=Nicolaides & Borden JACS 114, (1992), 8682  
 NU=3107(2),3051,3021,3019,1477,1463,1389,1242,1184,1005,983,913,801,738,517,510,  
 418 REF=Sim, Shaub, Chin, Dupuis JCP 95, (1991), 4315 HF298=39.1 Kcal  
 REF=Wu & Kern JPC 91 (1987), 6291 Max Lst Sq Error Cp @ 200 K 0.57%.  
 C3H5 SYMMETRIC T 9/96C 3H 5 0 OG 200.000 6000.000 B 41.07270 1  
 0.70094568E+01 0.13106629E-01-0.46533442E-05 0.74514323E-09-0.44350051E-13 2  
 0.16412909E+05-0.13946114E+02 0.14698036E+01 0.19034365E-01 0.14480425E-04 3  
 -0.35468652E-07 0.16647594E-10 0.18325831E+05 0.16724114E+02 0.19675772E+05 4

Table 4 (continued)

15552-77-9

C3H5 TERTIARY NONSYMMETRIC RAD (CH<sub>2</sub>=C\*CH<sub>3</sub>) STATWT=2. SIGMA=1. IA=1.2558815  
 IB=10.379297 IC=11.08304 NU=315,470.8,834.5,836,911.6,1018.8,1090.8,1356,1390,  
 1435,1448,1507,2830,2888,2902.5,2906.8,2999.7 IR=0.3945E-39 [V3=17.7 Kcal.  
 REF= Nicolaides & Borden JACS 114 (1992),8682] ROSYM=3.  
 REF=Ab-Initio Calculat. Karni, Oref & Burcat TAE #643 1989. HF298=56.8 Kcal  
 REF=Wo & Kern JPC 91 (1987),6291 Max Lst Sq Error Cp @ 6000 K 0.61%.  
 T-C3H5 CH3C\*=CH2 T 6/96C 3H 5 0 OG 200.000 6000.000 B 41.07270 1  
 0.61101805E+01 0.14673395E-01-0.53676822E-05 0.86904932E-09-0.51932006E-13 2  
 0.25532442E+05-0.83555712E+01 0.25544033E+01 0.10986798E-01 0.30174305E-04 3  
 -0.47253568E-07 0.19771073E-10 0.27150242E+05 0.13207592E+02 0.28582707E+05 4

6067-68-1

C3H5 SECONDARY RAD (CH<sub>3</sub>-CH=CH\*) ALLYL RADICAL SIGMA=1 STATWT=2 IA=1.4621  
 IB=8.8517 IC=9.7923 Ir=0.4336 ROSYM=3 [V3=705.5 cm<sup>-1</sup> REF=East & Radom JCP  
 106, (1997), 6655]. Nu=3258,3141,3091,3042,3033,1705,1514(2),1431,1288,1125,1074,  
 941,813,807,613,408 HF298=63.464 kcal HF0=66.33 kcal REF=Burcat G3B3 calc.  
 {HF298=62.8 Kcal REF=Wo & Kern JPC 91 (1992),6291} Max Lst Sq Error Cp @ 6000  
 K 0.59%.  
 C3H5 CH3CH=CH\* A12/04C 3.H 5. 0. 0.G 200.000 6000.000 B 41.07180 1  
 6.05091412E+00 1.34052084E-02-4.73450586E-06 7.55380897E-10-4.48421084E-14 2  
 2.90860210E+04-6.73692060E+00 3.33277282E+00 1.06102499E-02 2.17559727E-05 3  
 -3.47145235E-08 1.44476835E-11 3.03404530E+04 9.78922358E+00 3.19361425E+04 4

2417-82-5

C3H5 Cyclopropyl Radical STATWT=2 SIGMA=2 IA=3.5282671 IB=3.97392 IC=6.28245  
 NU=3042,3007,2994,2938,2933,1469,1432,1196,1150,1098,1080,1063,1044,899,831,764,  
 756,628 REF=Melius H4 HF298=66.9+/-2.5 REF=McMillen & Golden { HF298=69.29  
 REF=Melius H4} Max Lst Sq Error Cp @ 200 K \*\*1.25%\*\* @ 6000 K 0.55%.  
 C3H5 Cyclopropyl T02/03C 3.H 5. 0. 0.G 200.000 6000.000 B 41.07180 1  
 6.62512238E+00 1.36577057E-02-4.90066661E-06 7.90436486E-10-4.72860275E-14 2  
 3.03239999E+04-1.31845240E+01 2.15143774E+00 3.80171682E-03 6.14538989E-05 3  
 -8.83383102E-08 3.70565687E-11 3.24689062E+04 1.48309194E+01 3.36651949E+04 4

16136-85-9

C3H5Cl 1-Chloro-1-PrpeneE CHCl=CH-CH<sub>3</sub> SIGMA=1 STATWT=1 IA=2.0138 IB=34.8215  
 IC=36.3150 Ir=0.50042 ROSYM=3. [V(3)=752. cm<sup>-1</sup> REF=CH<sub>3</sub>-C<sub>2</sub>H<sub>3</sub> East & Radom JCP  
 106, (1997), 6655]. Nu=3227,3182,3125,3089,3039,1718,1519,1509,1444,1334,1289,  
 1125,1076,973,969,801,774,422,261,238 HF298=-8.100 kJ HF0=+4.937 kJ REF=Burcat  
 G3B3 calc {HF298=-12. kJ REF=Benson et al J Chem Thermo 5, (1973),411} Max Lst  
 Sq Error Cp @ 6000 K 0.52%.  
 C3H5Cl Burcat A 1/05C 3.H 5.CL 1. 0.G 200.000 6000.000 B 76.52450 1  
 7.93779996E+00 1.44893887E-02-5.14735839E-06 8.24668950E-10-4.91034104E-14 2  
 -4.57303808E+03-1.47604433E+01 4.42267408E+00 1.07886267E-02 2.92262847E-05 3  
 -4.48388716E-08 1.84566819E-11-2.95068417E+03 6.62986035E+00-9.74227465E+02 4

107-05-1

C3H5Cl 3-CHLORO-1-PROPENE-1 CH<sub>2</sub>=CH-CH<sub>2</sub>Cl SIGMA=1 STATWT=1 IA=3.9170 IB=30.624  
 IC=31.5649 Ir=2.9602 ROSYM=1 [V(3)=1341.cm<sup>-1</sup> REF=Ruscic & Burcat Unpublished]  
 Nu=3247,3183,3164,3159,3101,1729,1514,1470,1339,1302,1239,1129,1032,960,956,916,  
 738,595,405,284 HF298=0.369 kJ (0.0883 kcal) HF0=14.052 kJ REF=Burcat G3B3  
 calc {HF298=-6.4 kcal REF>Weismann & Benson estim. Prog.Energy Combust. Sci.  
 15, (1989),273} Max Lst Sq Error Cp @ 200 K 0.60%.  
 C3H5Cl CH<sub>2</sub>=CHCH<sub>2</sub>ClA 1/05C 3.H 5.CL 1. 0.G 200.000 6000.000 B 76.52450 1  
 8.52439580E+00 1.39387683E-02-4.94599494E-06 7.87953151E-10-4.66709395E-14 2  
 -3.80684034E+03-1.71514162E+01 3.46378742E+00 1.13302404E-02 4.01782107E-05 3  
 -6.44060622E-08 2.76922751E-11-1.73265523E+03 1.26490551E+01 4.44340075E+01 4

Table 4 (continued)

107-12-0

C3H5N ETHYL-CYANIDE (PROPIONITRILE) C2H5CN SIGMA=1 STATWT=1 IA=3.0049  
 IB=18.0447 Ir(CH3)=0.5117 ROSYM=3 [V(3)=1076 cm<sup>-1</sup> REF=Ruscic & Burcat]  
 Nu=3148,3144,3094,3070,3059,2350,1534,1526,1501,1440,1366,1301,1127,1103,1021,  
 845,796,549,397,224 HF298=12.71 kcal HF0=16.00 kcal REF=Burcat G3B3 calc.  
 {HF298=12.1 kcal REF=Stul Westrum & Sinke 1969; HF298=12.3 kcal REF=NIST  
 Webbook} Max Lst Sq Error Cp @ 1300 K 0.57%.  
 C3H5N Propionit A 1/05C 3.H 5.N 1. 0.G 200.000 6000.000 B 55.07854 1  
 7.04418234E+00 1.53008159E-02-5.44095595E-06 8.72156064E-10-5.19455789E-14 2  
 3.05885503E+03-1.15133490E+01 3.62429314E+00 1.26256761E-02 2.47719570E-05 3  
 -3.99054512E-08 1.66077777E-11 4.60780029E+03 9.10669692E+00 6.39739347E+03 4

3156-70-5

C3H5NO2 Nitro-Propylene STATWT = 1 IA = 9.5524 IB = 30.9429 IC = 39.9889  
 Ir(NO2) = 5.96 ROSYM = 2 V(2) = 1.5 kcal Ir(CH3) = 0.5166 ROSYM = 3  
 V(3) = 8.8 kcal NU = 3091,3001,2954,2954,2888,1696,1629,1477,1457,1448,  
 1400,1354,1228,1081,1072,971,955,887,831,762.655,575,382,362,223.  
 HF298 = 2.387 kcal REF = Melius Database 1988 D85J Max Lst Sq Error Cp  
 @ 1300 K 0.67%  
 NITROPROPYLENE C T11/97C 3.H 5.N 1.O 2.G 200.000 6000.000 B 87.07824 1  
 1.16044034E+01 1.73925254E-02-6.55603780E-06 1.08945442E-09-6.64543040E-14 2  
 -4.17082639E+03-3.40158247E+01 3.65175571E+00 2.01896036E-02 3.27504513E-05 3  
 -5.72328212E-08 2.41049017E-11-9.72583112E+02 1.18667163E+01 1.20117818E+03 4

13021-02-8

C3H5NO2 Nitro-Cyclo-Propane STATWT = 1 SYMNO = 2 IA = 10.5515 IB = 28.5698  
 IC = 32.4822 Ir(NO2) = 5.96 ROSYM = 2 V(2) = 4.7 kcal/mole NU = 3103,3095,  
 3019(2),2934,1571,1443,1407,1373,1325,1202,1118,1110,1075,1042,936,921,880,854,  
 828,770,730,645,483,309,289. REF = Holtzclaw, Harris & Bush J Raman Spect 9,  
 (1980),257 + Mochel, Britt & Boggs J. Chem. Phys. 58,(1973),3221 HF298=5.027  
 kcal HF0=9.91 kcal REF=Burcat G3B3 calc {HF298= 4.2 kcal REF = Stein,  
 NIST 94} Max Lst Sq Error Cp @ 200 K 0.91%.  
 C3H5NO2 NitroCy A 2/05C 3.H 5.N 1.O 2.G 200.000 6000.000 B 87.07734 1  
 1.28563199E+01 1.60379798E-02-5.91815626E-06 9.70787117E-10-5.87172699E-14 2  
 -3.30190816E+03-4.34060874E+01 2.06484531E+00 2.06827764E-02 5.54675716E-05 3  
 -9.75079697E-08 4.31809897E-11 6.77006688E+02 1.78174435E+01 2.52967018E+03 4

55-63-0

C3H5N3O9 NG Nitroglycerine STATWT = 1 SYMNO = 2 IA = 113.023087  
 IB = 216.411718 IC = 260.003555 (Ir(NO2) = 5.96 ROSYM = 2  
 V(3) = 9.1 kcal/mole)x3 NU = 3024,3014,2953,2941,2831,2142,3132,1537,1522,  
 1363,1359,1329,1318,1303,1231,1209,1160,1151,1145,1118,1093,1085,971,928,915,798,  
 701,676,654,639,627,622,582,478,470,463,409,379,348,317,312,276, 264,232,188,173,  
 97.7,62,60,54.1,44.4 REF = BURCAT, JPCRD 29 (1999)63-130 HF298 = -66.7 kcal  
 REF = Miroshnichenko et al, Bul Acad. Sci. USSR, Chem Sci. (1988),1778.  
 Max Lst Sq Error Cp @ 1300 K 0.59%  
 NITROGLICERINE T05/98C 3.H 5.N 3.O 9.G 200.000 6000.000 B 227.08752 1  
 3.24464077E+01 2.44149769E-02-9.67605267E-06 1.65298018E-09-1.02555476E-13 2  
 -4.65896112E+04-1.31431034E+02 5.70797625E+00 9.52017978E-02-7.18228583E-05 3  
 1.66304815E-08 3.01835927E-12-3.88975467E+04 7.78535957E+00-3.35645516E+04 4

Table 4 (continued)

15843-24-0

C3H5O PROPANAL RADICAL CH<sub>3</sub>CH<sub>2</sub>\*CO SIGMA=1 STATWT=2 IA=4.5640 IB=14.4953  
 IC=18.0265 Ir(CH<sub>3</sub>)=0.51267 ROSYM=3 V(3)=272 cm<sup>-1</sup> Ir(CO)=0.35506 ROSYM=2  
 V(3)=200 cm<sup>-1</sup> Nu=3143,3133,3085,3063,3055,1928,1528,1523,1477,1435,1335,1281,  
 1095,1054,981,807,738,625,240 HF298=-32.83 kJ HF0=-19.86 kJ REF=Janoschek &  
 Rossi, Int JCK 36 (2004), {HF298 = -36.02 kJ REF=THERM; HF298=-46.86 kJ  
 REF=NIST 94} Max Lst Sq Error Cp @ 6000 K 0.58%  
 C3H5O CH<sub>3</sub>CH<sub>2</sub>\*CO A10/04C 3.H 5.O 1. 0.G 200.000 6000.000 B 57.07120 1  
 6.52325448E+00 1.54211952E-02-5.50898157E-06 8.85889862E-10-5.28846399E-14 2  
 -7.19631634E+03-5.19862218E+00 6.25722402E+00-9.17612184E-03 7.61190493E-05 3  
 -9.05514997E-08 3.46198215E-11-5.91616484E+03 2.23330599E+00-3.94851891E+03 4

3122-07-4

C3H5O ACETONE RADICAL \*CH<sub>2</sub>COCH<sub>3</sub> SIGMA=1 STATWT=2 SYMNO=1. IA=7.7005 IB=9.3110  
 IC=16.4899 IR(CH<sub>3</sub>)=0.49327 ROSYM=3 V(3)=272 cm<sup>-1</sup> Ir(CH<sub>2</sub>)=.28265 ROSYM=2  
 (V(3)=230 cm<sup>-1</sup> est). NU=3283,3172,3166,3109,3051,1609,1508,1502,1482,1418,  
 1281,1076,1038,936,822,745,523,506,383 HF298=-33.34 kJ HF0=-20.62 kJ  
 REF=Janoschek Rossi Int JCK 36 (2004), {HF298=-3.36+/-0.5 KCAL REF=THERM}  
 MAX LST SQ ERROR Cp @ 6000 0.52%.  
 C3H5O CH<sub>3</sub>C(O)CH<sub>2</sub> A10/04C 3.H 5.O 1. 0.G 200.000 6000.000 B 57.07120 1  
 7.54410697E+00 1.43443222E-02-5.08381081E-06 8.13200521E-10-4.83673315E-14 2  
 -7.48672286E+03-1.14792587E+01 4.70187196E+00 5.51653762E-03 4.27505858E-05 3  
 -5.94680816E-08 2.40685378E-11-5.92845491E+03 7.12932590E+00-4.00985747E+03 4

38139-76-3

C3H5O \*CH<sub>2</sub>-CH(-O-)CH<sub>2</sub> PROPYLENE OXIDE RADICAL SIGMA=1 STATWT=2 IA=4.3360  
 IB=12.1010 IC=13.3195 Ir=0.2828 ROSYM=2 [V(3)=272 cm<sup>-1</sup> est] Nu=3289,3184,  
 3174,3138,3088,1544,1491,1414,1260,1194,1167,1152,1085,1001,907,832,735,533,411,  
 364 HF298=104.069 kJ HF0=118.072 kJ REF=Burcat G3B3 calc {HF298=110.33 KJ  
 REF=THERM} Max Lst Sq Error Cp @ 200 K 0.64%.  
 C3H5O \*CH<sub>2</sub>C<sub>2</sub>H<sub>3</sub>O A11/04C 3.H 5.O 1. 0.G 200.000 6000.000 B 57.07120 1  
 8.15052559E+00 1.42542561E-02-5.05387276E-06 8.08732845E-10-4.81184188E-14 2  
 8.72987262E+03-1.69520239E+01 3.53458477E+00 8.02398508E-03 4.85256807E-05 3  
 -7.23549959E-08 3.03822687E-11 1.08059525E+04 1.11545728E+01 1.25165081E+04 4

115-07-1

C3H6 PROPYLENE STATWT=1 SIGMA=1 IA=1.8133 IB=9.0187 IC=10.317 IR=0.3945  
 ROSYM=3 V3=698.46 cm<sup>-1</sup> NU=3091,3022,2991,2973,2932,1653,1459,1414,1378,1298,  
 1178,935,919,428,2953,1443,1045,990,912,575 REF=CHAO & ZWOLINSKI JPCRD 4, (1975)  
 251 HF298=4.88 kcal HF0=8.4 kcal REF=TRC(API #44),1988 {HF298=20.235+/-0.41  
 kJ REF=ATcT A} MAX LST SQR ERROR Cp @ 6000 K 0.60 %.  
 C3H6 propylene g 2/00C 3.H 6. 0. 0.G 200.000 6000.000 B 42.07974 1  
 6.03870234E+00 1.62963931E-02-5.82130800E-06 9.35936829E-10-5.58603143E-14 2  
 -7.41715057E+02-8.43825992E+00 3.83464468E+00 3.29078952E-03 5.05228001E-05 3  
 -6.66251176E-08 2.63707473E-11 7.88717123E+02 7.53408013E+00 2.40543339E+03 4

75-19-4

C3H6 CYCLOPROPANE STATWT=1 SIGMA=6 IA=IB=4.1766 IC=6.6358 NU=3038,1479,  
 1188,1126,1070,3102,854,3024(2),1438(2),1029(2),867(2),3082(2),1188(2),739(2)  
 REF=SHIMANOUCI HF298=53.3 KJ REF=Dorofeeva, Gurvich & Jorish JPCRD 15 (1986),  
 437. {HF298=53.415+/-0.54 kJ REF=ATcT A} MAX LST SQ ERROR Cp @ 200 K  
 \*\*\*1.55%\*\*\* @ 6000 K 0.59%  
 C3H6 cyclo- g 1/00C 3.H 6. 0. 0.G 200.000 6000.000 B 42.07974 1  
 6.21663437E+00 1.65393591E-02-5.90075838E-06 9.48095199E-10-5.65661522E-14 2  
 2.95937491E+03-1.36041009E+01 2.83278674E+00-5.21028618E-03 9.29583210E-05 3  
 -1.22753194E-07 4.99191366E-11 5.19520048E+03 1.08306333E+01 6.41047999E+03 4

Table 4 (continued)

89167-79-3

C3H6N2O2 n-Nitro-Azetidine SYMNO = 2 STATWT = 1 IA = 17.7086 IB = 36.1404  
 IC = 47.502 Ir(NO2) = 5.96 ROSYM = 2 V(2) = 12.5 kcal NU = 2982, 2973,  
 2964, 2925, 2914, 2911, 1641, 1507, 1481, 1464, 1431, 1318, 1284, 1263, 1214, 1188, 1182, 1148,  
 1131, 1113, 946, 902, 900, 827, 822, 806, 722, 593, 475, 247, 241.7, 136.7 HF298 = 27.28 kcal  
 REF = Melius Database 1988 D90A Max Lst Sq Error Cp @ 200 K 0.78%  
 N-NITRO-AZETIDIN T11/97C 3.H 6.N 2.O 2.G 200.000 6000.000 B 102.09292 1  
 1.28386051E+01 2.27540814E-02 -8.59766661E-06 1.42856214E-09 -8.70663456E-14 2  
 7.35548462E+03 -4.36199680E+01 4.36363512E+00 7.73075634E-03 9.68585080E-05 3  
 -1.36307741E-07 5.56913572E-11 1.14684500E+04 9.18578377E+00 1.37257378E+04 4

121-82-4

C3H6N6O6 RDX 1,3,5-Triazine Solid Cp 290-345 REF = Engineering Design Handbook  
 Military Pyrotechnics Series Part One AMCP 706-185 (1967) S298 = 33.94 cal  
 Graphic Integ HF298(solid) = 18.9 Kcal REF = NIST 98 (Krien, Licht, Zierath,  
 Thermochim. Acta, 6, (1973), 465-472) Max Lst Sq Error Cp @ 293 K 0.22 %  
 RDX Solid T 4/99C 3.H 6.N 6.O 6.S 293.000 478.500 D 222.11748 1  
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2  
 0.00000000E+00 0.00000000E+00 -2.26955822E+02 2.10620186E+00 -6.38009038E-03 3  
 8.94180990E-06 -4.63001831E-09 2.44460154E+04 8.96445093E+02 9.51079498E+03 4

121-82-4

C3H6N6O6 RDX 1,3,5-Triazine STATWT = 1 SYMNO = 6 IA = 137.8906  
 IB = 137.8906 IC = 245.5315 (Ir(NO2) = 5.97 ROSYM = 2 V(2) = 16.7 kcal)x3  
 NU = 2770, 2767(2), 2688, 2684(2), 1337, 1332(2), 1295(2), 1280, 1218(2), 1207, 1181, 1180,  
 1104(2), 1097, 1081, 1042, 1027, 1012(2), 907(2), 818, 807, 806, 762, 702(2), 638, 590, 583,  
 581, 554(2), 528, 501(2), 320, 307, 303, 302, 273, 266(2), 154, 152, 91.3, 90.2, 79.03  
 REF = Wu & Fried J Chem Phys 101, (1997), 8675 HF298 = 45.89 kcal  
 REF = Pepekina et al, Bull Acad Sci USSR Chem Sci (1974), 1707 Max Lst Sq Error  
 Cp @ 6000 K 0.54%  
 RDX 135 Triazine T 6/98C 3.H 6.N 6.O 6.G 200.000 6000.000 B 222.11748 1  
 3.27884812E+01 2.84393334E-02 -1.11821531E-05 1.88280824E-09 -1.15260232E-13 2  
 9.54327013E+03 -1.42802148E+02 1.46580269E+00 1.05297168E-01 -5.23365036E-05 3  
 -2.70780427E-08 2.44647856E-11 1.84793520E+04 2.07951964E+01 2.30921606E+04 4

123-38-6

C3H6O PROPIONALDEHYDE DATA FROM Chao et al 1986 EXTRAPOLATED TO 5000 K USING  
 WILHOIT'S POLYNOMIALS. HF298 = -45.90 KCAL REF = Stull Westrum & Sinke 1969 Max  
 Lst Sq Error Cp @ 5000 K 0.37%  
 C2H5CHO T 9/92C 3H 6O 1 0G 273.150 5000.000 B 58.08004 1  
 0.33137982E+01 0.26619606E-01 -0.10475596E-04 0.18815334E-08 -0.12761310E-12 2  
 -0.25459603E+05 0.96608447E+01 0.76044596E+01 -0.86403564E-02 0.73930097E-04 3  
 -0.79687398E-07 0.28004927E-10 -0.25489789E+05 -0.67643691E+01 -0.23097645E+05 4

67-64-1

C3H6O ACETONE (CH3-CO-CH3) STATWT = 1 SIGMA = 2 IAIBIC = 1390.63E-117 (Ir = 0.4888  
 ROSYM = 3 V3 = 272 cm-1)x2  
 NU = 3019(2), 2972, 2963, 2937(2), 1731, 1454, 1435, 1426, 1410, 1364(2), 1216, 1091, 1066,  
 891, 877, 777, 530, 484, 385 REF = CHAO et. al., JPCRD 15, (1986), 1369 HF298 = -214.814  
 +/- 0.26 kJ REF = ATcT A {HF298 = -51.9 KCAL REF = CHAO & ZWOLINSKI JPCRD 5 (1976),  
 319.} Max Lst Sq Error Cp @ 6000 0.6%  
 C3H6O Acetone ATcT AC 3.H 6.O 1. 0.G 200.000 6000.000 B 58.07914 1  
 7.29796974E+00 1.75656913E-02 -6.31678065E-06 1.02025553E-09 -6.10903592E-14 2  
 -2.95368927E+04 -1.27591704E+01 5.55638920E+00 -2.83863547E-03 7.05722951E-05 3  
 -8.78130984E-08 3.40290951E-11 -2.78325393E+04 2.31960221E+00 -2.58360384E+04 4

Table 4 (continued)

75-56-9

C3H6O PROPYLENEOXIDE Methyl-OXYRANE STATWT=1. SIGMA=1. IA=4.657 IB=12.561  
 IC=14.103 IR=.53 ROSYM=3 V3=895 cm<sup>-1</sup> NU=3065(2),3006,2975,2929,2846,1500,  
 1456(2),1406,1368,1263,1166,1142,1132,1102,1023,950,896,828,745,416,371  
 REF=SWALEN & HERSHBACH JCP 27,(1957),100 HF298=-92.76 kJ. REF=Stull, Westrum &  
 Sinke (1969) MAX LST SQ ERROR CP @ 200 K 0.69 %  
 C3H6O Me-Oxyrane A01/05C 3.H 6.O 1. 0.G 200.000 6000.000 B 58.07914 1  
 8.01491079E+00 1.73919953E-02-6.26027968E-06 1.01188256E-09-6.06239111E-14 2  
 -1.51980838E+04-1.88279964E+01 3.42806676E+00 6.25176642E-03 6.13196311E-05 3  
 -8.60387185E-08 3.51371393E-11-1.28446646E+04 1.04244994E+01-1.11564001E+04 4

503-30-0

C3H6O TRIMETHYLENE OXIDE (CYCLO), OXETANE SIGMA=2 STATWT=1 IA=6.9562  
 IB=7.1539 IC=12.5119 Nu=3146,3094,3070.6(2),3039,3028,1577,1546,1521,1399,  
 1323,1277,1247,1207,1171,1157,1056,1048,952,935,848,816,775,64.8 HF298=-81.086  
 kJ HF0=-61.49 kJ REF=Burcat G3B3 calc. {HF298=-19.25+/-2 kcal REF=NIST94;  
 HF298=-80.50 kJ REF=Dorofeeva et al Thermochim. Acta 194,(1992),9-46} Max Lst  
 Sq Error Cp @ 200 K \*1.3%\*  
 C3H6O OXETANE A11/04C 3.H 6.O 1. 0.G 200.000 6000.000 B 58.07914 1  
 6.80716906E+00 1.88824545E-02-6.79082475E-06 1.09713919E-09-6.57154952E-14 2  
 -1.36547629E+04-1.35382154E+01 5.15283752E+00-1.86401716E-02 1.29980652E-04 3  
 -1.58629974E-07 6.20668783E-11-1.13243512E+04 4.73561224E+00-9.75233898E+03 4

59123-15-8

C3H6O VINYL METHYL ETHER C2H3-O-CH3 SIGMA=1 STATWT=1 IA=2.1255 IB=18.6559  
 IC=20.1587 Ir(CH3)=0.50297 ROSYM=3 [V(3)=11 kJ REF=East & Radom JCP 106,  
 (1997),6655] Ir(CH3O-)=2.08244 ROSYM=1 V(3)=411. cm<sup>-1</sup> estim, NU=3379,3192,  
 3155,3142,3075,3018,1739,1532,1521,1508,1448,1359,1275,1186,1175,1120,984,893,  
 834,709,526,316 HF298=-100.378+/-4. kJ HF0=-82.54 kJ REF=Burcat G3B3 calc.  
 {HF298=-108.+/-8.4 kJ REF=NIST94} Max Lst Sq Error Cp @ 6000 K 0.53%  
 C3H6O C2H3-O-CH3 A01/05C 3.H 6.O 1. 0.G 200.000 6000.000 B 58.07914 1  
 7.36862196E+00 1.70579663E-02-6.02453419E-06 9.59230784E-10-5.68713111E-14 2  
 -1.56713547E+04-1.12908314E+01 5.33258600E+00 1.55080791E-03 5.77039781E-05 3  
 -7.46373993E-08 2.93544408E-11-1.41076819E+04 4.26255762E+00-1.20726710E+04 4

16545-68-9

C3H6O CYCLOPROPANOL C3H5-OH SIGMA=2 STATWT=1 IA=5.0221 IB=12.2088 IC=14.1629  
 Ir=0.141315 ROSYM=1 V(3)=1854. cm<sup>-1</sup> est according to Bozzelli JPC A 108,(2004)  
 ,8353 Nu=3728,3242,3226,3156,3146,3110,1530,1479,1437,1315,1239,1206,1200,1134,  
 1077,1059,994,935,842,822,763,409,403 HF298=-101.5 kJ HF0=-81.907 kJ  
 REF=Burcat G3B3 calc {HF298=-114.3 kJ REF=NIST 94} Max Lst Sq Error Cp @ 200  
 K 0.6%  
 C3H6O CyC3H5-OH A01/05C 3.H 6.O 1. 0.G 200.000 6000.000 B 58.07914 1  
 8.95739587E+00 1.60217198E-02-5.65131014E-06 9.01550505E-10-5.35370086E-14 2  
 -1.65852904E+04-2.45939234E+01 2.12818440E+00 8.44261433E-03 6.99012101E-05 3  
 -1.04542243E-07 4.42460530E-11-1.36496693E+04 1.64564771E+01-1.22080363E+04 4

Table 4 (continued)

287-27-4

C3H6S THIETHANE CY-C3H6S SIGMA=2 STATWT=1 A0=0.148 B0=0.222 C0=0.337  
 REF= C.J.Nielsen Acta Chem. Scan. A 31, (1977), 31. NU=2994(2), 2972, 2950, 2946,  
 2903, 1470, 1454, 1452, 1281, 1229, 1224, 1183, 1165, 1011, 986, 974, 933, 845, 823, 700, 677,  
 529, 114 REF=Shaw et.al. JPC 92, (1988), 6528 T0(STATWT)=3063(2)  
 HF298=14.48 kcal REF=Pedley & Naylor 1986 REF=Ching-Len Yu & S.H.Bauer Private  
 Communication Max Lst Sq. Error Cp @ 200 K \*\*\*1.10%\*\*\*.  
 C3H6S THIETHANE T05/97C 3.H 6.S 1. 0.G 200.000 6000.000 B 74.14664 1  
 8.39851867E+00 1.75807579E-02-6.34783803E-06 1.02801267E-09-6.16584833E-14 2  
 2.99017716E+03-2.17569867E+01 2.83653731E+00 4.35820504E-03 7.71681730E-05 3  
 -1.08731256E-07 4.49661338E-11 5.75902343E+03 1.34578417E+01 7.28657732E+03 4

2143-61-5

C3H7 n-Propyl Rad CH3CH2CH2\* SIGMA=1 STATWT=2 IA=2.5613 IB=9.4162 IC=10.8387  
 Ir(CH3)=0.4784 ROSYM=3 [V(3)=1253.9 cm-1 REF W. TSANG] Ir(CH2\*)=0.278 ROSYM=2  
 V(3)=0 NU=3258, 3161, 3119, 3112, 3047, 3033, 2938, 1536, 1528, 1500, 1490, 1436, 1379,  
 1284, 1187, 1093, 1064, 930, 890, 761, 465, 367 HF298=101.32+/-1. kJ HF0=119.149 kJ  
 REF+Ruscic G3B3 calc. {HF298= 100.5 KJ REF= WING TSANG JACS 107, (1985), 2872}  
 Max Lst Sq Error Cp @6000 K 0.55%  
 C3H7 n-propyl A 5/05C 3.H 7. 0. 0.G 200.000 6000.000 B 43.08768 1  
 6.49636579E+00 1.77337992E-02-6.24898046E-06 9.95389495E-10-5.90199770E-14 2  
 8.85973885E+03-8.56389710E+00 4.08211458E+00 5.23240341E-03 5.13554466E-05 3  
 -6.99343598E-08 2.81819493E-11 1.04074558E+04 8.39534919E+00 1.21859256E+04 4

2025-55=0

C3H7 ISO-Propyl Rad CH3-CH\*-CH3 SIGMA=2 STATWT=2 IA=2.2406 IB=10.1496  
 IC=11.3383 (Ir(CH3)=0.4745 ROSYM=3 V(3)=0)x2 Nu=3180, 3103(2), 3043(2), 2959,  
 2953, 1522, 1510.5(2), 1500, 1443, 1436, 1388, 1193, 1158, 1049, 955, 949, 890, 413, 361  
 HF298=90.19+/-2 kJ HF0=108.237 kJ REF=Ruscic G3B3 calc {HF298= 93.3 KJ.  
 REF= WING TSANG JACS 107, (1985), 2872} Max Lst Sq Error Cp @ 6000 K 0.62%  
 C3H7 i-propyl A 5/05C 3.H 7. 0. 0.G 200.000 6000.000 B 43.08768 1  
 5.30597255E+00 1.89854588E-02-6.74315384E-06 1.07993730E-09-6.42785036E-14 2  
 7.78748910E+03-2.23233935E+00 5.47421257E+00-8.42536682E-03 8.04607759E-05 3  
 -9.49287824E-08 3.59830971E-11 9.04939013E+03 3.40542323E+00 1.08473019E+04 4

107-08-4

C3H7I 1-iodopropane SIGMA=1 IA=8.29 IB=38.9476 IC=45.962 IR=6.27  
 POTENTIAL BARRIER V3= 698.5 cm-1 ROSYM=3 REF=BRINKMAN & BURCAT NU=2998, 2963,  
 2962(2), 2904, 2880, 2868, 1460, 1456(2), 1433, 1380, 1344, 1279, 1195, 1167, 1075, 1036,  
 1012, 880, 816, 764, 503, 390, 263, 189 REF=SHIMANOUCI JPCRD 9 (1980) 1221 HF0=-10.2  
 +/-2. KJ REF= BRAND & al. Chem Phys 76 (1983), 114 Max Lst Sq Error Cp @ 6000 K  
 0.613 %.  
 1-C3H7I T 5/97C 3H 7I 1 0G 200.000 6000.000 C 169.99305 1  
 8.75274672E+00 1.93877662E-02-6.96410211E-06 1.12226927E-09-6.71103091E-14 2  
 -8.16015913E+03-1.73406686E+01 4.99662911E+00 7.01218575E-03 5.68773142E-05 3  
 -7.77001229E-08 3.10455636E-11-6.01366014E+03 7.55650710E+00-3.84863125E+03 4

Table 4 (continued)

75-30-9

C3H7I 2-iodopropane SIGMA=1 IA=10.31 IB=38.2149 IC=45.6879 IR=0.5292  
 TWO EQUAL CH3 ROTORS ROSYM=3 POTENTIAL BARRIER V3=698.5 cm<sup>-1</sup> REF=BRINKMAN &  
 BURCAT NU=2997,2978,2961,2937,2925,2890,2882,1468(2)1459,1428,1389,1378,1325,  
 1210,1153,1113,1020,937,925,879,409,398,230,217 REF=KLABOE SPECTRACHIMICA ACTA  
 26A (1970), 87 HF0=-20.1+/-2. KJ REF=BRAND & al Chem Phys 76 (1983), 114  
 Max Lst Sq Error Cp @ 1300 K 0.613 %.

2-C3H7I	T 5/97C	3H	7I	1	OG	200.000	6000.000	C	169.99305	1
8.75725833E+00	1.88631159E-02	-6.76401581E-06	1.09030360E-09	-6.51918852E-14						2
-9.05136717E+03	-1.66958638E+01	6.01588010E+00	8.83549699E-03	4.05024381E-05						3
-5.47331103E-08	2.12607652E-11	-7.36100208E+03	1.91161348E+00	-4.91494664E+03						4

765-30-0

C3H7N cyclopropylamine (C3H5NH2) REF=DRAEGER HARRISON AND GOOD DATA EXTRAPO-  
 LATED THROUGH WILHOIT'S POLYNOMIALS HF298=77.37 KJ MAX LST SQ ERROR CP @  
 1400 K 0.95 % .

C3H5NH2	L 2/84C	3H	7N	1	OG	300.000	5000.00	B	57.09499	1
0.11077434E 02	0.15626516E-01	-0.52517407E-05	0.79408302E-09	-0.43887471E-13						2
0.43691211E 04	-0.35471283E 02	0.92693955E 00	0.35704415E-01	-0.35520043E-05						3
-0.24779276E-07	0.13902465E-10	0.75181836E 04	0.18755966E 02	0.93077042E+04						4

503-29-7

C3H7N CY -C3H6N:-H AZETIDINE SIGMA=2 STATWT=1 A0=0.220 B0=0.378 C0=0.382  
 NU=3358,3003,2961,2932,2920,2871,2862,1499,1458,1450,1341,1321,1252,1244,1196,  
 1180,1146,1088,1028,990,949,920,910,815,736,648,217 REF=Shaw et.al JPC 94,  
 (1990),118 HF298=23.47 kcal REF=Kamo et al Nippon Kagaknkai Shi 8, (1987),1560  
 REF TOTAL=Ching-Len Yu & S.H.Bauer Private Communication Max Lst Sq Error Cp @  
 200 K \*\*\*1.43%\*\*\*.

C3H7N AZETIDINE	T05/97C	3.H	7.N	1.	O.G	200.000	6000.000	B	57.09532	1
7.71995188E+00	2.08359439E-02	-7.51341908E-06	1.21565468E-09	-7.28540548E-14						2
7.40055773E+03	-2.05389040E+01	3.72047052E+00	-9.49272901E-03	1.21925375E-04						3
-1.56493514E-07	6.25256744E-11	1.03256972E+04	9.61790101E+00	1.18104951E+04						4

108-03-2

C3H7NO2 1-Nitro-Propane STATWT = 1 IA = 13.094016 IB = 35.457574  
 IC = 37.3826884 Ir(NO2) = 5.96 ROSYM = 2 V(2) = 0.08 kcal/mole  
 Ir(CH3) = 0.51666 ROSYM = 3 V(3) = 3.5 kcal/mole Ir(C2H5) = 2.104 ROSYM = 2  
 V(2)= 9.0 kcal NU = (3187,3088,3080,3031),2981,2905,2280,(1907),1567,1447,  
 (1415,1403,1392),1377,1232,1225,(1155,1140,1134,1068,1052),885,796,727,619,601,  
 569,(474,417,268)\*. In Parenthesis values added to IR bands. REF = NIST 97  
 HF298=-29.7 kcal REF= Pedley & Rylance 1977 Max Lst Sq Error Cp @ 1300 K 0.65%  
 C3H7NO2 T05/98C 3.H 7.N 1.O 2.G 200.000 6000.000 B 89.09412 1

1.27038541E+01	2.12000123E-02	-7.88951874E-06	1.29872564E-09	-7.87331819E-14						2
-2.09708557E+04	-3.93362344E+01	2.45041896E+00	2.99807749E-02	2.82471382E-05						3
-6.00704031E-08	2.66264111E-11	-1.71521009E+04	1.84229851E+01	-1.49455350E+04						4



Table 4 (continued)

627-13-4

C3H7ONO2 NPN n-Propyl-Nitrate STATWT = 1 IA = 15.235443 IB = 51.655271  
 IC = 55.1180418 Ir(NO2) = 5.96 ROSYM = 2 V(2) = 9.1 kcal/mole  
 Ir(CH3) = 0.51666 ROSYM = 3 V(3) = 3.5 kcal/mole Ir(C2H5) = 3.027 ROSYM = 2  
 V(2) = 9.0 kcal/mole NU= 3182,3088,3077,3049,3027,2955,2948,2099,1537,1430,  
 1413,1403,1401,1359,1341,1300,1161,1155,1129,1108,1105,1025,941,917,815,641,609,  
 541,461,359,301,244,179. REF = BURCAT TAE # 824A (1998) HF298 = -41.6 kcal  
 REF = Sull Westrum & Sinke Max Lst Sq Error Cp @ 1300 K 0.64%  
 C3H7NO3 NPN T05/98C 3.H 7.N 1.O 3.G 200.000 6000.000 B 105.09352 1  
 1.52256437E+01 2.22034122E-02-8.38746793E-06 1.39150880E-09-8.47131095E-14 2  
 -2.78718897E+04-5.27407711E+01 4.46362749E+00 2.95649058E-02 3.53085312E-05 3  
 -6.91816807E-08 3.01929999E-11-2.37681986E+04 8.34607830E+00-2.09338133E+04 4

16499-18-6

C3H7O N-PROPOXY RADICAL SIGMA=3 ESTIMATED USING THE NIST 1994 PROGRAM TO 1500K  
 EXTRAPOLATED USING WILHOIT'S POLYNOMIALS HF298=-9.0 KCAL Max Lst Sq Error Cp @  
 500 K 0.44%.  
 C3H7O N-PROPOXY T 3/96C 3H 7O 1 OG 298.150 5000.000 F 59.08798 1  
 0.84124958E+01 0.19520193E-01-0.71317071E-05 0.12393621E-08-0.82483889E-13 2  
 -0.87750718E+04-0.18293360E+02 0.91452571E+00 0.33601264E-01-0.12282254E-04 3  
 -0.10739947E-08 0.72924952E-12-0.61847956E+04 0.22563171E+02-0.45289500E+04 4

74-98-6

C3H8 PROPANE CH3CH2CH3 SIGMA=2 STATWT=1. IA=2.8899 IB=IC=10.5472  
 IR=.44202 ROSYM=3. V0=3.29 kcal NU=2977,2962,2887,1476,1462,1392,1158,869,369,  
 2967,1451,1278,940,2968,2887,1464,1378,1338,1054,922,2973,2968,1472,1192,748  
 HF298=-25.02+/-0.15 kcal HF0=-19.69 kcal REF=CHAO WILHOIT & ZWOLINSKI JPCRD 2,  
 (1973),427 {HF298=-104.68+/-0.6 REF=ATcT A} MAX LST SQ ERROR CP @ 200 K 0.64%  
 C3H8 g 2/00C 3.H 8. 0. 0.G 200.000 6000.000 B 44.09562 1  
 6.66919760E+00 2.06108751E-02-7.36512349E-06 1.18434262E-09-7.06914630E-14 2  
 -1.62754066E+04-1.31943379E+01 4.21093013E+00 1.70886504E-03 7.06530164E-05 3  
 -9.20060565E-08 3.64618453E-11-1.43810883E+04 5.61004451E+00-1.25900384E+04 4

71-23-8

1-C3H8O 1-PROPANOL C3H7OH SIGMA=1.753 STATWT=1 IAIBIC=1855.1  
 Ir(CH3)=0.5050 ROSYM=3 V(3)=1004. cm-1 Ir(OH)=0.1361 ROSYM=1 V(3)=279.8 cm-1  
 Ir(-CH2OH)=1.5635 ROSYM=1 V(3)=1105. Nu=3705,2971,2970,2941,2924,2911,2903,  
 2877,1465,1462,1461,1459,1394,1388,1330,1255,1227,1180,1075,1056,1003,917,880,  
 862,524,920,349. T0= 70.0 SIGMA=1.753 IAIBIC=1660.2 Ir=0.4591 ROSYM=3  
 V(3)=954.64 cm-1 Ir=0.1321 ROSYM=1 V(3)=279.8 Ir=1.493 ROSYM=3 V(3)=808 cm  
 Nu=3680,2940(7),1478,1463,1450(2),1393,1381,890,860,730,463,1341,1299,1272,  
 1220,1103,1066,1052,971,916 HF298=-255.2 kJ HF0=-231.342 kJ REF=CHAO et. al.  
 JPCRD 15 (1986),1369 Max Lst Sq Error Cp @ 200 K 0.69%.  
 C3H8O lpropanol g 2/00C 3.H 8.O 1. 0.G 200.000 6000.000 B 60.09502 1  
 8.52377408E+00 2.10371210E-02-7.48398370E-06 1.19958663E-09-7.14873013E-14 2  
 -3.50702414E+04-1.77857176E+01 5.41877541E+00-5.75566129E-04 8.51215375E-05 3  
 -1.11060442E-07 4.43007063E-11-3.28368377E+04 5.29974117E+00-3.06933301E+04 4

Table 4 (continued)

67-63-0

(CH<sub>3</sub>)<sub>2</sub>CHOH 2-PROPANOL SIGMA=3 IAIBIC=1831.0E-117 NU=3650,2940(6),2875,1475(2),1460(2),1387,1367,1340,1256(2),1153,1130,1072,955(2),940,818,488,427,373

(Ir(CH<sub>3</sub>)=0.5036 ROSYM=3 V(3)=1399 cm<sup>-1</sup>x2 Ir(OH)=0.1281 ROSYM=1 V(1)=30.4 cm<sup>-1</sup> V(2)=-86.2 cm<sup>-1</sup> V(3)=401.3 cm<sup>-1</sup> HF298=-272.7 KJ HF0=-248.59 kJ REF=CHAO et. al. JCPRD 15 (1986),1369 {HF298=-271.53+/-0.24kJ REF=ATcT A} Max Lst Sq Error Cp @ 200 K 0.56%.

C3H8O 2propanol	g	2/00C	3.H	8.0	1.	0.G	200.000	6000.000	B	60.09502	1	
							9.64183701E+00	2.00230715E-02	-7.11967189E-06	1.14138950E-09	-6.79935249E-14	2
							-3.74835623E+04	-2.56288343E+01	4.30755345E+00	1.02582798E-02	6.19565411E-05	3
							-9.02973802E-08	3.73936384E-11	-3.49249212E+04	7.55995822E+00	-3.27980843E+04	4

109-87-5

C3H8O2 CH<sub>3</sub>-O-CH<sub>2</sub>-O-CH<sub>3</sub> DiMethoxyMethane SIGMA=1 STATWT=1 IA=5.8896 IB=30.1703

IC=32.9248 Ir(CH<sub>3</sub>-1)=0.51501 Ir(CH<sub>3</sub>-2)=0.52847 Ir(CH<sub>3</sub>O-1)=4.03274

Ir(CH<sub>3</sub>O-2)=3.4016 ROSYM=3 and 2 V(3)=aprox 900.cm<sup>-1</sup> Nu=3151,3143,3096,3131,3030,3010,2988,2910,1557,1542,1536,1518,1515,1511,1495,1455,1316,1254,1237,1209,1190,1183,1142,1130,996,974,560,385,326 HF298=-345.967 kJ HF0=-321.133 kJ

REF=Burcat G3B3 calc {HF298=-348.2 +/-0.79 kJ REF=Pilcher & Fletcher Trans.

Farad Soc 65 (1969),2326} {HF298=-82.8+/-2.kcal REF=NIST 94; HF298=-81.83 kcal

REF=THERM; HF298=-83.53 kcal REF=THERGAS} Max Lst Sq Error Cp @ 6000 K 0.59%.

[Note: This is one of a very large number of possible conformers. It was chosen on basis of a MOPAC PM3 equilibration process.]

CH <sub>3</sub> -O-CH <sub>2</sub> -O-CH <sub>3</sub>	A11/04C	3.H	8.0	2.	0.G	200.000	6000.000	B	76.09442	1		
							8.95642008E+00	2.30964860E-02	-8.31918887E-06	1.33721431E-09	-7.96344608E-14	2
							-4.60512444E+04	-1.76089627E+01	6.78227799E+00	7.94775082E-03	5.06843864E-05	3
							-6.50264081E-08	2.46032899E-11	-4.43162724E+04	-9.93097382E-01	-4.16099797E+04	4

1115-12-4

C3N2O Oxopropandinitrile NC-CO-CN SIGMA=2 STATWT=1 IAIBIC=14666. E-117

NU=2230,1711,712,553,127.5,307,712,208.2,2230,1124,550,245.2 HF298=247.5+/-6.4

kJ HF0=246.5+/-6.4 kJ REF= Dorofeeva et al, 30, (2001), 475 Max Lst Sq Error Cp @ 1300 K 0.45%

C3N2O NC-CO-CN	T	6/03C	3.N	2.0	1.	0.G	200.000	6000.000	B	80.04498	1	
							1.02505353E+01	5.52056426E-03	-2.08011128E-06	3.46449568E-10	-2.11883184E-14	2
							2.60628607E+04	-2.36322120E+01	2.90255868E+00	3.60774698E-02	-5.74096105E-05	3
							4.90465390E-08	-1.66007074E-11	2.77164324E+04	1.21451730E+01	2.97672382E+04	4

504-64-3

C3O2 HF298=-93.64 KJ REF=TRC (API) April 30 1984

C3O2	L	7/88C	3O	2	0	OG	200.000	6000.000	B	68.03180	1	
							0.84617494E+01	0.48155296E-02	-0.18093067E-05	0.30078642E-09	-0.18372137E-13	2
							-0.14327160E+05	-0.17060508E+02	0.21966949E+01	0.31455190E-01	-0.50745522E-04	3
							0.43579038E-07	-0.14735014E-10	-0.12946099E+05	0.13298479E+02	-0.11262239E+05	4

12184-80-4

C4 SIGMA=2 STATWT=3 IB=16.3 NU=2570,1100,2170,440(2),200(2) T0=4000. STATWT=2

T0=6000. STATWT=6 T0=8000. STATWT=1 T0=14000. STATWT=2 T0=19564. STATWT=6

T0=24000. STATWT=8 T0=28000. STATWT=2 REF=TSIV HF298=1033.9 KJ

C4	R	79	C	4	0	0	OG	200.000	6000.000	B	48.04400	1
							0.56307710E 01	0.48313818E-02	-0.15041681E-05	0.20289460E-09	-0.10036092E-13	2
							0.12250094E 06	0.29887309E 01	0.33227750E 01	0.20259234E-01	-0.37345213E-04	3
							0.35685909E-07	-0.12771861E-10	0.12272364E 06	0.68097958E 01	0.12434933E 06	4

Table 4 (continued)

51104-87-1

C4Cl2 DichloroButadiyne DichloroDiacetylene ClCC-CCCl SIGMA=2 STATWT=1

IB=161.6125 Nu=2365,2259,1236,766,570(2),391,308(2),207(2),83.84(2)

HF298=453.592 kJ HF0=447.208 kJ REF=Burcat G3B3 calc MP2(full)/SCF=QC

Max Lst Sq Error Cp @ 1300 K 0.35%.

C4CL2	A04/05C	4.CL	2.	0.	0.G	200.000	6000.000	B	118.94820	1
1.17620201E+01	4.49306295E-03	-1.68019233E-06	2.78485278E-10	-1.69756991E-14						2
5.05450809E+04	-3.06261220E+01	3.66699045E+00	4.35315160E-02	-7.95853289E-05						3
7.22522258E-08	-2.50290031E-11	5.20982332E+04	7.46823673E+00	5.45542220E+04						4

87-68-3

C4Cl6 Perchloro-1,3-butadiene SIGMA=2 Ia=102.47612 Ib=201.1241

Ic=265.3158 Nu=1832,1764,1309,879,859,787,784,691,605,574,414,378,366,365,274,

271.5,227.7,180.4,168.4,129.15,111.7,68.47,61.56,29.2 REF=MOPAC6 PM3 calc.

HF298=-23.1 kcal REF=THERGAS est. { HF298=-2.55 kcal PM3 est} Max Lst Sq Error

Cp @ 1200 K 0.32% \*\* Internal rotation not considered. Estimated HF \*\*

C4CL6	Butadiene	T08/00C	4.CL	6.	0.	0.G	200.000	6000.000	D	260.76020	1
2.21980993E+01	5.83006041E-03	-2.25806563E-06	3.82826576E-10	-2.36983327E-14						2	
-1.93181619E+04	-7.45658167E+01	5.11650693E+00	7.63368754E-02	-1.23398475E-04						3	
1.00027196E-07	-3.19528806E-11	-1.56350963E+04	8.26053886E+00	-1.16243050E+04						4	

64788-23-4

C4F2 PerfluoroButadiyne PerfluoroDiacetylene FCC-CCF SIGMA=2 STATWT=1

IB=79.7196 Nu=2487,2390,1457,1100,569,523(2),344(2),292(2),121(2) HF298=215.31

HF0=210.191 kJ REF=Burcat G3B3 calc Max Lst Sq Error Cp @ 1300 K 0.40%

C4F2	A04/05C	4.F	2.	0.	0.G	200.000	6000.000	B	86.03961	1
1.10453397E+01	5.13392597E-03	-1.91094842E-06	3.15777482E-10	-1.92092174E-14						2
2.20569787E+04	-2.97095866E+01	2.65028548E+00	4.59479327E-02	-8.43662381E-05						3
7.74072161E-08	-2.70743107E-11	2.36682868E+04	9.76166049E+00	2.58955296E+04						4

685-63-2

C4F6 PERFLUORO 1-3 BUTADIENE SIGMA=1 SIGMAR=2 IA=42.1018 IB=80.1264

IC=116.0475 IR=132.823 V(2)=2850. NU=1796,1381,1138,933,702,660,529,464,396,

375,329,181,1765,1329,1189,972,633,547,520,422,293,259,204 REF=WURREY, BUCY

AND DURIG HF298=-240. kcal REF= Atkinson &amp; Stedman J. Chem. Soc (1962), 512

MAX LST SQ ERROR @ 1300 K 0.44 % .

C4F6	T12/82C	4F	6	0	OG	300.000	5000.0	B	162.034391
0.20649826E+02	0.63778609E-02	-0.24356023E-05	0.40486192E-09	-0.24477111E-13					2
-0.12834769E+06	-0.75434682E+02	0.61921721E+01	0.40591445E-01	-0.14628447E-04					3
-0.22981666E-07	0.15799126E-10	-0.12425062E+06	0.15772644E+00	-0.12077197E+06					4

697-11-0

C4F6 PERFLUOROCYCLOBUTENE SIGMA=2 IA=53.90 IB=64.95 IC=87.73 NU=1799,1418,

1387,1136,966,684,469.2,286,1182,493,337,174,98,1282,638,187,146,1259,1171,983,

579,429,238,217 REF=NIELSEN AND EL-SABEN JCP 23, (1955), 324. HF298=-289.4 kcal

REF= Atkinson &amp; Stedmann J. Chem. Soc (1962), 512. MAX LST SQ ERROR @ 1300 K

0.53%

F6C4	T12/82F	6C	4	0	OG	300.000	5000.000	B	162.03439	1
0.19723373E+02	0.81368275E-02	-0.30685842E-05	0.50541860E-09	-0.30311613E-13						2
-0.15313506E+06	-0.72023473E+02	0.60944862E+01	0.36527760E-01	-0.68788740E-05						3
-0.24970031E-07	0.14493539E-10	-0.14896744E+06	0.49672994E+00	-0.14563498E+06						4

Table 4 (continued)

115-25-3

C4F8 PERFLUOROCYCLOBUTANE ESTIMATED USING NIST 1994 TO 1000 K, EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS HF298=-1513.6 KJ Max Lst Sq Error Cp @ 500 K \*1.25%\*

C4F8 CY	T11/94C	4F	8	0	OG	298.150	5000.000	F	200.03123	1
0.25859659E+02	0.14057850E-01	-0.86342611E-05	0.18743110E-08	-0.13985280E-12						2
-0.19308325E+06	-0.10861981E+03	-0.64087603E+01	0.11778844E+00	-0.15735373E-03						3
0.11577968E-06	-0.37112295E-10	-0.18418883E+06	0.56186329E+02	-0.18204320E+06						4

355-25-9

C4F10 PERFLUOROBUTANE (FC-3-1-10) SIGMA=18 CALCULATED and EXTRAPOLATED USING NIST 94 AND BOZZELLI & RITTER'S PROGRAM. HF298=-510.85 KCAL Max Lst Sq Error Cp @ 1400 K 0.19%.

C4F10	T12/94C	4F	10	0	OG	298.150	5000.000	E	238.02803	1
0.30442529E+02	0.87222991E-02	-0.36625862E-05	0.67841011E-09	-0.46225435E-13						2
-0.26830628E+06	-0.12239409E+03	-0.43510861E+00	0.11003166E+00	-0.12712106E-03						3
0.66741713E-07	-0.13106885E-10	-0.26083419E+06	0.32565014E+02	-0.25707075E+06						4

53561-65-2

C4H RAD T0=0 STATWT=4. SIGMA=1. B0=0.1558 NU=3485,2283,2116,910,565(2), 473(2),204(2) T0=350. STATWT=2. NU=3474,2129,1864,889,695,424,186,565,473,204 REF=Kiefer, Sidhu, Kern, Xie, Chen & Harding (1992) LST SQ ERROR CP @ 1300 K 0.34% . HF298=192.0 KCAL

C4H	T12/91C	4H	1	0	OG	200.000	6000.000	B	49.05194	1
0.77680939E+01	0.49850386E-02	-0.17648839E-05	0.28217408E-09	-0.16779623E-13						2
0.93912126E+05	-0.14159577E+02	0.13210657E+01	0.38562824E-01	-0.71343174E-04						3
0.65319977E-07	-0.22607050E-10	0.95021629E+05	0.15554575E+02	0.96617600E+05						4

460-12-8

C4H2 BUTADIYNE STATWT=1. SIGMA=2. IB=19.1411 NU=3329(2),2184,874,2020,627(2) 4822),630(2),231) REF=Shimanouchi (Webbook) HF298=109.54 kcal REF=Burcat G3B3 calc.{HF298=110.9 kcal REF Kiefer Sidhu Kern et al Comb Sci Tech.82,(1992), 101-130} Max Lst Sq Error Cp @ 1300 K 0.34%.

C4H2 butadiyne	T07/04C	4.H	2.	0.	O.G	200.000	6000.000	B	50.05868	1
8.68978130E+00	6.69732229E-03	-2.34774865E-06	3.72759231E-10	-2.20554548E-14						2
5.19942624E+04	-2.20010465E+01	-5.84768273E-01	5.33506727E-02	-9.50805952E-05						3
8.37959674E-08	-2.80912179E-11	5.36111160E+04	2.09878997E+01	5.51203407E+04						4

764-42-1

C4H2N2 FUMARONITRILE trans-NC-CH=CH-CN SIGMA=2 STATWT=1 IA=1.7899 IB=56.8850 IC=58.6750 Nu=3213,3207,2357,2340,1680,1334,1304,1034(2),982,864,566,539,537, 391,258,137,127.4 HF298=331.+/-3 kJ HF0=334.8 kJ REF= Burcat G3B3 calc. {HF298=340+/-3 kJ REF=Boyd et al JPC 71,(1967),2187} Max Lst Sq Error Cp @ 1300 K 0.47%

C4H2N2 Fumaroni	T05/04C	4.H	2.N	2.	O.G	200.000	6000.000	B	78.07216	1
1.02609796E+01	1.05849090E-02	-3.83686580E-06	6.23219249E-10	-3.74697958E-14						2
3.56975913E+04	-2.56899378E+01	3.08972201E+00	3.01705916E-02	-2.22304023E-05						3
6.22606240E-09	3.38798598E-13	3.77312220E+04	1.14967588E+01	3.98094704E+04						4

Table 4 (continued)

2810-61-9

C4H3 E-1-butene-3-yne-1-yl Radical STATWT=2. SIGMA=1. IA=1.2292 IB=17.5117  
 IC=18.7408 NU=3496,3266,3050,2226,1653,1283,1029,824,817,683,635,587,537,351,  
 229 HF298=129.81 kcal HF0=130.34 kcal REF=Burcat G3B3 calc {HF298=130.8 kcal  
 REF=Klippenstein & Miller JPC A 109, (2005), 4285; HF298=131.38 kcal G3 calc and  
 HF298=125.96 kcal M-C calc REF=Krokidis et al IJCK 33, (2001), 808 ) Max Lst Sq  
 Error Cp @ 6000 K 0.40%

C4H3 E,1-butene-	T06/04C	4.H	3.	0.	0.G	200.000	6000.000	B	51.06662	1
8.44631306E+00	9.07291526E-03	-3.18681201E-06	5.06725048E-10	-3.00149855E-14						2
6.20007365E+04	-1.77938854E+01	5.54263934E-01	3.86185425E-02	-4.70818280E-05						3
3.06240321E-08	-7.90588421E-12	6.37974910E+04	2.10542043E+01	6.53200393E+04						4

63707-54-0

C4H3 i-1-butene-3-yne-2-yl Radical STATWT=2. SIGMA=1. IA=2.872 IB=20.2654  
 IC=20.5526 NU=3485,3154,3095,2034,1816,1466,997,911,882,626,580,446,251,140,  
 111 HF298=119.94 kcal HF0=119.92 kcal REF=Burcat G3B3 calc {HF298=119.3 kcal  
 REF=Klippenstein & Miller JPC A 1009, (2005), 4285; HF298=120.89 kcal G3 calc  
 and HF298=119.39 kcal M-C calc Krokidis et al IJCK 33, (2001), 808) Max Lst Sq  
 Error Cp @ 6000 K 0.40%

C4H3 1-butene-3	T06/04C	4.H	3.	0.	0.G	200.000	6000.000	B	51.06662	1
8.51181244E+00	9.03337808E-03	-3.17602594E-06	5.05276458E-10	-2.99379699E-14						2
5.71046116E+04	-1.51017769E+01	3.37964170E+00	2.70498840E-02	-2.90761572E-05						3
1.83027765E-08	-4.81164203E-12	5.83688723E+04	1.05464883E+01	6.03558069E+04						4

22112-56-7

C4H3 1,2,3-butatriene-4-yl CH<sub>2</sub>=C=C=CH\* Has the same configuration size  
 moments of inertia and vibrations as i-1-butene3-yne-2-yl, HF298=119.92 kcal.  
 REF=Burcat G3B3 calc {HF298=120.89 kcal G3 calc and HF298=119.39 kcal M-C calc)

687-97-4

C4H4 1-BUTEN-3YN STATWT=1. SIGMA=1. IA=2.6299 IB=17.8397 IC=19.4696  
 NU=3495,3265,3179,3160,2224,1691,1463,1336,1122,1013,945,899,715,631,588,559,  
 339,229 HF298=68.8 kcal HF0=70.37 kcal REF=Burcat G3B3 calc {HF298=70.5  
 kcal REF=NIST 2004 ROTH et al Chem Ber 124, (1991) 2499-2521} {A0=1.678094245  
 B0=.158273884 C0=.14442624 DJ=6.4E-08 DJK=-277.5E-08 DK=8499.2E-8 NU=3330,3116,  
 3068,3030,2111,1599,1415,1312,1096,874,625,539,217,974,927,677,618,304 HF0=75.3  
 kcal REF=TORNENG et al., SPECTROCHIM. ACTA 36A (1989) 975.} MAX LST SQ ERROR Cp  
 @ 6000 K 0.48%.

C4H4 1-butene-3	T06/04C	4.H	4.	0.	0.G	200.000	6000.000	B	52.07456	1
7.98456038E+00	1.20558816E-02	-4.23587475E-06	6.73646140E-10	-3.99059864E-14						2
3.11993029E+04	-1.67958975E+01	1.37368786E+00	2.88801256E-02	-1.46863874E-05						3
-3.91045446E-09	4.78133572E-12	3.30633344E+04	1.75941274E+01	3.46213066E+04						4

1120-53-2

CYCLOBUTADIENE SIGMA=4 STATWT=1 IAIBIC=360.E-117 NU=3050,1510,1120,900(3),  
 1100,570(2),1235,770,3030(2),1240,720,3040,1520,990 REF=DOROFEEVA, GURVICH &  
 JORISH JCPRD 15 (1986), 437. HF298=385 KJ MAX LST SQ ERROR Cp @ 6000 K 0.54%.

C4H4 CY	T 2/90C	4H	4	0	OG	200.000	6000.000	B	52.07576	1
0.80419352E+01	0.12520407E-01	-0.45234623E-05	0.73313766E-09	-0.44012214E-13						2
0.42510913E+05	-0.21127639E+02	0.12789207E+01	0.13420710E-01	0.41197797E-04						3
-0.69893781E-07	0.30724360E-10	0.45086412E+05	0.17678892E+02	0.46304593E+05						4

Table 4 (continued)

290-37-9

C4H4N2 PYRAZINE (SIX MEMBERED RING WITH N IN PARA POSITION) SIGMA=4 STATWT=1  
 IA=12.8266 IB=13.8011 IC=26.6277 NU= 3037,3031,3015,3014,1615,1579,1493,1404,  
 1337,1215,1227,1074,1010,1003,1001,995,982,935,801,748,695,584,435.7,380.6

REF= C. Melius Database #PJ11 HF298=46.8+-0.3 Kcal REF=Pedley, Nylor & Kirby  
 Max Lst Sq Error Cp @ 200 K \*\*1.06 %\*\*.

C4H4N2 PYRAZINE	T 9/96C	4H	4N	2	OG	200.000	6000.000	B	80.08924	1
	0.10551339E+02	0.16036746E-01	-0.58863657E-05	0.96422235E-09	-0.58315531E-13					2
	0.18418344E+05	-0.33943388E+02	0.13116930E+01	0.14100415E-01	0.64443831E-04					3
	-0.10163885E-06	0.43390536E-10	0.22143754E+05	0.19991866E+02	0.23550540E+05					4

289-95-2

C4H4N2 PYRIMIDINE (SIX MEMBERED RING WITH N IN ORTO POSITION) SIGMA=2 STATWT=1  
 IA=13.10379 IB=13.46 IC=26.57 NU=3045,3033,3015,3010,1608,1607.5,1466,1405,  
 1357,1214,1126,1083,1040,1039,1032,1010,985,978,813.7,704,671,610,411.7,371.3

REF=C.Melius Database #PI11 HF298=47.0+-0.2 Kcal REF=Pedley, Naylor & Kirby  
 Max Lst Sq Error Cp @ 200 K \*\*1.08 %\*\*.

C4H4N2 PYRIMIDINE	T 9/96C	4H	4N	2	OG	200.000	6000.000	B	80.08924	1
	0.10431658E+02	0.16150995E-01	-0.59292286E-05	0.97133853E-09	-0.58749686E-13					2
	0.18552038E+05	-0.33249214E+02	0.16371390E+01	0.11977423E-01	0.68383238E-04					3
	-0.10465037E-06	0.44218587E-10	0.22212482E+05	0.18656416E+02	0.23651183E+05					4

110-61-2

C4H4N2 SUCCINONITRILE NC-CH2-CH2-CN SIGMA=2 STATWT=1 IA=14.7588 IB=28.7459  
 IC=42.432984 Ir=8.4926 ROSYM=2 V(3)=1329. cm-1 NU=2952,2948,2899,2884,2441,  
 2439,1374,1354,1316,1304,1108,1096,1083,979,978,898,822,669,511,435,414,287,135  
 REF=PM3 HF298=209.7+/-0.9 kJ HF0=221.172 kJ REF=Rappaport Westrum & Andrews  
 JACS 93 (1971),4363 {NIST94 HF298=45. kcal; HF298=50.1 kcal Peddley & Reelance  
 1977} Max Lst Sq Error Cp @ 6000 K 0.52%

C4H4N2 SuccinonitrT12/03C	4.H	4.N	2.	O.G	200.000	6000.000	B	80.08804	1
	1.14626097E+01	1.43425847E-02	-5.26374167E-06	8.61140761E-10	-5.20073439E-14				2
	2.02962879E+04	-3.23404065E+01	2.92554100E+00	2.74517845E-02	9.39908894E-06				3
	-3.65605156E-08	1.81346873E-11	2.31092217E+04	1.41181715E+01	2.52209691E+04				4

110-00-9

C4H4O FURAN (CY) SIGMA=2 IAIBIC=1448.6 NU=3167,3161,3140,3129,1556,1491,  
 1384,1267,1180,1140,1066,1040,995,873,871,863,838,745,728,613,603 REF= Chao  
 et. al, JPCRD 15, (1986),1369 HF298=-8.29 KCAL REF=STULL WESTRUN & SINKE

Max Lst Sq Error Cp @ 200 K \*\*1.24%\*\*.

C4H4O FURAN	T03/97C	4.H	4.O	1.	O.G	200.000	6000.000	B	68.07516	1
	9.38935003E+00	1.40291241E-02	-5.07755110E-06	8.24137332E-10	-4.95319963E-14					2
	-8.68241814E+03	-2.79162920E+01	8.47469463E-01	1.31773796E-02	5.99735901E-05					3
	-9.71562904E-08	4.22733796E-11	-5.36785445E+03	2.14945172E+01	-4.17166616E+03					4

50888-73-8

C4H4O VINYL-KETENE H2C=CHCH=C=O SIGMA=1 STATWT=1 IA=2.0666 IB=35.5806  
 IC=37.6472 Ir=2.8084 ROSYM=1 [V(3)=3252. cm-1 REF=acrolein in Baadem et al.  
 Molec. Phys. 98, (2000), 329] Nu=3255,3196,3173,3167,2219,1702,1491,1375,1335,  
 1199,1128,1019,932,886,711,630,561,498,410,167 HF298=22.719 kJ HF0=31.980 kJ  
 REF=Burcat G3B3 calc. {HF298=1.82 kcal. REF=Zhong & Bozzelli JPC-A 102 (1998),  
 3537.} Max Lst Sq Error Cp @ 1300 K 0.56%.

C4H4O Vin-KETENE	A 1/05C	4.H	4.O	1.	O.G	200.000	6000.000	B	68.07396	1
	9.74850463E+00	1.37125055E-02	-5.05430099E-06	8.25446463E-10	-4.97385204E-14					2
	-1.55172564E+03	-2.40662801E+01	2.45069796E+00	2.60086795E-02	1.37550849E-06					3
	-2.17962924E-08	1.11438235E-11	8.71446510E+02	1.55762929E+01	2.73246650E+03					4

Table 4 (continued)

290-67-5

C4H4O2 1,4-Dioxin (Hexa-diene-ring) SIGMA=8 STATWT=1 IA=13.409619 IB=15.61557  
 IC=29.02519 NU=3273,3270,3253,3249,1787,1731,1437,1343,1319,1248,1078,1065,  
 1040,940,911,880,873,759,758,704,546,525,444,88 HF298=-86.+/-7 HF0=-71.5 kJ  
 REF=Zhu & Bozzelli JPCRD 32,(2003),1713 Max Lst Sq Error Cp @ 200 K 0.82  
 C4H4O2 1,4-Dioxin T02/04C 4.H 4.O 2. 0.G 200.000 6000.000 B 84.07336 1  
 1.11139149E+01 1.50834237E-02-5.43916242E-06 8.80792712E-10-5.28558988E-14 2  
 -1.54311253E+04-3.59861821E+01 1.14925397E+00 2.38202086E-02 3.55747174E-05 3  
 -7.14339238E-08 3.24758569E-11-1.19332134E+04 1.95762599E+01-1.03433636E+04 4

110-02-1

C4H4S THIOPHENE (CY) SIGMA=2 IAIBIC=4192. NU=3126,3125,3098(2),1507,1409,1360,  
 1256,1085,1083,1036,898,872,867,839,751,712,683,608,565,452 HF298=114.9 kJ  
 REF=Dorofeeva and Gurvich 1995 Max Lst Sq Error Cp @ 200 K 0.99%  
 C4H4S Thiophene T03/97C 4.H 4.S 1. 0.G 200.000 6000.000 B 84.14176 1  
 1.03361791E+01 1.31485110E-02-4.75133660E-06 7.70341282E-10-4.62623029E-14 2  
 9.14755147E+03-3.14959122E+01-5.33958016E-01 3.04279440E-02 1.57128681E-05 3  
 -5.21636175E-08 2.60141958E-11 1.25779686E+04 2.72103378E+01 1.38192148E+04 4

86181-68-2

N-C4H5 E-1,3-butadiene-1-yl RADICAL CH2=CHCH=CH\* STATWT=2 SIGMA=1  
 IA=1.7022 IB=18.3952 IC=20.0974 Ir=1.69319 V(3)=524 cm-1 ROSYM=1 NU=3267,  
 3249,3178,3164,3042,1707,1649,1464,1330,1269,1192,1036,960,929,857,810,729,565,  
 513,299 HF298=86.84 kcal HF0=89.321 kcal REF=Burcat G3B3 calc {HF298=85.97  
 kcal REF=Krokidis, Frenklach et al Int J Chem Kinet 33,(2001),808-820} Max  
 Lst Sq Error Cp @ 6000 K 0.50%.  
 C4H5 E-1,3dienlyl T05/04C 4.H 5. 0. 0.G 200.000 6000.000 B 53.08250 1  
 8.11183574E+00 1.42276370E-02-5.02419535E-06 8.00816580E-10-4.75459802E-14 2  
 4.00134524E+04-1.52704514E+01 3.28605952E+00 1.43352325E-02 2.78456642E-05 3  
 -4.84612551E-08 2.10628469E-11 4.19222504E+04 1.26653969E+01 4.36993353E+04 4

108179-96-0

I-C4H5 1,3-Butadiene-2-yl CH2=CHC\*=CH2 RADICAL SIGMA=1 STATWT=2 IA=1.9927  
 IB=19.1243 IC=20.5443 Nu=3279,3183,3154,3134,3098,1929,1518,1480,1398,1210,  
 1102,1000,941,915,881,737,575,529,494,228,217.5 HF298=75.34 kcal HF0=77.69  
 kcal REF=Burcat G3B3 calc Max Lst Sq Error Cp @ 6000 K 0.49%.  
 C4H5 1,3-Butadi T05/04C 4.H 5. 0. 0.G 200.000 6000.000 B 53.08250 1  
 8.58761100E+00 1.42683804E-02-5.04812095E-06 8.06555355E-10-4.79335634E-14 2  
 3.40836919E+04-1.96196761E+01 2.00881066E+00 2.50340684E-02 4.47930427E-06 3  
 -2.63989791E-08 1.34432880E-11 3.62069792E+04 1.59913722E+01 3.79123436E+04 4

89829-51-6

C4H5 1,2-Butadiene-4-yl \*CH2CH=C=CH2 RADICAL SIGMA=1 STATWT=2 IA=1.9936  
 IB=19.1221 IC=20.5430 Ir=0.35086 ROSYM=2 V(#)=900 cm-1 Nu=3279,3183,3154,  
 3134,3098,1929,1518,1480,1398,1210,1102,1000,941,915,881,737,575,529,494,228  
 HF298=75.34 kcal HF0=77.69 kcal REF=Burcat G3B3 calc Max Lst Sq Error Cp @  
 6000 K 0.49%.  
 C4H5 1,2-butadi T05/04C 4.H 5. 0. 0.G 200.000 6000.000 B 53.08250 1  
 8.62801071E+00 1.37278200E-02-4.83938983E-06 7.71244955E-10-4.57512509E-14 2  
 3.41638737E+04-1.90962775E+01 1.49752318E+00 3.09380729E-02-1.29703258E-05 3  
 -7.79553217E-09 6.57219652E-12 3.62176515E+04 1.82157058E+01 3.79123436E+04 4

Table 4 (continued)

3315-42-2

C4H5 1-Butayn-3-yl HCC-CH-CH3 SIGMA=1 STATWT=2 IA=2.1573 IB=19.0936  
 IC=20.7315 Ir=0.50605 ROSYM=3 [V(3)=2400 cm<sup>-1</sup> est.] Nu=3488,3169,3137,3059,  
 3020,2032,1522,1505,1431,1410,1164,1111,1019,876,602,598,557,420,314,216

HF298=316.53 kJ HF0=325.987 kJ REF=Janoschek & Rossi Int J. Chem. Kinet 2004  
 {HF298=295.0+/-9.2 kJ REF=McMillan & Golden 1982} Max Lst Sq Error Cp @ 1300 K  
 0.51%

C4H5 1-butyne-3yl A11/04C 4.H 5. 0. 0.G 200.000 6000.000 B 53.08250	1
9.21468577E+00 1.34950214E-02-4.82557552E-06 7.76743641E-10-4.64080569E-14	2
3.40842790E+04-2.25150877E+01 2.15910182E+00 3.04425273E-02-1.62521254E-05	3
-1.73750743E-10 2.43871422E-12 3.62155591E+04 1.46844795E+01 3.80695916E+04	4

109-97-7

C4H5N PYRROLE (CY) (AZOLE, IMIDOLE) SIGMA=2 IAIBIC=1586.5 NU=3527,3148,3140,  
 3125,3116,1530,1467,1422,1382,1287,1144,1134,1074,1048,1016,881,869,865,826,721,  
 710,618,601,474 HF298=108.18+/-0.81 KJ REF= Das et.al JPCRD 22, (1993), 659 Max  
 Lst Sq Error Cp @ 200 \*\*2.1%\*\*

C4H5N PYRROLE T 8/95C 4H 5N 1 0G 200.000 6000.000 B 67.09044	1
0.97727000E+01 0.16111112E-01-0.57690298E-05 0.92973976E-09-0.55604978E-13	2
0.82631988E+04-0.30359085E+02 0.38558756E+00 0.18943518E-01 0.52673009E-04	3
-0.91458921E-07 0.40445724E-10 0.11750328E+05 0.23102254E+02 0.13010989E+05	4

5500-21-0

C4H5N CYCLOPROPANE CARBONITRILE C3H5-CN SIGMA=2 IA=52.966 IB=245.88 IC=259.39  
 NU=222(2),527,543,736,808,821,880,941,1049,1070,1088,1125,1180,1195,1344,1442,  
 1468,2264,3040,3044,3052,3094,3120 REF=Dubnikova & Lifshitz J. Phys. Chem 102,  
 (1998),5876-5885 HF298=44.0+/-0.2 kcal REF=Fuchs Hallman Perlman  
 Canad. J. Chem. 60 (1982),1832. Max Lst Sq Error Cp @ 200 K 0.80%.

C4H5N CY S03/01C 4.H 5.N 1. 0.G 200.000 6000.000 B 67.09044	1
9.60414996E+00 1.64051790E-02-5.90335510E-06 9.54135951E-10-5.71660226E-14	2
1.75974846E+04-2.29869919E+01 2.25946164E+00 1.66431455E-02 4.50396029E-05	3
-7.61575623E-08 3.32182961E-11 2.04650359E+04 1.94239060E+01 2.21415333E+04	4

107-00-6

C4H6 1-Butayne Ethylacetylene HCC-C2H5 Calc. from TRC Table 10/93 to 1500 K and  
 extrapolated using Wilhoit's polynomials 800-6000 K. HF298=165.2 kJ HF0=178.8 kJ  
 Max Lst Sq Error Cp @ 2500 K 0.44%

C4H6 1 butyne L10/93C 4.H 6. 0. 0.G 200.000 6000.000 C 54.09044	1
7.81179394E+00 1.79733772E-02-6.61044149E-06 1.05501491E-09-6.19297169E-14	2
1.61770171E+04-1.59658015E+01 2.42819263E+00 2.49821955E-02 6.27370548E-06	3
-2.61747866E-08 1.26585079E-11 1.80248564E+04 1.36683982E+01 1.98688798E+04	4

503-17-3

C4H6 2-BUTAYN (DIMETHYLACETYLENE) STATWT=1 SIGMA=2 IA=1.0605 IB=IC=25.0029  
 Ir=0.2620 [V(3)=25. cm<sup>-1</sup> REF=B3LYP] (ONE ROTATION ONLY) NU=213(2),371(2),725,  
 1125,1029(2),1050(2),1380(2),1448(2),1468(2),2270,2916,2966(2),2976(3) REF=YOST  
 OSBORNE GARNER JACS 63, (1941),3492 HF298=34.97 kcal REF= Stull, Westrum &  
 Sinke 1969 {HF298=146.314+/-4. kJ REF=Burcat G3B3 calc; HF298=145.767+/-0.769  
 kJ REF=ATcT A} MAX LST SQ ERROR Cp @ 1300 K 0.60 %.

C4H6 Dimethyl Ac A 1/05C 4.H 6. 0. 0.G 200.000 6000.000 B 54.09044	1
7.26055302E+00 1.80160845E-02-6.47062409E-06 1.04411453E-09-6.24741250E-14	2
1.39644246E+04-1.29484347E+01 5.39211846E+00 2.98346178E-03 5.22542032E-05	3
-6.64726627E-08 2.56305331E-11 1.55148209E+04 1.71080366E+00 1.75974868E+04	4



Table 4 (continued)

106-99-0

1,3-C4H6 1,3-BUTADIENE CH2=CH-CH=CH2 SIGMA=2 STATWT=1 IA=1.9937 IB=19.0347  
 IC=21.0184 Ir=1.79466 V(3)=524 cm-1 ROSYM=1 HF298=26.49 kcal NU=3246(2),  
 3164.5(2),3158,3147,1730,1677,1496,1435,1331,1329,1241,1065,1011,1004,932,928,  
 907,782,540,516,297 REF=Burcat G3B3 calc Max Lst Sq Error Cp @ 200 K 0.58%.  
 C4H6 1,3-butadi T05/04C 4.H 6. 0. 0.G 200.000 6000.000 B 54.09044 1  
 7.62637466E+00 1.72523403E-02-6.09184911E-06 9.70800102E-10-5.76169721E-14 2  
 9.55306395E+03-1.48325259E+01 4.10599669E+00 5.05575563E-03 5.83885454E-05 3  
 -8.05950198E-08 3.27447711E-11 1.15092468E+04 8.42978067E+00 1.33302095E+04 4

590-12-2

C4H6 1,2-Butadiene CH2=C=CH-CH3 SIGMA=2 STATWT=1 Ia=2.4309 IB=20.1467  
 IC=21.4816 Ir=0.50734 V(3)=1230. ROSYM=3 Nu=3206,3144,3139,3129,3089,3039,  
 2078,1533,1514,1501,1435,1385,1164,1106,1072,1038,901,887,869,580,541,355,215  
 HF298=38.555 kcal REF=Burcat G3B3 {HF298=38.77 kcal REF=Prosen Maron & Rosini  
 J. Res NBS 46, (1951), 106-112} Max Lst Sq Error Cp @ 6000 K 0.53%.  
 C4H6 1,2-butadi T07/04C 4.H 6. 0. 0.G 200.000 6000.000 B 54.09044 1  
 8.13872997E+00 1.68655431E-02-5.97324908E-06 9.54915173E-10-5.67693708E-14 2  
 1.55467985E+04-1.77959041E+01 2.90828336E+00 1.79025349E-02 2.61486503E-05 3  
 -4.81598832E-08 2.11295844E-11 1.75928783E+04 1.23118106E+01 1.94015186E+04 4

822-35-5

C4H6 CYCLOBUTENE STATWT=1 SIGMA=2 IAIBIC=550\*10E-117 NU=3063,2941,1564,  
 1448,1185,1113,981,883,2955,1142,1000,909,327,3056,2934,1430,1294,1212,1013,890,  
 2961,1074,846,636 HF298=156.7 kJ REF=Dorofeeva, Gurvich & Jorish JPCRD 15(1986)  
 437. {HF298=156.88+/-1.48 REF=ATcT A} Max Lst Sq Error Cp @ 200 K \*\* 1.41%\*\*  
 C4H6 cyclo- g 8/00C 4.H 6. 0. 0.G 200.000 6000.000 54.09044 1  
 7.84858086E+00 1.80812930E-02-6.53186893E-06 1.05842182E-09-6.35254402E-14 2  
 1.46153466E+04-2.08980502E+01 2.91633480E+00-3.20585234E-03 1.00263587E-04 3  
 -1.34248191E-07 5.46670225E-11 1.74732235E+04 1.24816831E+01 1.88465706E+04 4

13676-58-9

C4H6CL2 1,4-DICHLOROBUTENE-1 CHCL=CH-CH2CH2CL SIGMA=1 STATWT=1 IA=17.2655  
 IB=98.3223 IC=110.5489 Ir(CH2CL)=14.1636 ROSYM=1 V3=1341. cm-1 REF=Ruscic &  
 Burcat Ir(CHCL=CH-)=8.9068 ROSYM=1 [V3=1420.cm-1 est from C3H7Br and C3H7Cl in  
 Bornstein Group II Molec. & Radicals Springer 2002 p.212] Nu=3232,3179,3161,  
 3106,3095,3016,1715,1512,1498,1389,1355,1332,1294,1248,1193,1090,1043,976,937,  
 880,818,783,663,471,391,319,231,169 HF298=-51.882 kJ HF0=-34.587 kJ REF=Burcat  
 G3B3 calc {HF298=-13.9 KCAL est. REF=Weissman & Benson Prog Energy Comb. Sci.  
 15, (1989), 273} Max Lst Sq Error Cp @ 200 K 0.55%.  
 C4H6CL2 1,4-DiCl A 1/05C 4.H 6.CL 2. 0.G 200.000 6000.000 B 124.99584 1  
 1.40516768E+01 1.60921842E-02-5.80441963E-06 9.39283307E-10-5.63156326E-14 2  
 -1.22360631E+04-4.07945919E+01 4.62931051E+00 2.13073668E-02 4.38338745E-05 3  
 -8.04356336E-08 3.58874909E-11-8.81241814E+03 1.23974998E+01-6.23988666E+03 4

Table 4 (continued)

760-23-6

C4H6CL2 3,4-DICHLOROBUTENE-1 CH<sub>2</sub>=CH-CHCl-CH<sub>2</sub>Cl SIGMA=1 STATWT=1 IA=24.4567  
 IB=63.7650 IC=84.7048 Ir(CH<sub>2</sub>Cl)=11.5823 ROSYM=1 [V3=1341. cm<sup>-1</sup> REF=Ruscic  
 Burcat] Ir(CH<sub>2</sub>=CH-)=3.089 ROSYM=1 [V(3)=1420.cm<sup>-1</sup> est from C3H7Br and C3H7Cl  
 in Bornstein Group II Molec. & Radicals Springer 2002 p.212] Nu=3263,3195,  
 3184,3170,3127,3098,1737,1508,1468,1368,1337,1336,1259,1196,1097,1076,1026,  
 1006,964,853,753,708,662,502,357,299,250,189 HF298=-53.572 kJ HF0=-36.121 kJ  
 REF=Burcat G3B3 calc {HF298=-16.5 kcal est. REF=Weissman & Benson Prog Energy  
 Comb. Sci. 15, (1989), 273} Max Lst Sq Error Cp @ 200 K 0.54%.

C4H6CL2 3,4-Dich	A 1/05C	4.H	6.CL	2.	0.G	200.000	6000.000	124.99584	1
1.40848232E+01	1.62550619E-02	-5.81516500E-06	9.32238501E-10	-5.54701708E-14					2
-1.24076239E+04	-4.17350351E+01	4.06180136E+00	2.62058396E-02	3.31510353E-05					3
-7.07152661E-08	3.26980783E-11	-8.98755786E+03	1.37617837E+01	-6.44318619E+03					4

1708-29-8

C4H6O 2,5-DIHYDROFURAN (1- OXOLENE CY) REF=Chao et. al. JPCRD 15, (1986), 1369  
 EXTRAPOLATED 1600-5000 K USING WILHOIT'S POLYNOMIALS HF298=-108.78 KJ  
 REF=Kudchadker, Kudchadker & Wilhoit TRC 1978 Key Chemicals Data Book- Furan,  
 Dihydrofuran, Tetrahydrofuran Max Lst Sq Error Cp @ 200 K 0.10%.

C4H6O 2,5DHFURAN	T 3/97C	4H	6O	1	0G	200.000	5000.000	B 70.09104	1
8.60658242E+00	2.08310051E-02	-8.42229481E-06	1.56717640E-09	-1.09391202E-13					2
-1.76177415E+04	-2.32464750E+01	2.67053463E+00	4.92586420E-03	8.86967406E-05					3
-1.26219194E-07	5.23991321E-11	-1.46572472E+04	1.45722395E+01	-1.30831522E+04					4

110-22-5

C4H6O4 Diacetylperoxide CH<sub>3</sub>-CO-O-O-CO-CH<sub>3</sub> SIGMA=2 STATWT=1 Calculated and  
 extrapolated 2000-6000 K from original tables using Wilhoit's Polynomials  
 HF298=-500+/-10.0kJ REF=Dorofeeva et al. JPCRD 30, (2001), 475. Max Lst Sq  
 Error Cp @ 2300 K 0.80 %.

CH3CO-OO-CO-CH3	T 8/03C	4.H	6.O	4.	0.G	200.000	6000.000	C 118.08804	1
1.47808728E+01	2.21808904E-02	-8.32215014E-06	1.39901235E-09	-8.64737754E-14					2
-6.68299981E+04	-4.65855726E+01	3.60213807E+00	3.52492892E-02	2.10387409E-05					3
-5.57591215E-08	2.58211049E-11	-6.28644087E+04	1.54613635E+01	-6.01358348E+04					4

1708-32-3

C4H6S 2,5-DIHYDROTHIOPHEN REF=DOROFEEVA & GURVICH JPCRD 24, (1995), 1351 EXTRA-  
 POLATED USING WILHOIT'S POLYNOMIALS HF298=86.9 KJ Max Lst Sq Error Cp @ 200 K  
 0.85%.

2,5 C4H6S	T 3/97C	4.H	6.S	1.	0.G	200.000	5000.000	B 86.15764	1
1.00854835E+01	1.90975958E-02	-7.20771905E-06	1.28890804E-09	-8.80278600E-14					2
5.53885520E+03	-2.96760237E+01	1.04681536E+00	2.39100306E-02	4.05153733E-05					3
-7.65294400E-08	3.42334612E-11	8.85389773E+03	2.14459803E+01	1.04516081E+04					4

2669-61-6

C4H7 tt-1-Butene-1-yl \*CH=CHCH<sub>2</sub>CH<sub>3</sub> SIGMA=1 STATWT=2 IA=3.4110 IB=19.5128  
 IC=20.1897 Ir(CH<sub>3</sub>)=0.511592 ROSYM=3 V(3)=1049.3 cm<sup>-1</sup> Ir(C<sub>2</sub>H<sub>5</sub>)=2.0821  
 ROSYM=2 V(3)=524.6 cm<sup>-1</sup> NU=3257,3124,3115,3090,3047,3030,3023,1696,1536,1527,  
 1512,1435,1365,1309,1270,1150,1100,1030,920,828,801,782,655,420,331  
 HF0=62.8 =/-0.75 kcal HF0(cc)=63.3+/-0.75 kcal REF=G3B3LYP calc Miller JPC-A,  
 108, (2004), 2268-2277 Max Lst Sq Error Cp @ 6000 K 0.55%

C4H7 tt-1buten-	T05/04C	4.H	7.	0.	0.G	200.000	6000.000	B 55.09838	1
8.15646382E+00	1.90308835E-02	-6.73262214E-06	1.07333098E-09	-6.36886441E-14					2
2.55826427E+04	-1.61428872E+01	4.19857522E+00	1.19616999E-02	4.23864923E-05					3
-6.30299109E-08	2.59475110E-11	2.75256555E+04	8.57181248E+00	2.95712937E+04					4

Table 4 (continued)

95045-33-3

C4H7 trans-1-Butene-2-yl CH<sub>2</sub>=C\*CH<sub>2</sub>CH<sub>3</sub> SIGMA=1 STATWT=2 IA=3.1683 IB=20.4680  
 IC=21.5460 Ir=0.511592 ROSYM=3 V(3)=979.3 cm<sup>-1</sup> NU=3171,3131,3128,3057(2),  
 3043,2963,1761,1535,1526,1488,1446,1435,1351,1288,1140,1100,1029,970,881,841,  
 788,555,366,286,217 HF0=59.4+/-0.75 kcal HF0(cis)=59.3 kcal REF=G3B3LYP  
 calc Miller JPC-A,108,(2004),2268-2277 Max Lst Sq Error Cp @ 6000 K 0.56%  
 C4H7 trans-1-Bu T05/04C 4.H 7. 0. 0.G 200.000 6000.000 B 55.09838 1  
 8.16688868E+00 1.95680375E-02-6.95694878E-06 1.11504166E-09-6.64079384E-14 2  
 2.37537003E+04-1.77041242E+01 3.77145965E+00 1.46544157E-02 3.70080802E-05 3  
 -5.72714455E-08 2.36641011E-11 2.58014506E+04 9.11906641E+00 2.78022108E+04 4

17787-91-6

C4H7 trans-2-Butene-2yl CH<sub>3</sub>C\*=CHCH<sub>3</sub> SIGMA=1 STATWT=2 IA=1.9855 IB+23.2224  
 IC=24.1643 (Ir(CH<sub>3</sub>)=0.511592 ROSYM=3)x2 V(3)=489.7 cm<sup>-1</sup> V(3)=454.8 cm<sup>-1</sup>  
 Nu=3134,3089,3081,3065,3035,3017,2982,1789,1520,1514,1506,1488,1432,1426,1310,  
 1127,1079,1072,1056,998,849,736,461,248,211 HF0=57.3+/-0.75 kcal HF0(cis)=58.1  
 kcal REF=G3B3LYP calc Miller JPC-A,108,(2004),2268-2277 Max Lst Sq Error  
 Cp @ 6000 K 0.59%  
 C4H7 t-2Buten-2ylT05/04C 4.H 7. 0. 0.G 200.000 6000.000 B 55.09838 1  
 7.26612168E+00 1.99858497E-02-7.12030976E-06 1.14276142E-09-6.81206632E-14 2  
 2.31915554E+04-1.09941637E+01 7.61389036E+00-9.06922602E-03 8.28486476E-05 3  
 -9.61203624E-08 3.59333528E-11 2.44971584E+04-5.90519467E+00 2.69231159E+04 4

2154-62-3

C4H7 trans-3-BUTEN-1-YL CH<sub>2</sub>=CHCH<sub>2</sub>CH<sub>2</sub>\* RADICAL SIGMA=1 STATWT=2 IA=3.3944  
 IB=19.4491 IC=19.9854 IR=2.105394 V(3)=384.7 cm<sup>-1</sup> ROSYM=2 NU=3269,3234,  
 3167,3157,3148,3027,2956,1729,1491,1484,1469,1354,1331,1254,1125,1084,1056,1034,  
 940,905,804,657,471,419,323,136 HF0=52.8+/-0.7 kcal HF0(cis)=53.3+/-0.7 kcal  
 REF=G3B3LYP calc Miller JPC-A,108,(2004),2268-2277 Max List Sq Error Cp @  
 6000 K 0.54%.  
 C4H7 3butene-1yl T05/04C 4.H 7. 0. 0.G 200.000 6000.000 B 55.09838 1  
 8.49073768E+00 1.91056974E-02-6.74370664E-06 1.07343267E-09-6.36251837E-14 2  
 2.04659294E+04-1.74555814E+01 5.07355313E+00 5.27619329E-03 6.23441322E-05 3  
 -8.54203458E-08 3.45890031E-11 2.24615054E+04 5.60318035E+00 2.46070249E+04 4

15819-46-2

C4H7 CH<sub>2</sub>\*CHCHCH<sub>3</sub> trans-1-Methylallyl RADICAL SIGMA=1 STATWT=2 IA=2.2024  
 IB=21.0963 IC=22.7812 IR=0.5116918 ROSYM=3 V(3)=279.8 cm<sup>-1</sup> Nu=3259,3168,  
 3166,3136,3110,3050,3014,1548,1536,1504,1501,1440,1358,1297,1223,1151,1038,1002,  
 1001,890,777,737,546,505,286,218 HF0=36.7+/-0.7 kcal HF0(cis)=37.4+/-0.7 kcal  
 REF=G3B3LYP calc Miller JPC-A,108,(2004),2268-2277 Max Lst Sq Error Cp @ 200 K  
 0.57%  
 C4H7 1-me-allyl T05/04C 4.H 7. 0. 0.G 200.000 6000.000 B 55.09838 1  
 8.08107449E+00 1.95526544E-02-6.93149115E-06 1.10889183E-09-6.59584410E-14 2  
 1.22822959E+04-1.67137903E+01 4.54746808E+00 4.63771460E-03 6.61340221E-05 3  
 -8.97456502E-08 3.61716165E-11 1.43843217E+04 7.30313471E+00 1.63702936E+04 4

98705-00-1

T-C4H7 \*CH<sub>2</sub>CH=CHCH<sub>3</sub> RADICAL 2-Butyl-1yl This radical does not exist and it  
 transits to 1-MethylAllyl which is a resonative specie,thus more stable.  
 REF=Miller JPC-A,108,(2004),2268-2277

Table 4 (continued)

15157-95-6

C4H7 2-METHYL-ALLYL \*CH<sub>2</sub>C(CH<sub>3</sub>)=CH<sub>2</sub> RADICAL SIGMA=2 STATWT=2 IA=8.4666  
 IB=9.5538 IC=17.4983 IR=3.09356 ROSYM=3 V(3)=279.8cm<sup>-1</sup> Nu=3258,3255,3172,  
 3164,3129,3108,3049,1558,1526,1524,1510,1444,1390,1352,1072,1059,1037,981,855,  
 791,758,556,549,482,430,407 HF0=37.1+/-1.5 kcal REF=G3B3LYP calc Miller  
 JPC-A,108,(2004),2268-2277 Max List Sq Error Cp @ 6000 K 0.54%  
 C4H7 2-methylal T05/04C 4.H 7. 0. 0.G 200.000 6000.000 B 55.09838 1  
 8.34970451E+00 1.92508033E-02-6.81360221E-06 1.08484853E-09-6.42422082E-14 2  
 1.24406647E+04-1.87060633E+01 2.38739541E+00 2.06784631E-02 2.89299685E-05 3  
 -5.37553477E-08 2.35670326E-11 1.47584145E+04 1.55529104E+01 1.65497991E+04 4

4548-06-5

C4H7 CYCLOBUTYL RADICAL SIGMA=2 STATWT=2 IA=7.0475 IB=7.7257 IC=13.2005  
 Nu=3204,3131,3081,3019,3015,2999,2994,1526,1496,1489,1331,1304,1260,1230,1225,  
 1199,1046,1020,1010,978,916,912,795,761,751,240,90 HF0=59.6+/-0.7 kcal  
 REF=G3B3LYP calc Miller JPC-A,108,(2004),2268-2277 Max List Sq Error Cp @  
 200 K \*\*\*\* 1.18% \*\*\*\*.  
 C4H7 cyclobutyl T05/04C 4.H 7. 0. 0.G 250.000 6000.000 B 55.09838 1  
 8.09128993E+00 2.02621283E-02-7.25107191E-06 1.16753044E-09-6.97639239E-14 2  
 2.33277928E+04-1.99030399E+01 4.52750826E+00-8.02608115E-03 1.13185713E-04 3  
 -1.46032732E-07 5.85457045E-11 2.59670561E+04 7.19739565E+00 2.76992393E+04 4

391208-88-1 ?

C4H7O 2-BUTANONE RAD CH<sub>3</sub>-CH\*CO-CH<sub>3</sub> SIGMA=1 STATWT=2 IA=8.3576 IB=23.2184  
 IC=30.5369 Ir(CH<sub>3</sub>)=0.51535 ROSYM=3 V(3)=498. cm<sup>-1</sup> REF=Bronstein 2002  
 Ir(CH<sub>3</sub>)=0.50717 ROSYM=3 V(3)=498 cm<sup>-1</sup> Ir(CH<sub>3</sub>CH-)=3.06886 ROSYM=1 V(3)=1234  
 cm<sup>-1</sup> REF=Bronstein 2002 Nu=3177,3163,3155,3107,3056,3049,3019,1624,1514,1509,  
 1506,1497,1444,1415,1409,1228,1146,1050,1044,995,968,798,666,598,524,414,258  
 HF298=-18.163+/-1.9 kcal HF0=-13.78 kcal REF=Burcat G3B3 calc {HF298=-4.92 KCAL  
 REF=THERM} Max Lst Sq Error Cp @ 6000 K 0.53%  
 C4H7O 2-Butanone A 8/05C 4.H 7.0 1. 0.G 200.000 6000.000 B 71.09778 1  
 9.85652328E+00 1.98872938E-02-7.08691627E-06 1.13373982E-09-6.73665286E-14 2  
 -1.37492202E+04-2.22301667E+01 5.97007491E+00 9.72931391E-03 5.08157852E-05 3  
 -7.16606546E-08 2.88687546E-11-1.16733080E+04 2.85386447E+00-9.13992430E+03 4

309966-76-5

C4H7O 2-METYL,ALLYL OXY RADICAL H<sub>2</sub>C=C(CH<sub>3</sub>)CH<sub>2</sub>O\* SIGMA=1 STATWT=2 IA=10.5803  
 IB=20.5589 IC=28.7201 Ir(CH<sub>3</sub>)=0.51444 ROSYM=3 [V(3)=711. cm<sup>-1</sup> REF=East Radom,  
 JCP 106,(1997),6655] Ir(CH<sub>2</sub>O\*)=2.96655 ROSYM=1 [V(3)=1050. vm<sup>-1</sup> est from  
 Bornstein, Group II Molec & Radicals Vol 24 Springer 2002] Nu=3233,3257,3139,  
 3099,3038,2970,2841,1740,1525,1506,1476,1437,1381,1344,1289,1157,1089,1074,1032,  
 977,934,823,802,707,559,410,390,262 HF298=55.748 kJ HF0=75.378 kJ REF=Burcat  
 G3B3 calc {HF298=12.35 KCAL REF=THERM} Max Lst Sq Error Cp @ 6000 K 0.54%.  
 C4H7O 2-Methyl-A A 8/05C 4.H 7.0 1. 0.G 200.000 6000.000 B 71.09778 1  
 1.02561681E+01 2.00758775E-02-7.17606810E-06 1.15056131E-09-6.84810174E-14 2  
 1.87761041E+03-2.60316687E+01 3.43287860E+00 2.32281283E-02 2.72682151E-05 3  
 -5.29221716E-08 2.32310074E-11 4.50163234E+03 1.29269253E+01 6.70485886E+03 4

106-98-9

C4H8 1-BUTENE CH<sub>2</sub>=CH-CH<sub>2</sub>-CH<sub>3</sub> SPECTROSCOPIC DATA NOT AVAILABLE. REF= CHAO & HALL  
 Private Communication HF298=-0.544 kJ {HF298=-0.031+/-0.47 REF=ATcT A}  
 MAX LST SQ ERROR Cp @ 4500 K \*\*\*1.45\*\*\* %.  
 C4H8 T 6/83C 4H 8 0 OG 300.000 5000. B 56.104 1  
 0.20535841E+01 0.34350507E-01-0.15883197E-04 0.33089662E-08-0.25361045E-12 2  
 -0.21397231E+04 0.15556360E+02 0.11811380E+01 0.30853380E-01 0.50865247E-05 3  
 -0.24654888E-07 0.11110193E-10-0.17904004E+04 0.21075639E+02-0.06494670E+03 4

Table 4 (continued)

115-11-7

CH<sub>2</sub>=C(CH<sub>3</sub>)<sub>2</sub> ISOBUTENE SPECTROSCOPIC DATA NOT AVAILABLE REF=CHAO & HALL  
 Private Communication HF298=-17.15 kJ {HF298=-17.574+/-0.52 REF+ATcT A}  
 MAX LST SQ ERROR Cp @ 4500 K \*\*\* 1.27\*\*\* % .

H8C4	T 6/83H	8C	4	0	OG	300.000	5000.0	B	56.104	1
0.44609470E+01	0.29611487E-01	0.13077129E-04	0.26571934E-08	0.20134713E-12						2
-0.50066758E+04	0.10803180E+01	0.26471405E+01	0.25902957E-01	0.81985354E-05						3
-0.22193259E-07	0.88958580E-11	0.40373069E+04	0.12689550E+02	0.20626591E+04						4

624-64-6

C<sub>4</sub>H<sub>8</sub> 2-BUTENE-TRANS CH<sub>3</sub>-CH=CH-CH<sub>3</sub> SPECTROSCOPIC DATA NOT AVAILABLE REF= CHAO  
 & HALL Private Communication HF298=-10.96 kJ {HF298=-11.185+/-0.5 REF=ATcT A}  
 MAX LST SQ ERROR Cp @ 4500 K \*\*\*1.52 %\*\*\* .

C <sub>4</sub> H <sub>8</sub> TRANS	T 6/83C	4H	8	0	OG	300.000	5000.00	B	56.104	1
0.82797676E+00	0.35864539E-01	0.16634498E-04	0.34732759E-08	0.26657398E-12						2
-0.30521033E+04	0.21355710E+02	0.12594252E+01	0.27808424E-01	0.87013932E-05						3
-0.24402205E-07	0.98977710E-11	0.29647742E+04	0.20514290E+02	0.13181775E+04						4

590-18-1

C<sub>4</sub>H<sub>8</sub> 2-BUTENE-CIS CH<sub>3</sub>-CH=CH-CH<sub>3</sub> SPECTROSCOPIC DATA NOT AVAILABLE REF= CHAO  
 & HALL Private Commun. HF298=-7.41 kJ {Hf298=-7.340+/-0.52 kJ REF=ATcT A}  
 MAX LST SQ ERROR Cp @ 4500 K\*\*\* 1.5 %\*\*\*.

C <sub>4</sub> H <sub>8</sub> CIS	T 6/83C	4H	8	0	OG	300.000	5000.	B	56.104	1
0.11097383E+01	0.35542578E-01	0.16481703E-04	0.34412202E-08	0.26411468E-12						2
-0.26507607E+04	0.19366680E+02	0.24108791E+01	0.25147773E-01	0.98473047E-05						3
-0.22716758E-07	0.86585895E-11	0.27758694E+04	0.14097700E+02	0.89121300E+03						4

287-23-0

C<sub>4</sub>H<sub>8</sub> CYCLOBUTANE VALUES FROM Dorofeeva, Gurvich & Jorish JPCRD 15 (1986), 437.  
 EXTRAPOLATED USING WILHOIT'S METHOD. HF298=28.4 KJ Max Lst Sq Error Cp @ 1300 K  
 0.48 %.

C <sub>4</sub> H <sub>8</sub> CY	T 1/90C	4H	8	0	OG	200.000	5000.000	B	56.10752	1
0.59858453E+01	0.26809962E-01	0.10846260E-04	0.20133589E-08	0.14020730E-12						2
-0.56733861E+03	0.12313076E+02	0.38114076E+01	0.96804077E-02	0.12791623E-03						3
-0.16305543E-06	0.64830904E-10	0.18710969E+04	0.85966860E+01	0.34157154E+04						4

505-60-2

C<sub>4</sub>H<sub>8</sub>Cl<sub>2</sub>S S(CH<sub>2</sub>CH<sub>2</sub>Cl)<sub>2</sub> MUSTARD SYMNO=2 STATWT=1 IA=12.48279 IB=238.3000  
 IC=248.7121 Nu=3002,3001,2955,2953,2943(2),2906(2),1468,1466,1465,1461,1345,  
 1328,1275,1271,1252,1226,1131,1125,1023,993,984,964,790,758,754,746,709.6,692,  
 325,318,207.6,198.9,109.4,108.9,59.4,53.1,34.9 HF298=-29.82 kcal REF=MELIUS  
 Database P28L BAC/MP4 calc. 1988 Max Lst Sq Error Cp @ 6000 K 0.52%

MUSTARD S(CH <sub>2</sub> CH <sub>2</sub> S03/01CL 2.S 1.C 4.H 8.G	200.000	6000.000	B	159.07892	1
1.61928145E+01	2.41315425E-02	8.73508032E-06	1.41727945E-09	8.51392369E-14	2
-2.22775039E+04	-5.17666230E+01	7.43521829E+00	1.61310615E-02	7.70227933E-05	3
-1.16433505E-07	4.87658485E-11	1.84131265E+04	9.21100356E-01	1.50059210E+04	4

2691-41-0

C<sub>4</sub>H<sub>8</sub>N<sub>8</sub>O<sub>8</sub> HMX Octogen Solid-beta Cp 290-345 REF= Yin,Ziru,Ganghe,Chengyun  
 17th Internat. Pyrotech. Seminar 1991 Vol 1, 515-521 S298=33.94 cal Graphic  
 Integ HF298(solid)=17.9 Kcal/mol REF=NIST 98 Max Lst Sq Error Cp @ 293 K 0.22  
 %

beta HMX	HF298 C	4.H	8.N	8.O	8.S	273.000	544.000	D	296.15664	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
0.00000000E+00	0.00000000E+00	1.98869800E+01	-1.81294708E-01	1.61616631E-03						3
-3.42368773E-06	2.30310099E-09	2.53647933E+03	-8.79398440E+01	9.00757832E+03						4

Table 4 (continued)

2691-41-0

C4H8N8O8 HMX Octogen SIGMA= 128. STATWT = 1. Ia = 166.71154 Ib = 333.65031  
 Ic = 355.174455 4 (Ir(NO2) = 5.96 V2 = 16.7 kcal/mole) NU = 3110,3076,  
 3034,2992,2979,2977,2914,2912,2076,2062,2051,1968,1892,1747,1726,1706,1464,1412,  
 1406,1397,1385,1382,1367,1366,1356,1338,1312,1271,1258,1224,1179,1167,1141,1127,  
 1109,1071,1046,1021,1005,1004,990,963,819,776,758,736,714,696,676,662,638,625,  
 624,608,544,494,471,434,358,348,338,312,256,218,143,130,122,108,97.1,80.3,74.6,  
 64.6,55.5,393. HF298= 44.9 kcal REF = BURCAT TAE Report # 824 1998  
 {HF298=65.7+/-7.2 kcal REF=o. Dorofeeva & P. Tolmach, Thermochim Acta 240, (1994)  
 47-66} Max Lst Sq Error Cp @ 6000 K 0.63%  
 C4H8N8O8 HMX T 6/98C 4.H 8.N 8.O 8.G 200.000 6000.000 F 296.15664 1  
 3.44746335E+01 4.64515729E-02-1.79061365E-05 2.98652447E-09-1.81854443E-13 2  
 7.27250557E+03-1.48183270E+02 8.14013076E+00 8.33153720E-02 2.72627839E-05 3  
 -9.98161338E-08 4.69225870E-11 1.63985782E+04-3.22778664E+00 2.25944283E+04 4

513-42-8

C4H8O 2-METHYL,ALLYL ALCOHOL SIGMA=1 STATWT=1 IA=10.9165 IB=21.2985  
 IC=28.9536 Ir(CH3)=0.49 ROSYM=3 V(3)=1254. NU=3754,3235,3158,3135,3100,3037,  
 3023,2966,1744,1541,1528,1505,1487,1454,1436,1330,1262,1244,1111,1077,1062,993,  
 977,933,823,726,557,426,401,262,250,188 HF298=-38.514 HF0=-38.51 KCAL  
 REF=Burcat G3B3 calc Max Lst Sq Error Cp @ 6000 K 0.54%  
 C4H8O Methyl Al T 7/04C 4.H 8.O 1. 0.G 200.000 6000.000 B 72.10572 1  
 1.05847949E+01 2.25064337E-02-7.95991069E-06 1.27168200E-09-7.55781638E-14 2  
 -2.45297393E+04-3.10486089E+01 3.74727997E+00 1.98199995E-02 4.63745935E-05 3  
 -7.56066224E-08 3.19921712E-11-2.16544825E+04 9.31161697E+00-1.93808867E+04 4

78-93-3

C4H8O 2-BUTANONE C2H5-CO-CH3 IAIBIC=6268.4E-117 SIGMA=1 NU=2983(4),2941,  
 2910(2),2884,1716,1460(2),1422,1413(2),1373,1346,1263(2),1182,1108,1089,997,952,  
 934,768,760,590,460,413,260 IR(C2H5)=2.621 ROSYM=1 POTENTIAL BARRIER C2H5  
 V(1)=667.8 cm-1 V(3)=334.2 cm-1 IR(CH3-CH2)=0.5119 ROSYM=3 POTENTIAL BARRIER  
 V(3)=919.2 cm-1 IR(CH3)=0.5071 ROSYM=3 POTENTIAL BARRIER V(3))=181.3 cm-1  
 NEL=60 REF=CHAO et al JPCRD 15, (1986) 1369 Max Lst Sq Error Cp @ 1300 K 0.63%  
 HF298=-56.97 KCAL REF=Stull, Sinke & Westrum  
 C4H8O T 5/92C 4H 8O 1 0G 200.000 6000.000 B 72.10692 1  
 0.10155224E+02 0.22543521E-01-0.81766338E-05 0.13266807E-08-0.79735407E-13 2  
 -0.33635513E+05-0.25571125E+02 0.63433693E+01 0.94237046E-02 0.55004487E-04 3  
 -0.73507239E-07 0.28504736E-10-0.31332537E+05 0.88015186E-01-0.28668253E+05 4

21490-63-1

C4H8O trans-2,3-DIMETHYL-OXYRANE (trans-DIMETHYL-ETHYLENE-OXIDE) SIGMA=2  
 STATWT=1 IA=6.8602 IB=24.7368 IC=27.544 (Ir(CH3)=0.5077 ROSYM=3 V(3)=1254.  
 cn-1)x2 NU=3134,3132,3112,3112,3102,3097,3050,3049,1543,1526,1521,1513,1499,  
 1441,1438,1384,1299,1205,1183,1157,1136,1049,1044,979,920,827,762,470,458,283,  
 247 HF298=-32.90 kcal HF0=-27.11 kcal REF=Burcat G3B3 calc Max Lst Sq Error  
 Cp @ 6000 K 0.54%.  
 C4H8O Di-Methyl T 7/04C 4.H 8.O 1. 0.G 200.000 6000.000 B 72.10572 1  
 1.03381768E+01 2.25389675E-02-8.02838070E-06 1.28860864E-09-7.68280865E-14 2  
 -2.17087991E+04-3.13135418E+01 3.97206991E+00 1.28761957E-02 6.71545910E-05 3  
 -9.89399808E-08 4.09976684E-11-1.87300487E+04 7.87415863E+00-1.65563315E+04 4

Table 4 (continued)

106-88-7

C4H8O ETHYL-OXYRANE Ethyl Ethylene-Oxide SIGMA=1 STATWT=1 IA=6.2787 IB=27.2375  
 IC=27.7877 Ir(C2H5)=3.65274 ROSUM=3 V(3)=1254. cm-1 Nu=3181,3122,3115,3102,  
 3098,3078,3048,3043,1558,1539,1530,1518,1465,1440,1368,1308,1285,1201,1179,1155,  
 1140,1071,1042,961,931,869,819,777,454,399,243,218 HF298=-27.71 kcal  
 HF0=-21.83 kcal REF=Burcat G3B3 calc Max Lst Sq Error Cp & 6000 K 0.57%.  
 C4H8O Ethyl OXY T 7/04C 4.H 8.O 1. 0.G 200.000 6000.000 B 72.10572 1  
 9.75283779E+00 2.36899014E-02-8.50522197E-06 1.36844358E-09-8.16432018E-14 2  
 -1.90579489E+04-2.69575674E+01 4.93938398E+00 5.44816194E-04 1.01222605E-04 3  
 -1.34563349E-07 5.40808612E-11-1.60974477E+04 6.34373652E+00-1.39466499E+04 4

109-99-9

C4H8O TETRAHYDROFURAN (OXOLAN CY) SIGMA=2 REF=Chao et.al JPCRD 15, (1986), 1369  
 EXTRAPOLATED 1600-5000 K USING WILHOIT'S POLYNOMIALS HF298=-184.18 KJ  
 REF=Kudchadker, Kudchadker & Wilhoit TRC 1978 Key Chemicals Data Book- Furan,  
 Dihydrofuran, Tetrahydrofuran Max Lst Sq Error Cp @ 200 K 0.12%.  
 C4H8O T.H.FURAN T 3/97C 4H 8O 1 0G 200.000 5000.000 B 72.10692 1  
 6.97323971E+00 2.88949921E-02-1.16992973E-05 2.17090268E-09-1.51075478E-13 2  
 -2.67236416E+04-1.44239686E+01 4.08780471E+00-1.16647870E-02 1.44507977E-04 3  
 -1.83315676E-07 7.25734431E-11-2.38006675E+04 1.16117821E+01-2.21516361E+04 4

123-91-1

C4H8O2 1,4-DIOXANE SIGMA=4 IA=16.3132 IB=17.4452 IC=30.0912 NU=2934,2933.5,  
 2931,2930.7,2855,2850,2847,2841,1485,1479,1471,1465,1419,1398,1382,1342,1302,  
 1293,1260,1216,1158,1150,1135,1094,1038,1003,887,871,849,829,598,475.7,418.6,  
 397,258.4,237 HF298=-75.15+/-1.6 kcal REF=C. MELIUS DATABASE D94T Max Lst Sq  
 Error Cp @ 200 K 0.86%.  
 C4H8O2 DIOXANE T03/97C 4.H 8.O 2. 0.G 200.000 6000.000 B 88.10632 1  
 1.09080022E+01 2.65730193E-02-9.70934955E-06 1.58519471E-09-9.56379521E-14 2  
 -4.38420203E+04-3.79862937E+01 3.64975602E+00 3.21199783E-03 1.12973931E-04 3  
 -1.50581748E-07 6.00072918E-11-3.97765405E+04 9.86785750E+00-3.78167324E+04 4

6993-75-5

C4H8O4 ETHANOIC (ACETIC) ACID DIMER (CH3COOH)2 IAIBIC=1.6141 E-112 Brot=5.3613  
 ROSYM=3 V(3)=168.2 cm-1 NU=3193,3032,2949,1675,1436,1436,1370,1283,1018,886,  
 624,448,196,110,3140,3028,2956,1715,1413,1413,1359,1295,1013,886,624,480,188,  
 2990,1413,1050,934,635,67,47,3000,1436,1112,912,623,115 HF298=-222.04 KCAL.  
 REF=CHAO & ZWOLINSKI JPCRD 7, (1978), 363 Max Lst Sq Error Cp @ 0.55%.  
 (CH3COOH)2 g10/00C 4.H 8.O 4. 0.G 200.000 6000.000 B 120.10392 1  
 1.58244708E+01 2.61835690E-02-9.46100863E-06 1.53338095E-09-9.20479892E-14 2  
 -1.19039137E+05-5.11094706E+01 7.75423757E+00 1.38948935E-02 8.32892300E-05 3  
 -1.20015842E-07 4.90658451E-11-1.15185585E+05-1.22178403E+00-1.11734228E+05 4

293-30-1

C4H8O4 1,3,5,7 Tetra-Oxocane (Octahedron-ring) SIGMA=8 REF=Dorofeeva Thermochim  
 Acta 200, (1992), 121-150 Data from Dorofeeva extrapolated to 5000 K using  
 Wilhoit's polynomials. HF298=-620.2 kJ Max Lst Sq Error Cp @ 200 K 0.63%  
 C4H8O4 Tetraoxoca T11/99C 4.H 8.O 4. 0.G 200.000 5000.000 B 120.10512 1  
 1.23990610E+01 3.33828188E-02-1.36133532E-05 2.53106627E-09-1.76207962E-13 2  
 -8.13386934E+04-4.28948598E+01 3.51394172E+00 1.62812222E-02 1.01537862E-04 3  
 -1.46551354E-07 5.97417135E-11-7.69994933E+04 1.27220188E+01-7.45924895E+04 4

Table 4 (continued)

110-01-0

C4H8S TETRAHYDROTHIOPHEN SIGMA=2 REF=Dorofeeva & Gurvich JPCRD 25, (1995), 1351  
EXTRAPOLATED USING WILHOIT'S POLYNOMIALS HF298=-34.1 KJ Max Lst Sq Error Cp @  
200 K 0.86 %.

C4H8S T.H.THIOPHE T 3/97C 4.H 8.S 1. 0.G 200.000 5000.000 B 88.17352	1
1.05353487E+01 2.35320902E-02-8.77376230E-06 1.56515072E-09-1.06979035E-13	2
-9.48200844E+03-3.23144630E+01 1.55153937E+00 2.25556797E-02 5.70166001E-05	3
-9.59127084E-08 4.15407376E-11-5.90019315E+03 1.99054134E+01-4.10126393E+03	4

505-29-3

C4H8S2 1,4 DITHIANE SIGMA=2 IAIBIC=51450. NU=2944,2936,2905(2),2955(2),  
2919(2),1418,1410,1408,1404,1297,1283,1275,1206(2),1156,1152,1110,999,994,944,  
904,894,821,694,669,653,628,480,374,333,253,277,169 HF298=0.0 KJ

REF=Dorofeeva & Gurvich JPCRD 24, (1995), 1351 Max Lst Sq Error Cp @ 200 K 0.65%

1,4-C4H8S2 T03/97C 4.H 8.S 2. 0.G 200.000 6000.000 B 120.23952	1
1.36035997E+01 2.38171520E-02-8.63455848E-06 1.40243589E-09-8.43096867E-14	2
-6.54885251E+03-4.84322813E+01 1.50684634E+00 3.27456314E-02 4.42731895E-05	3
-8.78680150E-08 3.94466672E-11-2.14083750E+03 1.96208497E+01 0.00000000E+00	4

505-23-7

C4H8S2 1,3 DITHIANE SIGMA=1 IAIBIC=51236. NU=2958,2936,2905,2900(2),2860,2838,  
2818,1432,1426,1417,1387,1285,1272,1244,1210,1180,1175,1152,1090,1010,1009,921,  
887,815,792,748,679,672,636,470,336,315,312,217,167 HF298=-10.0 KJ

REF=Dorofeeva & Gurvich JPCRD 24, (1995), 1351 Max Lst Sq Error Cp @ 200 K 0.66%

1,3-C4H8S2 T03/97C 4.H 8.S 2. 0.G 200.000 6000.000 B 120.23952	1
1.37583597E+01 2.38041270E-02-8.65896154E-06 1.40951445E-09-8.48640095E-14	2
-7.81751735E+03-4.84750572E+01 1.60889846E+00 3.27014397E-02 4.42707028E-05	3
-8.76314400E-08 3.92785746E-11-3.37238305E+03 1.99277613E+01-1.20271670E+03	4

2492-36-6

N-C4H9 N-BUTYL RADICAL. SIGMA=2 STATWT=2 IA=3.4245 IB=22.3499 IC=23.6384

Ir(CH3)=0.49 V3=1254 cm-1 ROSYM=3 NU=3257,3160,3110,3107,3075,3047,3041,3039,  
3013,1539,1529,1523,1515,1489,1438,1382,1344,1311,1299,1210,1102,1076,1031,958,  
875,808,741,523,396,259,248,129 HF298=19.55 kcal HF0=25.09 kcal REF=Ruscic  
G3B3 calc {HF298=19.0 kcal REF=NIST 94; HF298=15.9 kcal REF=TRC/84} MAX LST  
SQ ERROR CP @ 6000 K 0.57% .

C4H9 n-butyl T 7/04C 4.H 9. 0. 0.G 200.000 6000.000 B 57.11426	1
8.97401527E+00 2.39704154E-02-8.48703645E-06 1.35644127E-09-8.06234913E-14	2
5.19161526E+03-2.31075609E+01 4.73737837E+00 9.69051565E-03 6.63846383E-05	3
-9.24799302E-08 3.74006099E-11 7.57382332E+03 4.91063455E+00 9.83838903E+03	4

2348-55-2

s-C4H9 sec-Butyl Radical Sigma=1 STATWT=2 Ia=3.1891 Ib=23.1992 Ic=24.6259

Rotor 1 Ir=0.48 V(3)=1253. cm-1 ROSYM=3 Rotor 2 Ir=0.48 V(3)=0.0 ROSYM=3

Rotor 3 Ir=1.4 V3=0.0 ROSYM=1 Nu=3164,3118,3111,3102,3047,3044,3013,2956,  
2926,1536,1528,1518,1505,1502,1441,1438,1427,1331,1286,1139,1143,1086,1033,997,  
987,854,777,428,413,263 HF298=16.78 kcal REF=Burcat G3B3 calc

{HF298=69.0+/-4.2 kJ HF0=93.78 kJ REF=Tsang JACS 107 (1985), 2872-2880.} Max  
Lst Sq Error Cp @ 6000 K 0.60 %.

C4H9 s-butyl T 6/04C 4.H 9. 0. 0.G 200.000 6000.000 B 57.11426	1
7.72287211E+00 2.43427284E-02-8.65476475E-06 1.38712529E-09-8.26084187E-14	2
4.15004489E+03-1.43949625E+01 5.42089393E+00-9.12146870E-04 8.84998581E-05	3
-1.12115531E-07 4.38222782E-11 6.28927311E+03 5.04210029E+00 8.44598852E+03	4



Table 4 (continued)

4630-45-9

C4H9 iso-BUTYL RADICAL CH<sub>3</sub>CH(CH<sub>3</sub>)CH<sub>2</sub>\* STATWT=2 SIGMA=2 Ia=10.0033 Ib=10.6623  
 Ic=18.2551 FIRST ROTOR = SECOND ROTOR ROSYM=3 V(3)=1254. cm<sup>-1</sup> IR=0.49  
 NU=3255,3157,3114,3112,3110,3109,3045,3040,2913,1541,1532,1522,1518,1489,1439,  
 1424,1347,1338,1217,1191,1104,991,976,953,913,818,515,399,372,357,260  
 HF298=73.78 kJ+/-3. REF=Burcat G3B3 calc {HF298=70+/-4.2 kJ HF0=94.26 kJ  
 REF=Wing Tsang JPCRD 19 (1990), 1-68} Max Lst Sq Error Cp @ 6000 K 0.55%  
 C4H9 isobutyl rad T 6/04C 4.H 9. 0. 0.G 200.000 6000.000 B 57.11426 1  
 9.61250942E+00 2.28581786E-02-8.06391309E-06 1.28556553E-09-7.62730799E-14 2  
 4.15218608E+03-2.66485099E+01 3.34476784E+00 2.31869650E-02 3.28261040E-05 3  
 -5.96398514E-08 2.58980820E-11 6.66201200E+03 9.68860372E+00 8.87422590E+03 4

1605-73-8

C4H9 T-C4H9 (CH<sub>3</sub>)<sub>3</sub>C\* STATWT=2 SIGMA=3 Ia=10.5267 Ib=10.5895 Ic=19.4800,  
 THREE EQUIV FREE ROTORS (ROSYM=3, V(3)=0.0, Ir=0.47)x3 Nu=3098.5(2),3093,3053,  
 3048.5(2),2955,2945,2944,1523.7(2),1517,1502,1500(2),1454,1428,1426,1311,1307,  
 1108,1019,1016,981,950.7(2),762,381,376,252 HF298=55.04 kJ HF0=76.8 kJ  
 {HF298=52.04 kJ HF0=77.35 kJ REF=Tsang JPCRD 19, (1990), 1-68.} Max Lst Sq Error  
 Cp @ 1300 K 0.64%  
 C4H9 t-butyl T 6/04C 4.H 9. 0. 0.G 200.000 6000.000 B 57.11426 1  
 6.72557390E+00 2.53649194E-02-9.05306262E-06 1.45474620E-09-8.67934112E-14 2  
 2.57430692E+03-8.89920414E+00 6.45910754E+00-1.02015930E-02 1.06310577E-04 3  
 -1.25717030E-07 4.75543216E-11 4.43420391E+03 1.30648608E+00 6.61981524E+03 4

123-75-1

C4H9N PYRROLIDINE (TETRAHYDROPYRROLE, TETRAMETHYLENEIMINE) IAIBIC=3330.5  
 IR=1.119 ROSYM=2. V(2)=280. cm<sup>-1</sup> NU=3367,2970(2),2882(4),2818(2),1480(2),  
 1468(2),1418,1348,1299,1284,1239,1220,1205,1171,1136,1105,1080,1053,1025,980,  
 925,909,872,844,792,612,570,145 HF298=-3.59+/-0.80 KJ REF=Das et. al JPCRD 22  
 (1993), 659 Max Lst Sq Error Cp @ 200 K \*\*1.47%\*\*  
 C4H9N PYRROLIDINE T 3/95C 4H 9N 1 0G 200.000 6000.000 B 71.12220 1  
 0.91914472E+01 0.27301993E-01-0.98874802E-05 0.16049052E-08-0.96462592E-13 2  
 -0.59280463E+04-0.26546544E+02 0.55475933E+01-0.20299796E-01 0.17343060E-03 3  
 -0.21528524E-06 0.84721240E-10-0.23303304E+04 0.56593427E+01-0.43177529E+03 4

627-05-4

C4H9NO2 1-Nitro-Butane SIGMA=1 STATWT=1 IA = 17.914472 IB = 52.800976  
 IC = 57.4685911 Ir (NO<sub>2</sub>) = 5.96 ROSYM = 2 V(2) = 0.08 kcal/mole  
 Ir(CH<sub>3</sub>) = 0.51666 ROSYM = 3 V(3) = 3.5 kcal/mole Ir(C<sub>2</sub>H<sub>5</sub>) = 2.104 ROSYM = 2  
 V(2) = 9.0 kcal Ir(C<sub>3</sub>H<sub>7</sub>) = 2.22 ROSYM = 3 V(3) = 13.64 kcal  
 NU = (3157,3092,3083,3062,3060,3056),2970,2889,2760,2276,1568,1440,(1425,1408,  
 1405,1400,1394),1379,(1374,1346,1278,1241),1211,(1191,1160),1123,(1088,1054,  
 1033),900,860,752,712,611,(535,446,368,243). HF298 = -34.4 kcal  
 REF=Stein, NIST 94 Max Lst Sq Error Cp @ 6000 K 0.70%  
 NITRO-BUTANE T05/98C 4.H 9.N 1.O 2.G 200.000 6000.000 B 103.12100 1  
 1.27918861E+01 2.96302599E-02-1.10618131E-05 1.81914243E-09-1.10094356E-13 2  
 -2.40186756E+04-4.05022397E+01 4.50296897E+00 1.41859282E-02 9.14552906E-05 3  
 -1.29431188E-07 5.23563809E-11-1.98606730E+04 1.15748426E+01-1.73106533E+04 4

Table 4 (continued)

19062-98-7

C4H9O N-BUTOXY RADICAL SIGMA=1 STATWT=2 IA=6.3735 IB=35.0962 IC=37.9720  
 Ir(CH3)=0.50841 V(3)=2400 cm-1 ROSYM=3 Ir(C2H5)=4.79876 V(3)=2400 cm-1  
 ROSYM=2 Ir(-CH2O)=3.19759 V(3)=2400 cm-1 ROSYM=2 NU=3113,3109,3082,3064,3043,  
 3032,3026,2041,2888,1541,1531,1525,1510,1444,1427,1389,1377,1343,1331,1275,1215,  
 1134,1097,1054,1032,962,883,856,761,533,477,343,251 HF298=-56.35 kcal HF0=-29.0  
 kcal REF=Burcat G3B3 {HF298=-13.9 KCAL NIST 94} Max Lst Sq Error Cp @  
 1300 K 0.67%.

C4H9O n-butoxy r	A08/04C	4.H	9.0	1.	0.G	200.000	6000.000	B	73.11366	1	
						1.21336180E+01	2.43954328E-02	-9.04409323E-06	1.48350965E-09	-8.96467065E-14	2
						-1.29883091E+04	-3.89685328E+01	5.61984431E+00	2.12772932E-03	1.02679749E-04	3
						-1.34097807E-07	5.25493048E-11	-9.21442557E+03	4.46683857E+00	-6.77732206E+03	4

26397-42-2

C4H9O I-BUTOXY RADICAL 2 METHYL PROPOXY RADICAL (CH3)2CHCH2O\* SIGMA=9 STATWT=2  
 IA=11.0039 IB=23.0220 IC=30.9306 (Ir(CH3)=0.51033 ROSYM=3. V3=2400 cm-1)x2  
 Nu=3133,3115,3105,3099,3042,3036,3028,2938,2874,1541,1533,1523,1520,1448,1430,  
 1395,1388,1358,1327,1236,1204,1144,1083,1030,978,945,933,825,608,496,412,342,  
 263,242 HF298=-15.552 kcal HF0=-36.703 kJ REF=Burcat G3B3 calc Max Lst Sq  
 Error Cp @ 1300 K 0.65%.

C4H9O i-butoxy r	A08/04C	4.H	9.0	1.	0.G	200.000	6000.000	B	73.11366	1	
						1.16309708E+01	2.47981574E-02	-9.01550536E-06	1.46714720E-09	-8.83214518E-14	2
						-1.37854612E+04	-3.81956151E+01	3.80297372E+00	1.56874209E-02	6.81105412E-05	3
						-9.83346774E-08	3.95261902E-11	-1.00832243E+04	9.78963305E+00	-7.82602559E+03	4

26397-42-2

C4H9O S-BUTOXY-2 RADICAL CH3CH(O\*)CH2CH3 SIGMA=1 STATWT=2 IA=9.7561  
 IB=24.5156 IC=31.2736 Ir(CH3)=0.51107 ROSYM=3 V(3)=2400. cm-1 Ir(CH3)=0.509545  
 ROSYM=3 V(3)=2400. cm-1 Ir(C2H5)=3.87374 ROSYM=2 V(3)=2400. cm-1 Nu=3141,  
 3139,3125,3113,3076,3056,3049,3038,2849,1539,1527,1525,1518,1511,1437,1423,1360,  
 1318,1254,1202,1179,1079,1074,1042,1003,948,939,801,777,469,437,366,247  
 HF298=-16.693 kcal HF0=-10.31 kcal REF=Burcat G3B3 calc {HF298=-17.5 KCAL  
 REF=NIST 94} Max Lst Sq Error Cp @ 1300 K 0.65%.

C4H9O s-butoxy r	A09/04C	4.H	9.0	1.	0.G	200.000	6000.000	B	73.11366	1	
						1.23515300E+01	2.40070435E-02	-8.82800485E-06	1.44359362E-09	-8.71114711E-14	2
						-1.46466302E+04	-4.13524913E+01	4.43662987E+00	1.00289940E-02	8.56583118E-05	3
						-1.18678067E-07	4.74411822E-11	-1.07133878E+04	8.21507294E+00	-8.40019580E+03	4

3141-58-0

C4H9O T-BUTOXY RADICAL (CH3)3CO\* SIGMA=3 STATWT=2 IA=17.0722 IB=17.1074  
 IC=18.9493 (Ir(CH3)=0.51216 ROSYM=3 V3=2400 cm-1)x3 NU=3154,3142,3134.5(2),  
 3126,3199,3063,3055,3049,1545,1523,1519,1515,1508,1493,1440,1407,1400,1265,1192,  
 1179,1026,1011,969,936,906,888,736,429,409,405,328,322 HF298=-20.775 kcal  
 HF0=-14.435 kcal REF=Burcat G3B3 calc {HF298=-22.0 KCAL REF=NIST 94} Max Lst  
 Sq Error Cp @ 1300 K 0.59%.

C4H9O T butoxy r	T08/04C	4.H	9.0	1.	0.G	200.000	6000.000	B	73.11366	1	
						1.27371509E+01	2.33707342E-02	-8.50516678E-06	1.38519973E-09	-8.34398061E-14	2
						-1.66940150E+04	-4.53156321E+01	2.77057100E+00	2.68033175E-02	4.12718360E-05	3
						-7.22054739E-08	3.02642276E-11	-1.27079262E+04	1.21532856E+01	-1.04543262E+04	4

Table 4 (continued)

3395-62-8

C4H9O2 tert-Butyl-Peroxy Radical SIGMA=3 STATWT=2 IA=18.7345711 IB=29.2614186  
 IC=29.5062781 (Ir(CH3)=0.5169832 ROSYM=3 V(3)=1329.1 cm-1)x3 Ir(O-O)=2.8516  
 ROSYM=3 V(3)=314.8 cm-1 Nu=3178(2),3176,3086,3084,3083(2),3082,3080,1442,  
 1417(2),1412,1406,1403,1402,1398(3),1321,1293,1220,1010(2),976,958(2),912,815,  
 607,466,435,378,333,278 REF=PM3 + Wang HF298=-102.97+/-15. kJ REF=Thergas  
 Rough Estimate. HF0=-74.3 kJ Max Lst Sq Error Cp @ 200 K & 6000 K 0.51%.

C4H9O2 PeroxyTe T 9/03C 4.H 9.O 2. 0.G 200.000 6000.000 B 89.11306 1  
 1.38099210E+01 2.37496067E-02-8.42862219E-06 1.34570534E-09-7.98783159E-14 2  
 -1.87367759E+04-4.65324829E+01 4.55297174E+00 2.41748992E-02 5.52718373E-05 3  
 -9.49679000E-08 4.13649243E-11-1.51365186E+04 6.88006921E+00-1.23843738E+04 4

106-97-8

N-C4H10 N-BUTANE \*\*\*This is an equilibrium mixture of 1/3 trans and 2/3 gauche  
 through STATWT. T0=760 cal for gauche is included in V of C3H5\*\*\* STATWT=1/3  
 SIGMA=2 IA=3.6865 IB=24.704 IC=23.093 Ir=0.52483 ROSYM=3 V(3)=1154. cm-1  
 Ir=0.40633 ROSYM=3 V(3)=1154. cm-1 Brot1=1.5443 Brot2=-0.10258 Brot3=0.06043  
 Brot4=-0.00612 ROSYM=1 V(1)=401. V(2)=-40.97 V(3)=1152.7 cm-1 NU=2965,2872,  
 2853,1460,1442,1382,1361,1151,1059,842,432,2968,2930,1461,1257,948,731,2965,  
 2912,1460,1300,1180,803,2968,2780,2853,1461(2),1379,1290,1009,964,271  
 For Gauche T0=0 STATWT=2/3 SIGMA=2 IA=6.589 IB=20.299 IC=17.05 Internal rot as  
 for trans Nu=2968(4),2920(2),2870(2),2860(2),1460(4),1450(2),1380(2),1370,1350,  
 1281,1233,1168,1133,1077,980(2),955,827,788,747,469,320 REF = CHEN, WILHOIT &  
 ZWOLINSKI JPCRD 4, (1975), 859 HF298=-125.79 kJ HF0=-98.463 kJ REF=TRC 10/85  
 {HF298=-125.865+/-0.38 kJ REF=ATcT A} MAX LST SQ ERROR Cp @ 200 K 0.66 %.

C4H10 n-butane g12/00C 4.H 10. 0. 0.G 200.000 6000.000 B 58.12220 1  
 9.44547835E+00 2.57856620E-02-9.23613194E-06 1.48631762E-09-8.87891206E-14 2  
 -2.01383773E+04-2.63477585E+01 6.14474013E+00 1.64500242E-04 9.67848789E-05 3  
 -1.25486208E-07 4.97846257E-11-1.75989467E+04-1.08058878E+00-1.51289733E+04 4

75-28-5

I-C4H10 ISOBUTANE (2-METHYLPROPANE) STATWT=1 SIGMA=81 IA=18.648 IB=10.777  
 IC=10.777 IR=3X(0.51364) V3=3851. cal V6=-150. cal NU=2962(5),2904,2880,  
 1477,1394,1177,797,433,2958,1450,981(3),2894(2),1477(2),1475(2),1371(2),1330(2),  
 1166(2),966(2),367(2), (TORSION 256,220(2)) HF298=-134.648+/-0.63 kJ REF=CHEN,  
 WILHOIT & ZWOLINSKI Thermochim Acta 10 (1974), 359 {HF298=-134.355+/-0.4 kJ  
 REF=ATcT A} MAX LST SQ ERROR Cp @ 200 K 0.64 % .

C4H10 isobutane g 8/00C 4.H 10. 0. 0.G 200.000 6000.000 B 58.12220 1  
 9.76991697E+00 2.54997141E-02-9.14142587E-06 1.47328201E-09-8.80799697E-14 2  
 -2.14052667E+04-3.00329670E+01 4.45479140E+00 8.26058864E-03 8.29886433E-05 3  
 -1.14647616E-07 4.64569994E-11-1.84593929E+04 4.92740653E+00-1.62354727E+04 4

107-44-8

C4H10FO2P SARIN CH(CH3)2OP(O)FCH3 SIGMA=1 IA=30.7204 IB=67.1005 IC=73.1898  
 NU=2962,2959,2958,2947,2941,2927,2921,2885,2878,2872,1475,1467,1460,1456,1435,  
 1431,1411,1399,1372,1355,1352,1287,1167,1143,1123,1024,922,917,908,904,842,827,  
 751,636,511,457,413,382,353,309,276,255,244,223,192,146.8,82,40.1 REF=C.MELIUS  
 DATABASE BACMP4 #2417 Q2U HF298=-230.2+/-9.57 KCAL Max Lst Sq Error Cp @ 1300 K  
 0.56%.

C4H10FO2P SARIN T 9/96 WARNING! G 200.000 6000.000 D 140.09437 1  
 0.18578606E+02 0.30137329E-01-0.10920099E-04 0.17729267E-08-0.10654834E-12 2  
 -0.12429242E+06-0.68579536E+02 0.52448929E+01 0.45868801E-01 0.21805453E-04 3  
 -0.61857475E-07 0.28400543E-10-0.11952678E+06 0.55156043E+01-0.11584048E+06 4

Table 4 (continued)

110-85-0

C4H10N2 1,4-Piperazine SIGMA=4 STATWT=1 IA=17.7816 IB=18.6214 IC=33.2233  
 Nu=3498,3454,3097(2),3072(2),3051,3047,2910.2900,1529,1523,1510(2),1499,1496,  
 1443,1416,1378,1365,1361,1315,1246,1206,1180,1166,1137,1082,1046.5(2),932,890,  
 880,850,826,773,579,476,447,412,263,261 HF298=32.058 kJ HF0=70.650 kJ  
 REF=Burcat G3B3 calc {HF298=225+/-3.6 kJ Zhang et al Acta Chimica Sin. 39,  
 (1981),485.} Max Lst Sq Error Cp @ 200 K 0.94%.  
 C4H10N2 1,4-PIPE A03/05C 4.H 10.N 2. 0.G 200.000 6000.000 B 86.13568 1  
 1.04879953E+01 3.14741038E-02-1.12833865E-05 1.81933575E-09-1.08829314E-13 2  
 -2.32285856E+03-3.70632811E+01 3.22862722E+00 3.00564238E-03 1.30125796E-04 3  
 -1.73154524E-07 6.91836772E-11 1.91930968E+03 1.18480207E+01 3.85564609E+03 4

71-36-3

C4H10O-N 1-BUTANOL SIGMA=3 STATWT=1 IAIBIC=8444.0E-117 NU=3300,2290(9),1470,  
 1450(4),1294(7),1250,1070,1050,955(4),890(3),446,392,350 INTERNAL ROTATIONS  
 CH3-C3H6OH ROSYM=1 IR=0.485 POTENTIAL BARRIER V(3)=1140 cm-1 NEL=60  
 C2H5-C2H4OH ROSYM=1 IR=2.038 POTENTIAL BARRIER V(3)=1140 cm-1 NEL=60  
 C3H7-CH2OH ROSYM=1 IR=1.835 POTENTIAL BARRIER V(3)=1140 cm-1 NEL=60  
 C4H9-OH ROSYM=1 IR=0.127 POTENTIAL BARRIER V(3)=258.8 cm-1 NEL=60  
 HF298=-274.68 kJ REF=Chao et. al, JCPRD 15, (1986), 1369 Max Lst Sq Error  
 Cp @ 1300 K 0.77%  
 C4H10O-N T07/96C 4H 100 1 0G 200.000 6000.000 B 74.12280 1  
 0.13084060E+02 0.26489386E-01-0.10030766E-04 0.16703993E-08-0.10204842E-12 2  
 -0.39853115E+05-0.42581058E+02 0.59455772E+01 0.23216158E-02 0.10865741E-03 3  
 -0.14026051E-06 0.54446937E-10-0.35620542E+05 0.52265747E+01-0.33036174E+05 4

78-92-2

C4H10O-S 2-BUTANOL (D,L) SYMNO=3 STATWT=1 IAIBIC=7910.E-117 NU=3682,2980(6),  
 2943(2),2891,1450(4),1394,1380(2),1350,1314,1290,1250,1145,1110,1080,1034,992,  
 970,912,820,780,500,435,382,274 INTERNAL ROTATIONS  
 CH3-C2H4OHCH3 ROSYM=1 IR=0.5043 POTENTIAL BARRIER V(3)=1084.2 cm-1 NEL=60  
 C2H5CHOH-CH3 ROSYM=1 IR=0.5043 POTENTIAL BARRIER V(3)=1399.3 cm-1 NEL=60  
 C2H5-CHOHCH3 ROSYM=1 IR=3.027 POTENTIAL BARRIER V(3)= 752.3 cm-1 NEL=60  
 C4H9-OH ROSYM=1 IR=0.127 POTENTIAL BARRIER V(3)= 279.7 cm-1 NEL=60  
 HF298=-292.63 kJ REF=Chao et. al, JCPRD 15, (1986), 1369 Max Lst Sq Error  
 Cp @ 6000 K 0.57%  
 C4H10O-S T07/96C 4H 100 1 0G 200.000 6000.000 B 74.12280 1  
 0.11644218E+02 0.25565041E-01-0.91441752E-05 0.14708132E-08-0.87878387E-13 2  
 -0.40944516E+05-0.32554307E+02 0.52699764E+01 0.14103965E-01 0.70685163E-04 3  
 -0.10285799E-06 0.42246905E-10-0.37834271E+05 0.72163727E+01-0.35194974E+05 4

62958-68-3

C4H10O-T 2METHYL-2PROPANOL SIGMA=54 IAIBIC=5961.7E-117 NU=3643,2980(6),  
 2910(2),2880,1472(5),1450,1395,1374(2),1330,1230,1215,1140,1106(2),1013(3),919,  
 748,462(2),424,356,344 INTERNAL ROTATIONS THREE EQUIVALENT ROTATIONS + 1  
 CH3-COH(CH3)2 ROSYM=1 IR=0.5145 POTENTIAL BARRIER V(3)=1329.1 cm-1 NEL=60  
 C4H9-OH ROSYM=1 IR=0.1291 POTENTIAL BARRIER V(3)= 314.8 cm-1 NEL=60  
 HF298=-312.63 kJ REF=Chao et. al, JCPRD 15, (1986), 1369 Max Lst Sq Error Cp  
 @ 6000 K 0.547%  
 C4H10O-T T07/96C 4H 100 1 0G 200.000 6000.000 B 74.12280 1  
 0.12195905E+02 0.25213437E-01-0.89531088E-05 0.14332117E-08-0.85400239E-13 2  
 -0.43495400E+05-0.39715527E+02 0.41048907E+01 0.23022720E-01 0.53016433E-04 3  
 -0.87928571E-07 0.37588572E-10-0.40159890E+05 0.77499347E+01-0.37600349E+05 4

Table 4 (continued)

75-91-2

C4H10O2 tert-Butyl Hydroperoxy (CH<sub>3</sub>)<sub>3</sub>COOH SIGMA=3 STATWT=1 IA=18.7883288  
 IB=31.1526946 IC=31.4487605 (IR(CH<sub>3</sub>)=0.5172455 ROSYM=3 V(3)=1329.1 cm<sup>-1</sup>)x3  
 IR(OH)=0.147536 ROSYM=1 V(3)=314.8 cm<sup>-1</sup> NU=3988,3987,3183,3182,3097,3090(2),  
 3086(2),3085,1514,1454,1432,1413(2),1411,1404,1402,1394(2),1318,1282,1277,1014,  
 1010,974,956(2),941,877,812,536,491,443,376,374,347,274 REF=PM3 + Wang  
 HF298=-247.78+/-10 kJ HF0=-215.13 kJ REF=Thergas {HF298=-246.5+/-5 kJ  
 REF=Kozlov & Rabinovich Tr Khim Khim Tekhnol. (1964) 189-193}. Max Lst Sq Error  
 Cp @ 6000 K 0.47%.

C4H10O2 T 9/03C 4.H 10.O 2. 0.G 200.000 6000.000 B 90.12100 1  
 1.46292637E+01 2.51457268E-02-8.80947061E-06 1.39841089E-09-8.27380629E-14 2  
 -3.64714576E+04-5.20089703E+01 3.08440835E+00 3.82884213E-02 2.86328998E-05 3  
 -7.10015659E-08 3.32770291E-11-3.25506989E+04 1.16695693E+01-2.98009143E+04 4

594-27-4

C4H12Sn TetraMethylStanum SN(CH<sub>3</sub>)<sub>4</sub> SIGMA(external)=12 STATWT=1  
 IA=IB=IC=35.1336 (IB=0.50857 ROSYM=3 V3=154. cm<sup>-1</sup>)x3 IB=0.50857 ROSYM=3  
 V3=147. cm<sup>-1</sup> Nu=2928(3),2926(5),2859,2857(3),1444.5(3),1435(5),1257,1246,  
 768(3),766(2),656.5(3),486(3),465,136(3),126(2) HF298=-20.502+/-4.2 kJ  
 HF0=+11.00 kJ REF=Allendorf & Melius JPC A 109(2005),4939 Max Lst Sq Error  
 Cp @ 6000 K 0.55%

Sn(CH<sub>3</sub>)<sub>4</sub> A 6/05SN 1.C 4.H 12. 0.G 200.000 6000.000 B 178.84808 1  
 1.38790401E+01 2.92000977E-02-1.04178179E-05 1.67323152E-09-9.97829904E-14 2  
 -8.81907052E+03-4.02553679E+01 6.19363827E+00 3.87714034E-02 5.88990229E-06 3  
 -3.20231048E-08 1.54029293E-11-6.03168664E+03 2.46477535E+00-2.46576166E+03 4

871-33-0

C4H12Sn DiEthylDiHydroxyStanum (C<sub>2</sub>H<sub>5</sub>)<sub>2</sub>SnH<sub>2</sub> SIGMA(external)=2 STATWT=1  
 IA=18.0524 IB=56.3213 IC=68.6493 Ir(C<sub>2</sub>H<sub>5</sub>)=3.2144 ROSYM=1 V3=430.2 cm<sup>-1</sup>  
 Ir(C<sub>2</sub>H<sub>5</sub>)=3.02226 ROSYM=1 V3=447.7 cm<sup>-1</sup> Ir(CH<sub>3</sub>)=0.4968 ROSYM=3 V3=1025 cm<sup>-1</sup>  
 Ir(CH<sub>3</sub>)=0.5069 ROSYM=3 V3=14002.5 cm<sup>-1</sup> Nu=2915.5(2),2898(2),2892.5(2),  
 2863.5(2),2849.5(2),1760,1752,1475(2)1470(2),1439(2),1396.5(2),1236,1233,  
 1221(2),1002,996,938,933,931(2),704,677,672,580,513,463,449,347,244,211,207.5  
 HF298=56.484+/-7.6 kJ HF0=90.910 kJ REF=Allendorf & Melius JPC A 109(2005),4939  
 Max Lst Sq Error Cp @ 1300 K 0.57%

H2Sn(C<sub>2</sub>H<sub>5</sub>)<sub>2</sub> A 6/05SN 1.C 4.H 12. 0.G 200.000 6000.000 B 178.84808 1  
 1.53342568E+01 2.85972363E-02-1.03797982E-05 1.67880820E-09-1.00479429E-13 2  
 -3.20700314E+02-4.91843361E+01 5.22643062E+00 3.83917158E-02 2.00663186E-05 3  
 -5.18248688E-08 2.32704274E-11 3.44291836E+03 7.61234779E+00 6.79342499E+03 4

1071-98-3

C4N2 CARBON SUBNITRID (2-BUTYNEDINITRILE) SIGMA=2 STATWT=1 B0=0.044891 cm<sup>-1</sup>  
 Nu=2333,2267,2241,1154,640,504(2),471(2),263(2),107(2) REF=Khanna et al Spectro-  
 chim Acta 43A, (1987),421 & Brown et al JPC 93(1989),5679 HF298=529.2+/-0.8 kJ  
 REF=TRC 12/93 Max Lst Sq Error Cp @ 1300 K 0.43%

C4N2 g 6/01C 4.N 2. 0. 0.G 200.000 6000.000 B 76.05628 1  
 1.04153519E+01 5.71823954E-03-2.12579288E-06 3.50943265E-10-2.13327917E-14 2  
 6.00000379E+04-2.67166250E+01 2.17476309E+00 4.76126863E-02-8.98016589E-05 3  
 8.41509508E-08-2.97993323E-11 6.15242900E+04 1.16619961E+01 6.36477676E+04 4

Table 4 (continued)

12595-82-3

C5 SIGMA=2 STATWT=1 IB=32.7 Nu=1600,400,1950,1540,520(2),330(2),130(2)  
 HF0=1040.+/-60. kJ HF298=1050.92 KJ REF=Gurvich 1991. Max Lst Sq Error Cp  
 @ 1200 K 0.45%

C5	g 8/00C	5.	0.	0.	0.G	200.000	6000.000	B	60.05350	1
	9.57455603E+00	3.86017176E-03	-1.47557854E-06	2.48048107E-10	-1.52659550E-14					2
	1.23054088E+05	-2.37138042E+01	3.35869799E+00	3.24352369E-02	-5.93062255E-05					3
	5.60118909E-08	-2.03076689E-11	1.24376816E+05	6.04923346E+00	1.26396415E+05					4

678-26-2

C5F12 PERFLUOROPENTANE (FC-4-1-12) SIGMA=18 CALCULATED and EXTRAPOLATED USING  
 NIST 94 AND BOZZELLI & RITTER'S PROGRAM. HF298=-607.86 KCAL Max Lst Sq Error Cp  
 @ 1400 K 0.18%

C5F12	FC 41-12	T12/94C	5F	12	0	0G	298.150	5000.000	E	288.03584	1
	0.36667427E+02	0.11143649E-01	-0.46707310E-05	0.86434283E-09	-0.58866364E-13						2
	-0.31952055E+06	-0.15059131E+03	0.41651260E+00	0.12785646E+00	-0.14464730E-03						3
	0.74809522E-07	-0.14534599E-10	-0.31055833E+06	0.32067147E+02	-0.30588830E+06						4

104602-63-3

C5H RAD T0=0. STATWT=4. IB=35.5335 NU=712.(2),557.(2),637.(2),843.,3329.,  
 2290.,586.(2),2200.,1570. SIGMA=1. T0=4000. STATWT=2. REF=DUFF & BAUER  
 MAX LST SQ ERROR CP @ 400 K 0.88 % . HF0=185.4 KCAL.

C5H	T12/81C	5H	1	0	0G	300.000	5000.000	C	61.0629	1
	0.86957493E+01	0.60543008E-02	-0.20160105E-05	0.28928926E-09	-0.14700995E-13					2
	0.90310687E+05	-0.21029110E+02	0.16348248E+01	0.25095381E-01	-0.12066364E-04					3
	-0.10465111E-07	0.88099883E-11	0.92124875E+05	0.15135100E+02	0.93598280E+05					4

117992-78-6

C5H2 RAD SIGMA=2. T0=0 STATWT=3. IB=37.7286 NU=627(2),350(2),1900,630(2),  
 3329(2),1800,550(2),1570,450(2),843 T0=1576.4 STATWT=2. T0=2624. STATWT=1.  
 REF=DUFF & BAUER MAX LST SQ ERROR CP @ 400 K 0.62 % .HF0=165. KCAL

C5H2	T12/81C	5H	2	0	0G	300.000	5000.000	C	62.0709	1
	0.11329175E+02	0.74240565E-02	-0.26281887E-05	0.40825410E-09	-0.23013326E-13					2
	0.78787062E+05	-0.36184340E+02	0.30623217E+01	0.27099982E-01	-0.10091697E-04					3
	-0.12727451E-07	0.91672191E-11	0.81149687E+05	0.70842413E+01	0.83156537E+05					4

591755-73-6

C5H2Cl2O 3,4-DICHLORO-2,4-CYCLOPENTADIENE-1-ONE SIGMA=2 IA=42.3909 IB=71.0170  
 IC=113.407915 NU=3286,3285,1814,1652,1620,1278,1218,1136,1103,929,886,863,766,  
 713,695,629,529,479,422,378,292,176,148,143 HF298=-12.17 kJ HF0=-5.59 kJ  
 REF=Janoschek J. Mol.Struct 661-2,(2003),635 Max Lst Sq Error Cp @ 1300 K 0.44%

C5H2Cl2O	3,4-Cyc	T06/03C	5.H	2.O	1.CL	2.G	200.000	6000.000	B	148.97418	1
	1.57844051E+01	1.13161217E-02	-4.17819275E-06	6.87366689E-10	-4.17039260E-14						2
	-7.74449233E+03	-5.36347657E+01	1.25636860E+00	5.24381406E-02	-4.28285490E-05						3
	1.08399553E-08	1.86208134E-12	-3.81291739E+03	2.10643718E+01	-1.46370622E+03						4

591768-87-5

C5H2Cl3 TRI-CHLORO-1,3,4-CYCLOPENTADIENYL RADICAL STATWT=2 SIGMA=2  
 Ia=41.11508 Ib=112.3192 Ic=153.4698 Nu=3289,3288,1505,1496,1365,1269,  
 1239,1103,1051,912,821,799,737,620,601,594,472,381,375,325,200,169,161,125  
 HF298=152.68 kJ HF0=158.05 kJ REF=Janoschek J. Mol.Struct 661-2,(2003),635  
 Max Lst Sq Error Cp @ 1300 K 0.40%.

C5H2Cl3	1,3,4 tr	T 6/03C	5.H	2.CL	3.	0.G	200.000	6000.000	B	168.42748	1
	1.68990170E+01	1.02613023E-02	-3.78469676E-06	6.22286260E-10	-3.77437852E-14						2
	1.18158638E+04	-5.72327613E+01	1.95135592E+00	5.38396460E-02	-4.68814466E-05						3
	1.40727391E-08	9.77870650E-13	1.57742002E+04	1.92546669E+01	1.83630785E+04						4

Table 4 (continued)

115236-82-3

C5H3 1,3PENTADIYNE-5-YL RAD SIGMA=2 STATWT=2 IA=.2813 IB=39.0398 IC=39.3211  
 NU=3012,3102,1410,1090,935,3005,615,629,870,1950,2100,1200,480,220,530,350,200,  
 300 REF=DUFF & BAUER MAX LST SQ ERROR CP @ 1300 K 0.47 %. HF298=602.58 KJ  
 ESTIMATED BY USING BOZZELLI & RITTER'S PROGRAM FROM 1,3 PENTADIYNE

C5H3	T 2/92C	5H	3	0	OG	200.000	6000.000	C	63.07882	1
0.10296658E+02	0.10470124E-01	0.37746103E-05	0.61077326E-09	0.36621089E-13						2
0.68439389E+05	0.27338507E+02	0.15946538E+01	0.43378369E-01	0.56253789E-04						3
0.41304029E-07	0.12456939E-10	0.70491079E+05	0.15644812E+02	0.72473303E+05						4

78596-35-7

C5H3 1,4-PENTADIYNE-3-YL RADICAL (HCCCH\*CCH) SIGMA=2 STATWT=2 IA=2.8885  
 IB=30.7707 IC=33.659 NU=138,330(2),347,483,484,560,612,644,645,886,1058,1324,  
 1718,1817,2993,3242,3245 REF=Sandia BAC/MP4 Database by C. Melius, Private Commu  
 HF298=134.945+/-10.3 KCAL Max Lst Sq Error Cp @ 1300 K 0.39%

C5H3	1,4DIYNE3YL	T 3/94C	5H	3	0	OG	200.000	6000.000	B	63.07882	1
0.11453917E+02	0.92730586E-02	0.33071124E-05	0.53138989E-09	0.31710350E-13						2	
0.63604544E+05	0.32238569E+02	0.32458342E-01	0.59449660E-01	0.93606717E-04						3	
0.76931684E-07	0.24822627E-10	0.65960596E+05	0.22810663E+02	0.67906573E+05						4	

474977-33-8

C5H3 CYCLOPENTATRIENE-YL (RADICAL OF 1,2,4-CYCLOPENTATRIENE NONSYM) STATWT=2  
 SIGMA=1 IA=7.56527 IB=9.649169 IC=17.21444 NU=464,481,685,687,768,770,864,  
 965,1001,1136,1161,1241,1345,1366,3047,3063,3084 REF=Sandia BAC/MP4 Database  
 of C. Melius Private Communication HF298=166.771+/-17.8 KCAL Max Lst Sq Error  
 Cp @ 200 K 0.81%

C5H3	CY	T 3/94C	5H	3	0	OG	200.000	6000.000	B	63.07882	1
0.10397501E+02	0.10548283E-01	0.38462526E-05	0.62738447E-09	0.37836482E-13						2	
0.79435481E+05	0.30539213E+02	0.30279743E+00	0.31376032E-01	0.30789383E-05						3	
-0.35937535E-07	0.19474441E-10	0.82652282E+05	0.26395722E+02	0.83921947E+05						4	

591755-74-7

C5H3Cl3O 1-hydroxy-1,3,4-trichloro-cyclopentadiene SIGMA=1 IA=56.3622  
 IB=129.8008 IC=158.7470 Ir=0.1424 V(3)=1116.8 cm-1 ROSYM=1 NU=3702,3281,  
 3280,1666,1633,1322,1300,1210,1204,1164,1066,939,899,865,803,789,639,625,521,  
 501,435,430,351,332,295,245,171,136,91 HF298=-104.72 kJ HF0=-93.65 kJ  
 REF=Janoschek Fabian J Mol Struct 661/2 (2003),635 Max Lst Sq Error Cp @ 1300 K  
 0.36%

C5H3Cl3O	1-hydroxy	T06/03C	5.H	3.O	1.CL	3.G	200.000	6000.000	B	185.43482	1
1.97505887E+01	1.23107559E-02	4.45238080E-06	7.22906086E-10	4.34762350E-14						2	
-2.01911038E+04	7.16503477E+01	4.45787154E-01	7.64329241E-02	8.51510547E-05						3	
4.54054089E-08	8.84467176E-12	1.54582149E+04	2.52357971E+01	1.25948492E+04						4	

7129-66-0

C5H3N CYANO VINYL ACETYLENE HCC-CH=CH-CN SIGMA=1 STATWT=1 IA=1.7817  
 IB=57.4233 IC=59.2050 No Internal Rotation Nu=3492,3209,3181,2341,2222,1669,  
 1335,1304,1052,1034,981,860,641,623,558,543,521,384,256,134,126 HF298=422.6 kJ  
 HF0=426.538 kJ REF=Burcat G3B3 calc {HF298=416.3 kJ REF=MACKIE & COLKET  
 22 COMB. SYMP. 1990} Max Lst Sq Error Cp @ 6000 0.44%

C5H3N	CyanoVinyl	A01/05C	5.H	3.N	1.	O.G	200.000	6000.000	B	77.08406	1
1.12214716E+01	1.21359183E-02	4.33358316E-06	6.96955569E-10	4.16178238E-14						2	
4.63247595E+04	3.05570137E+01	1.68494050E+00	4.34233565E-02	4.45293097E-05						3	
2.43654701E-08	5.26531282E-12	4.87437574E+04	1.75458535E+01	5.08284058E+04						4	

Table 4 (continued)

4729-01-5

C5H4 1,3 PENTADIYNE HCC-CC-CH3 SIGMA=3 STATWT=1 IA=0.5256 IB=IC=41.3285  
 No Internal Rotor NU=3497,3102(2),3038,2363,2183,1501(2),1440,1192,1063(2),  
 690(2),686,575(2),346(2),158(2) HF298=411.835 kJ HF0=416.82 kJ REF=Burcat  
 G3B3 calc {HF298=95.5 kcal REF=NIST 91} Max Lst Sq Error Cp @ 6000 K 0.48%  
 C5H4 1,3 DiYne A 1/05C 5.H 4. 0. 0.G 200.000 6000.000 B 64.08526 1  
 9.31656215E+00 1.37165199E-02-4.87209640E-06 7.80513961E-10-4.64725769E-14 2  
 4.56259628E+04-2.31942358E+01 2.12483066E+00 3.62486885E-02-3.30843646E-05 3  
 1.74658596E-08-3.85998715E-12 4.75470659E+04 1.34500476E+01 4.95321196E+04 4

24442-69-1

C5H4 1,4 PENTADIYNE SIGMA=2 IA=4.3656 IB=29.7157 IC= 33.5673 NU=138,313,330,  
 341,558,605,606,629,632,908,953,1004,1254,1359,1486,2248,2256,3020,3046,3495(2)  
 HF298=108.022 kcal HF0=109.22 kcal REF=Burcat G3B3 calc. {HF298=111.083+/-4.34  
 kcal. REF=Sandia BAC/MP4 Database of. Melius, Private Communication.} Max Lst  
 Sq Error Cp @ 6000 K 0.43%  
 C5H4 1,4 DIYNE A 1/05C 5.H 4. 0. 0.G 200.000 6000.000 B 64.08526 1  
 1.01601157E+01 1.27915774E-02-4.50070751E-06 7.16461181E-10-4.24716335E-14 2  
 5.02537981E+04-2.60574377E+01 5.79688527E-01 4.87731655E-02-5.94800335E-05 3  
 4.04270841E-08-1.11749295E-11 5.24687091E+04 2.11761240E+01 5.43584707E+04 4

21986-03-8

C5H4 PENTATETRAENE CH2=C=C=CH2 SIGMA=4 STATWT=1 IA=0.5758 IB=40.3081  
 IC=40.3088 Nu=3213(2),3142(2),2245,1970,1538,1463,1344,1025(2),850(2),761,699,  
 601(2),360(2),162(2) HF298=444.466 kJ HF0=449.702 kJ REF=Burcat G3B3 calc  
 {HF298=115.1 kcal REF=NIST 91} Max Lst Sq Error Cp @ 6000 K 0.48%  
 C5H4 TETRAENE A 1/05C 5.H 4. 0. 0.G 200.000 6000.000 B 64.08526 1  
 9.72209830E+00 1.34135944E-02-4.77702792E-06 7.66673595E-10-4.57075766E-14 2  
 4.93744234E+04-2.60458810E+01 1.80277794E+00 3.60967201E-02-2.72177915E-05 3  
 7.91927363E-09 4.78650599E-13 5.15394138E+04 1.46808125E+01 5.34567064E+04 4

33555-85-0

C5H4 1,2-PENTADIENE-4-YNE CH2=C=CHCCH SIGMA=1 STATWT=1 IA=3.1964 IB=32.3450  
 IC=34.9654 NU=140,305,355,360,587,628,690,727,877,905,910,995,1097,1320,1440,  
 1978,2154,2971,2991,3042,3273 REF= BAC/MP4 Database By C. Melius Private  
 Communication. HF298=103.574 kcal REF=Burcat G3B3 calc {HF298=106.107+/-5.88  
 kcal REF=C. Melius database} Max Lst Sq Error Cp @ 6000 K .48%.  
 C5H4 1,2diene-4yneA 2/05C 5.H 4. 0. 0.G 200.000 6000.000 B 64.08526 1  
 1.02698973E+01 1.30734761E-02-4.68904953E-06 7.56153447E-10-4.52307822E-14 2  
 4.78277442E+04-2.75295590E+01 8.65430272E-01 4.15170326E-02-3.54484283E-05 3  
 1.30559494E-08-6.24737386E-13 5.03045116E+04 2.04152757E+01 5.21201629E+04 4

98206-69-0

C5H4 1,2,4-CYCLOPENTATRIENE NOSYM SIGMA=1 IA=7.8241 IB=10.128436 IC=17.642  
 NU=344,378,613,627,803,808,878,934,935,958,1070,1091,1098,1276,1339,1443,1548,  
 3022,3034,3070,3073 HF298=131.808+/-5.6 kcal REF=Sandia BAC/MP4 Database of  
 C. Melius, Private Commun. {HF298=131.129 kcal Burcat G3B3 calc 2005}.  
 Max Lst Sq Error Cp @ 200 K 0.9%  
 C5H4 CY T 3/94C 5H 4 0 0G 200.000 6000.000 B 64.08676 1  
 0.10106809E+02 0.13457466E-01-0.48862383E-05 0.79465424E-09-0.47821691E-13 2  
 0.61714735E+05-0.30155332E+02 0.98338482E+00 0.21429446E-01 0.33390071E-04 3  
 -0.66941379E-07 0.30563346E-10 0.64905174E+05 0.20682801E+02 0.66327982E+05 4



Table 4 (continued)

189230-13-5

C5H4N 1,3-Pentadiene-4-cyano-1-yl RADICAL \*CH=CH-CH=CH-CN SIGMA=1 STATWT=2  
 IA=3.0692 IB=56.2707 IC=59.3398 Ir(\*CH=CH-)=2.4298 ROSYM=1 [V(3)=1049. cm<sup>-1</sup>  
 REF=Langowski et al THEOCHEM 258, (1992), 341] Nu=3263, 3198, 3186, 3126, 2337, 1671,  
 1636, 1338, 1328, 1254, 1144, 1035, 1005, 919, 864, 843, 683, 567, 505, 437, 315, 201, 146  
 HF298=120.106 kcal REF=Burcat G3B3 calc QCISD/SCF=QC {HF298=114+/-3 KCAL  
 REF=Mackie & Colket, 22 COMB. Symp 1990}. Max Lst Sq Error Cp @ 6000 K 0.45%.  
 C5H4N linear A 4/05C 5.H 4.N 1. 0.G 200.000 6000.000 B 78.09200 1  
 1.17573715E+01 1.38995464E-02-4.96374665E-06 7.95190495E-10-4.73266222E-14 2  
 5.56216989E+04-3.16348822E+01 2.68686526E+00 3.53836353E-02-1.44995476E-05 3  
 -1.03289761E-08 8.19905828E-12 5.82605257E+04 1.59522259E+01 6.04896625E+04 4

29761-81-7

C5H4N META PYRIDYL RADICAL SIGMA=1 STATWT=2 IA=12.7172 IB=14.5379 IC=27.2550  
 Nu=3206, 3198, 3190, 3175, 1629, 1560, 1484, 1453, 1343, 1286, 1213, 1119, 1074, 1050, 988,  
 983, 945, 921, 785, 688, 662, 578, 424, 391 HF298=96.855 kcal HF0=99.94 kcal  
 REF=Burcat G3B3 calc QCISD/SCF=QC {HF298=91.6 KCAL (FOR ORTHO AND PARA RAD.  
 ADD -1.5 KCAL) Mackie & Colket, 22 COMB. SYMP 1990; HF298=93.4 kcal (m,p)  
 REF=Kiefer Zhang et al JPC A 101, (1997), 7061; HF298=93 kcal REF=NIST 94} Max  
 Lst Sq Error Cp @ 200 K 0.94%.  
 C5H4N m-Pyridyl A 2/05C 5.H 4.N 1. 0.G 200.000 6000.000 B 78.09200 1  
 1.03712938E+01 1.59574619E-02-5.80322295E-06 9.44993706E-10-5.69257795E-14 2  
 4.37175356E+04-3.13526019E+01 1.38066475E+00 1.47207328E-02 6.04123921E-05 3  
 -9.62107504E-08 4.11105614E-11 4.73100961E+04 2.09747610E+01 4.87390502E+04 4

13177-38-3

C5H4O CYCLOPENTADIENE-1-ONE SIGMA=2 A=0.273 B=0.131 C=0.088 NU=209,448,  
 (458), 640, (632), 714, 729, (822), 839, 943, 945, 949, (1068, 1136, 1332, 1678, 1724, 1727,  
 1789, 1870), 3161, 3171, 3204, 3206 HF298=13.2 kcal REF=(in parenthesis EXPERIM.  
 M. JACOX JPCRD 19, (1990), 1532) + Wang & Brezinsky JPC-A 102, (1998), 1530.  
 Max Lst Sq Error Cp @ 400 K 0.55%  
 C5H4O CY CPD-ONE T 8/99C 5.H 4.O 1. 0.G 200.000 6000.000 B 80.08616 1  
 1.00806824E+01 1.61143465E-02-5.83314509E-06 9.46759320E-10-5.68972206E-14 2  
 1.94364771E+03-2.94521623E+01 2.64576497E-01 3.34873827E-02 1.67738470E-06 3  
 -2.96207455E-08 1.54431476E-11 5.11159287E+03 2.35409513E+01 6.64245999E+03 4

39763-18-3

C5H4O2 ketene 2 propylene 4-aldehyde O=CHCH=CHCH=C=O SIGMA=1 STATWT=1  
 Ia=3.5671 Ib=97.1357 Ic=100.7247 Ir=2.6874 ROSYM=1 V(3)=0. Nu=3202, 3196,  
 3160, 2881, 2225, 1785, 1680, 1460, 1408, 1341, 1257, 1183, 1159, 1090, 1034, 993, 853, 678,  
 656, 535, 516, 408, 313, 249, 191, 104 HF298=-25.295 kcal REF=Burcat G3B3 calc.  
 {HF298=-31.02 kcal. REF=Zhong & Bozzelli JPC-A 102 (1998), 3537}. Max Lst Sq  
 Error Cp @ 1300 K 0.54%.  
 C5H4O2 Ketene A 4/05C 5.H 4.O 2. 0.G 200.000 6000.000 B 96.08406 1  
 1.23494140E+01 1.64232866E-02-5.96752256E-06 9.70925018E-10-5.84449615E-14 2  
 -1.81142267E+04-3.38091251E+01 3.71974617E+00 2.85214829E-02 8.94530795E-06 3  
 -3.30625737E-08 1.55936947E-11-1.51266538E+04 1.36793612E+01-1.27288656E+04 4

Table 4 (continued)

336800-69-2

C5H5 1-PENTYNE-3-ENE-5-YL RADICAL HCC-CH=CH-CH2\* SIGMA=1 STATWT=2 IA=2.0303  
 IB=35.1257 IC=37.1560 Ir(CH2\*)=9.31775 ROSYM=2 V3=1049. cm-1 estim  
 Nu=3490,3261,3176,3170,3160,2106,1563,1484,1348,1301,1214,1109,1011,933,847,772,  
 615,587,555,470,443,398,173 HF298=384.93 kJ HF0=393.17 kJ REF=Burcat G3B3  
 calc. {HF298=97.1+/-2.0 kcal REF=NIST-94} Max Lst Sq Error Cp @ 6000 K 0.44%  
 C5H5 1Yne3Ene5Yl A 1/05C 5.H 5. 0. 0.G 200.000 6000.000 B 65.09320 1  
 1.12334577E+01 1.37755916E-02-4.88589306E-06 7.81744763E-10-4.65008043E-14 2  
 4.16520916E+04-3.05396799E+01 1.04253561E+00 4.42423548E-02-3.60781742E-05 3  
 1.09482099E-08 7.03473990E-13 4.43154478E+04 2.14097777E+01 4.62959333E+04 4

2143-53-5

C5H5 CYCLOPENTADIENYL RADICAL SIGMA=2 STATWT=2 IA=9.06849 IB=9.9295  
 IC=18.998 NU=484,496.6,652.7,702.3,709.7,766.7,814.5,833.6,893.5,902.6,917.3,  
 954.9,982,1080,1201,1275.3,1337,1364,1404,3024.4,3029.4,3039,3048,3061  
 HF298=266.1 KJ REF=Ab-Initio Calc Karni,Oref & Burcat JPCRD 20 (1991), 665  
 Max Lst Sq Error Cp @ 6000 K 0.52%  
 C5H5 CY T12/89C 5H 5 0 0G 200.000 6000.000 B 65.09470 1  
 0.10844072E+02 0.15392831E-01-0.55630422E-05 0.90189440E-09-0.54156619E-13 2  
 0.26950886E+05-0.35254983E+02-0.95902849E+00 0.31396777E-01 0.26724050E-04 3  
 -0.68942183E-07 0.33301983E-10 0.30779441E+05 0.29072780E+02 0.32004580E+05 4

2180-69-0

C5H5N 1-Cyano-1,3-Butadiene CN-CH=CH-CH=CH2 SIGMA=1 STATWT=1 IA=3.1563  
 IB=58.5404 IC=61.6968 Ir(CH2=CH-)=2.54839 ROSYM=1 [V(3)=1049. cm-1 (3 kcal)  
 REF=Langowski et al THEOCHEM 258, (1992), 341.] Nu=[3150,3097,3075,3012,2921,  
 2223,1627,1568,1430,1366,1302,1238,1143,1063,1009,993,940,887,780,674,] 573,496,  
 460,318,208,144 HF298=238.944 kJ HF0=250.607 kJ REF=[Webbook IR]+ Burcat  
 G3B3 calc {HF298=239.3 kJ REF=NIST 94} Max Lst Sq Error Cp @ 6000 K 0.51%.  
 C5H5N 1-Cyano A 2/05C 5.H 5.N 1. 0.G 200.000 6000.000 B 79.09994 1  
 1.18240384E+01 1.67108077E-02-6.02084839E-06 9.70590626E-10-5.80113765E-14 2  
 2.35732846E+04-3.37413725E+01 2.78936308E+00 3.21194174E-02 3.46293916E-06 3  
 -3.07848335E-08 1.58396908E-11 2.65017082E+04 1.51281661E+01 2.87382006E+04 4

110-86-1

C5H5N PYRIDINE (AZINE) SIGMA=2 IAIBIC=5696.6 NU=3094.2,3086.9,3072.8,3042.4,  
 3030.1,1583.9,1580.5,1483.4,1441.9,1362.3,1227,1218,1143.3,1079,1071.9,1031.7,  
 1007,991.4,980,936.6,880,744,700.3,652,601.4,403.3,373 HF298=140.37+/-0.54 KJ  
 REF=Das et al. 1993 Max Lst Sq Error Cp @ 200 K \*\*1.2%\*\*  
 C5H5N PYRIDINE T 3/95C 5H 5N 1 0G 200.000 6000.000 B 79.10144 1  
 0.10737274E+02 0.18411346E-01-0.67089960E-05 0.10937092E-08-0.65928113E-13 2  
 0.11511982E+05-0.35580435E+02 0.12333682E+01 0.14084676E-01 0.73775044E-04 3  
 -0.11405870E-06 0.48433017E-10 0.15439523E+05 0.20414274E+02 0.16882534E+05 4

N/A

2,4-C5H4OH 1-HYDROXY-2,4-CYCLOPENTADIENE-1-YL RADICAL Ab-Initio Calculations  
 Karni Oref & Burcat JPCRD 20 (1991), 665. SIGMA=1 STATWT=2 IA=10.736637  
 IB=24.951617 IC=35.688254 ROSYM=2 INT ROT POTENTIAL V2=1213. IR=0.1336  
 NU=295.6,365.8,510.4,593.4,615.4,680.6,717.3,724.5,831.7,884.8,897.6,905.5,939,  
 1060.8,1087,1208.5,1272.6,1284.8,1365,1503.8,1467,3028,3043.8,3054,3074.5,  
 3482.6 HF298=15.9 kcal REF=Wang&Brezinsky JPC,102, (1998), 1530. Max. List Sq  
 Error Cp @ 200 K 0.71%  
 C5H4OH CYCLO RAD T 8/99C 5.H 5.O 1. 0.G 200.000 6000.000 B 81.09410 1  
 1.33741248E+01 1.51996469E-02-5.45685046E-06 8.80944866E-10-5.27493258E-14 2  
 2.20358027E+03-4.59569069E+01-1.28398054E+00 4.90298511E-02-1.35844414E-05 3  
 -2.92983743E-08 1.90820619E-11 6.37364803E+03 3.08073591E+01 8.00114499E+03 4

Table 4 (continued)

136936-20-4

1,3-C<sub>5</sub>H<sub>5</sub>O 1-OXYL-1,3-CYCLOPENTADIENE RADICAL Ab-Initio Calculations Karni,Oref  
 Burcat JPCRD 20 (1991) 665. SIGMA=1 STATWT=2 IA=11.147244 IB=21.976487  
 IC=35.267015 NU=191.35,386.3,417.8,520.8,607,637,774.7,867.7,899.5,925.6,989,  
 1024.4,1129,1150,1218,1267.4,1321.6,1341.6,1375.4,1422,2868,2900.7,3025.4,3037,  
 3051,787.6,797 HF298=59.8 KJ Max Lst Sq Error Cp @ 6000 0.53%.

1,3C5H5O RADICAL	T 4/91C	5H	5O	1	OG	200.000	6000.000	B	81.09410	1
0.12606535E+02	0.16747067E-01	-0.61097587E-05	0.99674576E-09	-0.60111834E-13						2
0.14114657E+04	-0.42604911E+02	0.23043601E+00	0.32322572E-01	0.28900908E-04						3
-0.70680613E-07	0.33407174E-10	0.55554724E+04	0.25330946E+02	0.71922458E+04						4

136936-21-5

1,4-C<sub>5</sub>H<sub>5</sub>O 1-OXYL-1,4-CYCLOPENTADIENE RADICAL Ab-Initio calculations Karni,Oref  
 Burcat JPCRD 20(1991) 665. SIGMA=1 STATWT=2 IA=11.180668 IB=24.926636  
 IC=35.551016 NU=224.8,338.5,410,562.5,620,653,729,751,826,862,896,920.6,939,  
 1038,1144.4,1145,1197.6,1243,1285.4,1337,1385.7,1433,2854,2881.6,3027,3046,  
 3055.8 HF298=103.3 KJ Max Lst Sq Error Cp @ 6000 K 0.53%

1,4C5H5O RADICAL	T 4/91C	5H	5O	1	OG	200.000	6000.000	B	81.09410	1
0.12711510E+02	0.16650171E-01	-0.60741189E-05	0.99090150E-09	-0.59758183E-13						2
0.66172961E+04	-0.43161680E+02	0.45438248E-01	0.33871750E-01	0.25637288E-04						3
-0.67844135E-07	0.32508364E-10	0.10797244E+05	0.26058142E+02	0.12424063E+05						4

136936-19-1

2,4-C<sub>5</sub>H<sub>5</sub>O 1-OXYL-2,4-CYCLOPENTADIENE RADICAL Ab-Initio Calculations Wang &  
 Brezinsky JPC, 102, (1998), 1530. SIGMA=2 STATWT=2 A=0.245 B=0.132 C=0.094  
 Nu=176,397,523,626,690,766,798,804,878,947,968(2),1055,1066,1090,1118,1276,1311,  
 1363,1574,1603,1871,2843,3030,3038,3062,3068 HF298=52.8 kcal

2,4-c-C <sub>5</sub> H <sub>5</sub> O	D 9/97C	5H	5O	1	0OG	300.000	3000.000	B	81.09410	1
0.85405312E+01	0.22989510E-01	-0.95437563E-05	0.17061612E-08	-0.97459360E-13						2
0.22263699E+05	-0.20818825E+02	-0.30777600E+01	0.52581679E-01	-0.28856513E-04						3
-0.33885479E-08	0.63361399E-11	0.25510455E+05	0.39591522E+02	0.26570048E+05						4

206255-24-5

C<sub>5</sub>H<sub>5</sub>O<sub>2</sub> 2-pentenedialehyde-1-yl radical O=C\*CH=CHCH<sub>2</sub>CHO ESTIMATED FROM GROUP  
 ADDITIVITY DATA AND EXTRAPOLATED FROM 2000 to 5000 K USING Wilhoit's POLYNO-  
 MIALS REF=Zhong & Bozzelli JPC-A 102 (1998), 3537. HF298=-19.99 kcal.

C <sub>5</sub> H <sub>5</sub> O <sub>2</sub> 2-pentene	T 8/99C	5.H	5.O	2.	O.G	298.150	5000.000	E	97.09350	1
1.46629817E+01	1.65541793E-02	-6.29149065E-06	1.11259736E-09	-7.44617493E-14						2
-1.63990894E+04	-4.40514968E+01	-3.53400779E+00	8.32842318E-02	-1.14653205E-04						3
9.02774159E-08	-2.94687646E-11	-1.18588987E+04	4.67266279E+01	-1.00593011E+04						4

206255-23-4

C<sub>5</sub>H<sub>5</sub>O<sub>2</sub> 2-pentenedialehyde-4-yl radical O=CHCH=CHCH\*CHO ESTIMATED FROM GROUP  
 ADDITIVITY DATA AND EXTRAPOLATED FROM 2000 to 5000 K USING Wilhoit's POLYNO-  
 MIALS REF=Zhong & Bozzelli JPC-A 102 (1998), 3537. HF298=-17.89 kcal.

C <sub>5</sub> H <sub>5</sub> O <sub>2</sub> 2-pentene	T 8/99C	5.H	5.O	2.	O.G	298.150	5000.000	E	97.09350	1
1.56927684E+01	1.57719181E-02	-6.01048812E-06	1.06457071E-09	-7.13241582E-14						2
-1.54871075E+04	-5.03606092E+01	-3.16128127E+00	8.34432454E-02	-1.14264559E-04						3
8.92804044E-08	-2.89089773E-11	-1.06704590E+04	4.41383953E+01	-8.75093782E+03						4

Table 4 (continued)

10563-01-6

C5H6 1,2,4 Pentatriene CH<sub>2</sub>=CH-CH=C=CH<sub>2</sub> Vinyl-Allenyl. STATWT=1 SIGMA=1  
 IA=2.45998 IB=36.2587 IC=38.1169 Ir=2.8948339 Int Rot Barrier V(2)=699.5 cm<sup>-1</sup>  
 ROSYM=2 NU=3099,3060,3045,2999,2991,2982,1950,1624,1449,1428,1401,1320,1281,  
 1173,1083,993,902,870,851,704,658,547,492,395,327,162 REF=Klaboe et al, Spectr-  
 ochimica Acta 30A (1974),1527 HF(298)=60.3 kcal REF=NIST-94 estimate.

Max Lst Sq Error Cp @ 6000 K 0.54 %

C5H6 Vinyl-Allen	T02/02C	5.H	6.	0.	0.G	200.000	6000.000	B	66.10264	1	
						1.01926736E+01	1.80721370E-02	-6.49266545E-06	1.04421432E-09	-6.22835300E-14	2
						2.57023788E+04	-2.67860465E+01	2.70515049E+00	2.98831529E-02	2.74090664E-06	3
						-2.51726901E-08	1.25975560E-11	2.82287948E+04	1.40821373E+01	3.03439649E+04	4

646-05-9

C5H6 1-PENTEN-3-YNE SIGMA=3 HF298=59.6 KCAL REF=NIST 1991 TO 1500 K EXTRAPOLATED  
 TO 5000 K USING WILHOIT'S POLYNOMIALS Max Lst Sq Error Cp @ 500 K \*\*1.3%\*\*

C5H6 1en-2yne	T 4/94C	5H	6	0	0G	298.150	5000.000	E	66.10264	1	
						0.11961729E+02	0.14213107E-01	-0.37135572E-05	0.53054857E-09	-0.32337040E-13	2
						0.24700248E+05	-0.36324258E+02	0.18057462E+01	0.29748651E-01	0.88584433E-05	3
						-0.31819540E-07	0.14349539E-10	0.28108939E+05	0.19197135E+02	0.29991713E+05	4

2004-69-5

C5H6 3-PENTEN-1-YNE SIGMA=3 HF298=61.3 KCAL REF=NIST 1991 TO 1500 K EXTRAPOLATED  
 TO 5000 K USING WILHOIT'S POLYNOMIALS Max Lst Sq Error Cp @ 500 K \*\*1.6%\*\*

The method does not differentiate between the Cis and the Trans isomers.

C5H6 3en-1yne	T 4/94C	5H	6	0	0G	298.150	5000.000	E	66.10264	1	
						0.12461757E+02	0.14686414E-01	-0.48422257E-05	0.80222734E-09	-0.52391736E-13	2
						0.25378034E+05	-0.39930098E+02	0.16581871E+01	0.36047209E-01	-0.79525384E-05	3
						-0.15547159E-07	0.88371326E-11	0.28847420E+05	0.18120095E+02	0.30847182E+05	4

542-92-7

C5H6 CYCLOPENTADIENE STATWT=1 SIGMA=2 IAIBIC=1996\*10E-117 NU=3091,3075,  
 2886,1500,1378,1365,1106,994,915,802,1100,941,700,516,3105,3043,1580,1292,1239,  
 11090,959,805,2900,925,891,664,350 REF=Dorofeeva, Gurvich & Jorish JPCRD 15,  
 (1986) 437. HF298=134.3 KJ from Pedley, Naylor and Kirby. Max Lst Sq Error  
 Cp @ 6000 K 0.58 %.

CYCLOPENTADIENE	T 1/90C	5H	6	0	0G	200.000	6000.000	B	66.10264	1	
						0.99757848E+01	0.18905543E-01	-0.68411461E-05	0.11099340E-08	-0.66680236E-13	2
						0.11081693E+05	-0.32209454E+02	0.86108957E+00	0.14804031E-01	0.72108895E-04	3
						-0.11338055E-06	0.48689972E-10	0.14801755E+05	0.21353453E+02	0.16152485E+05	4

504-29-0

C5H6N2 2-AMINO-PYRIDINE SIGMA=2 STATWT=1 IA=14.22 IB=30.312 IC=44.465  
 NU=3499,3399,3036,3019,3005,3000,1631,1612,1594,1486,1439,1314,1290,1193,1122,  
 1091,1027,1023,1001,989,967,855,824,775,744,615,589,541,497,411,385,331,207.5  
 HF298=28.35 KCAL REF=C.MELIUS DATABASE BACMP4 PF11 Binkerton, Pilcher, Al-Takhin  
 J.Chem.Thermodyn 16 (1984) 373 HF298=28.0+/-0.2 KCAL Max Lst Sq Error Cp @ 200  
 K 0.6 %

C5H6N2	T 9/96C	5H	6N	2	0G	200.000	6000.000	B	94.11612	1	
						0.13806658E+02	0.20732346E-01	-0.74781249E-05	0.12110605E-08	-0.72674834E-13	2
						0.78210347E+04	-0.50686216E+02	-0.37783801E+00	0.42946164E-01	0.15869990E-04	3
						-0.59636577E-07	0.29397526E-10	0.12433786E+05	0.26323931E+02	0.14266192E+05	4

Table 4 (continued)

80156-16-7

C5H5OH 2,4-CYCLOPENTADIENE-1-OL Ab-Initio Calculations Karni, Oref Burcat JPCRD 20(1991) 665. SIGMA=1 STATWT=1 IA=12.53933 IB=24.829069 IC=33.91959 NU=300, 368.4,520.3,542.6,705.8,768.6,791.7,809.5,842.3,888.6,979.6,1012.8,1018,1019, 1096.8,1117.8,1206.6,1241.3,1290.5,1343.8,1334.5,1540,1603,1889.8,3021.5,3030, 3048.6,3057.6,3436.6 ROSYM=1 BROT=21.07 INT ROT POTENTIAL BARRIER V1=30.4 V2=86.14 V3=401. Max Lst Sq Error Cp @ 6000 K 0.54%. HF298=7.9 KJ.

2,4-C5H5OH	T 4/91C	5H	6O	1	OG	200.000	6000.000	B	82.10204	1
	0.12073957E+02	0.19167781E-01	-0.69148807E-05	0.11197648E-08	-0.67186779E-13					2
	-0.47916482E+04	-0.40662174E+02	0.15607391E+01	0.22274522E-01	0.57195791E-04					3
	-0.99408942E-07	0.43757325E-10	-0.83475005E+03	0.19351929E+02	0.95014619E+03					4

103905-53-9

C5H5OH 1,3-CYCLOPENTADIENE-1-OL Ab-Initio Calculations Karni, Oref Burcat JPCRD 20(1991) 665. SIGMA=1 STATWT=1 IA=10.761122 IB=26.5896 IC=36.79168 NU=341.8, 363,424,527.4,603,714,793,865.4,874.7,887.3,928.3,935,1001.6,1089,1119,1151.4, 1206.8,1254,1312,1383.4,1412,1545,1606,2866.5,2899.5,3021.5,3032.6,3053,3466 ROSYM=2 IR=0.1336 INT ROT POTENTIAL BARRIER V2=1213. HF298=-24.3 KJ

Max Lst Sq Error Cp @ 6000 K 0.6%

1,3-C5H5OH	T 4/91O	1C	5H	6	OG	200.000	6000.000	B	82.10204	1
	0.12696134E+02	0.18618412E-01	-0.67184339E-05	0.10881502E-08	-0.65298439E-13					2
	-0.88025224E+04	-0.44039241E+02	-0.22499411E-01	0.36512400E-01	0.22970166E-04					3
	-0.65452226E-07	0.31611123E-10	-0.46272736E+04	0.25340697E+02	-0.29226016E+04					4

103905-54-0

C5H5OH 1,4-CYCLOPENTADIENE-1-OL Ab-Initio Calculation by Karni, Oref & Burcat JPCRD 20 (1991) 665. SIGMA=1 STATWT=1 IA=10.995026 IB=26.446161 IC=36.88101 NU=335,369.3,379,607,616,742.7,795,795.4,850.3,889.3,926,935,999,1074.5,1112, 1147.6,1195.5,1252,1298,1387,1421.8,1550,1626,2851.6,2880,3030.3,3036.5,3057.6, 3472 ROSYM=2 IR=0.1336 INT ROT POTENTIAL BARRIER V2=1213. HF298=-27.2 KJ. Max Lst Sq Error Cp @ 6000 K 0.6%

1,4 C5H5OH	T 4/91O	1C	5H	6	OG	200.000	6000.000	B	82.10204	1
	0.12734997E+02	0.18582251E-01	-0.67050926E-05	0.10859592E-08	-0.65165720E-13					2
	-0.91625548E+04	-0.44227527E+02	-0.84687145E-01	0.36826867E-01	0.22761297E-04					3
	-0.65709925E-07	0.31839396E-10	-0.49692504E+04	0.25639055E+02	-0.32713894E+04					4

6067-72-7

C5H7 1,4-Pentadiene-3-yl H2C=CH-\*CH-CH=CH2 SIGMA=2 STATWT=2 IA=2.6277 IB=36.9599 IC=39.5876 [Ir(CH2=CH-)=2.40673 ROSYM=1 V(3)=4547 cm-1 ~13. kcal REF=Sebbar Bockhorn & Bozzelli, PCCP 4, (2002), 3691]x2 Nu=3256(2), 3169, 3167, 3160, 3145, 3143, 1613, 1547, 1506, 1463, 1315.5(2), 1293, 1269, 1185, 1037, 1019, 989, 929, 864, 844, 831, 630, 588, 492, 452, 257 HF298=205.445 kJ HF0=223.086 kJ REF=Burcat G3B3 calc {HF298=53. kcal REF= Weissman & Benson Prog. Energy Combust. Sci 15, (1989), 273} Max Lst Sq Error Cp @ 6000 K 0.64%

C5H7 1,4-Pentad	A 1/05C	5.H	7.	0.	OG	200.000	6000.000	B	67.10908	1
	1.01206141E+01	2.19623708E-02	-8.13808356E-06	1.32677709E-09	-7.97014062E-14					2
	1.97304588E+04	-2.73862410E+01	2.36470149E+00	2.39388874E-02	3.85164588E-05					3
	-7.07659775E-08	3.11379069E-11	2.27262660E+04	1.71124336E+01	2.47104544E+04					4

3808-35-3

C5H7 1,3-PENTADIENE-5-YL RADICAL H2C=CH-CH=CH-CH2\* SIGMA=1 STATWT=2

It is not clear if this radical exists or is unstable. In all attempts to calculate it, it converged to the 1,4-Pentadiene-3-yl form.

Table 4 (continued)

690994-72-0

C5H7 CYCLO-1-PENTEN-1-YL RADICAL SIGMA=1 STATWT=2 IA=10.7046 IB=11.1602  
 IC=20.8356 Nu=3236,3225,3202,3050,3030,3027,3014,1522,1502,1499,1420,1337,  
 1315,1295,1235,1153,1115,1086,10036,1005,949,920,912,815,809,725,634,598,448,129  
 HF298=172.623 kJ HF0=192.745 kJ REF=Burcat G3B3 calc {HF298=166.88 kJ REF=Therm}  
 Max Lst Sq Error Cp @ 200 K \*\*1.2%\*\*,@ 6000 K 0.59%.

C5H7 CYCLO-1-pe A 9/04C 5.H 7. 0. 0.G 200.000 6000.000 B 67.10908	1
9.74013709E+00 2.15079576E-02-7.71169114E-06 1.24352828E-09-7.43887470E-14	2
1.56355223E+04-2.89664925E+01 2.31203194E+00 7.01023600E-03 9.35725543E-05	3
-1.33744658E-07 5.55553794E-11 1.91721662E+04 1.72892593E+01 2.07617132E+04	4

10577-65-8

C5H7 CYCLO-1-PENTEN-4-YL RADICAL SIGMA=2 STATWT=2 IA=10.6032 IB=11.3563  
 IC=20.9321 Nu=3228,3219,3195,2965,2964,2963(2),2960,1698,1497,1491,1407,1346,  
 1314,1292,1142,1140,1135,1044,969,958,930,923,913,788,741,685,390,313,209  
 HF298=223.94 kJ HF0=243.815 kJ REF=Burcat G3B3 calc Max Lst Sq Error Cp @  
 6000 K 0.59%.

C5H7 CYCLO-1-pe A 9/04C 5.H 7. 0. 0.G 200.000 6000.000 B 67.10908	1
8.58774652E+00 2.23806578E-02-7.98587176E-06 1.28324922E-09-7.65681699E-14	2
2.23083592E+04-2.28844345E+01 2.84227879E+00 7.67441692E-03 8.13034074E-05	3
-1.15127705E-07 4.74968151E-11 2.52319161E+04 1.37757573E+01 2.69336656E+04	4

129793-02-8

C5H7CL 5-CHLORO-1,3-PENTADIENE (CH<sub>2</sub>=CHCH=CHCH<sub>2</sub>CL) SIGMA=1 STATWT=1 IA=6.8726  
 IB=90.6353 IC=92.1071 Ir(-CH<sub>2</sub>CL)=9.0981 ROSYM=1 V(3)=1341 cm<sup>-1</sup> (From  
 CH<sub>3</sub>CH<sub>2</sub>CL) Ir(CH<sub>2</sub>=CH-)=3.2561 ROSYM=1 V(3)=1000. cm<sup>-1</sup> est. Nu=3250,3179,3167,  
 3162,3159,3147,3103,1731,1686,1511,1476,1351,1340,1325,1291,1233,1166,1104,1052,  
 990,981,937,915,865,693,636,502,439,336,214,181.5 HF298=18.884+/-1.9 kcal  
 HF0=18.22 kcal REF=Burcat G3B3 calc {HF298=17.0 KCAL REF=Weismann & Benson  
 Prog. Energy Comb. Sci. 15, (1989), 273 HF298=12.8 kcal REF=NIST 94} Max Lst Sq  
 Error Cp @ 200 K 0.52%

C5H7CL A08/05C 5.H 7.CL 1. 0.G 200.000 6000.000 B 102.56178	1
1.30978247E+01 1.98955652E-02-7.14299948E-06 1.14829942E-09-6.84572130E-14	2
1.12151286E+03-3.78578820E+01 4.13048625E+00 2.41562471E-02 4.12699083E-05	3
-7.66549750E-08 3.40285660E-11 4.45228842E+03 1.30293308E+01 6.98666019E+03	4

108402-57-9 ??

C5H7CL<sub>2</sub> 1,5-DICHLOROPENTENE-1-YL-3 (\*ClCHCH<sub>2</sub>CH=CHCH<sub>2</sub>Cl) SIGMA=1 STATWT=2  
 IA=15.2698 IB=161.6032 IC=172.2463 Ir(-CH<sub>2</sub>CL)=14.2488 ROSYM=1 V(3)=1341.  
 cm<sup>-1</sup> Ir(\*ClCH-)=11.8413 ROSYM=1 V(3)=1500. cm<sup>-1</sup> est. Ir(\*CHCLCH<sub>2</sub>-)=21.9836  
 ROSYM=1 V(3)=1000. cm<sup>-1</sup> est. NU=3242,3177,3161,3157,3105,3047,2991,1744,1511,  
 1480,1375,1348,1331,1308,1297,1238,1182,1116,1073,1041,1013,958,925,809,718,681,  
 539,470,332,311,263,252,110.3 HF298=26.512+/-1.9 kcal HF0=30.77 kcal  
 REF=Burcat G3B3 calc {HF298=14.7 kcal REF=Weismann & Benson Prog. Energy Comb.  
 Sci. 15, (1989), 273} Max Lst Sq Error Cp @ 200 K 0.46%

C5H7CL <sub>2</sub> A08/05C 5.H 7.CL 2. 0.G 200.000 6000.000 B 138.01448	1
1.70600425E+01 1.75885302E-02-6.28267330E-06 1.01040123E-09-6.03280289E-14	2
6.31476542E+03-5.14696018E+01 5.23200814E+00 3.31354262E-02 2.66047406E-05	3
-6.82885772E-08 3.26323749E-11 1.01930845E+04 1.31714456E+01 1.33412802E+04	4

Table 4 (continued)

N/A

C5H7NO 2-METHYL-3-OXO-BUTYRO-NITRIL CH3-C=O-CH(CH3)-CN ROSYM=2x3 ESTIMATED  
 USING NIST 1994 FROM [C-(C)(CN)(CO)(H)]=[C-(C)2(CN)(H)]; [CO-(C)2]; 2x[C-(H)3]  
 HF298=-108.7 KJ Max Lst Sq Error H-H298 @ 300 K 0.69%

C5H7NO	T10/94C	5H	7N	1O	1G	298.150	5000.000	E	97.11672	1
0.11348162E+02	0.26153783E-01	0.10147863E-04	0.18274196E-08	0.12448116E-12						2
-0.18497976E+05	-0.27546501E+02	0.70321296E+01	0.17114461E-01	0.43753706E-04						3
-0.64537212E-07	0.25693936E-10	-0.16201998E+05	0.23072915E-01	-0.13073530E+05						4

62224-37-7

C5H7O Cyclo-1-penten-4-oxy Radical C5H7-O\* SIGMA=1 STATWT=2 Ia=13.4135  
 Ib=22.9617 Ic=31.3589 Nu=3217,3194,3086.5(2),3037,3033,2902,1701,1508,1504,  
 1372,1328,1306,1265,1171,1170,1142,1092,1075,987,979,976,974,906,868,813,765,  
 696,676,403,392,354,75.4 HF298=95.04 kJ HF0=117.53 kJ REF=G3B3 calc  
 {HF298=9.38 kcal REF=THERM; THERGAS HF298=26.41 kcal; PM3 HF298=11.10 kcal;  
 AM1 HF298=15.68 kcal} Max Lst Sq Error Cp @ 200 K \*\*1.06%.\*\*

C5H7O Cy C5H7-O*	A10/04C	5.H	7.O	1.	0.G	200.000	6000.000	B	83.10848	1
1.18245290E+01	2.25156780E-02	-8.11965644E-06	1.31442052E-09	-7.88442567E-14						2
5.47509398E+03	-3.89405519E+01	2.16396289E+00	1.45387805E-02	8.65448177E-05						3
-1.31349889E-07	5.55584547E-11	9.60790169E+03	1.87490468E+01	1.14305666E+04						4

2004-70-8

C5H8 1,3-PENTADIENE H2C=CH-CH=CH-CH3 SIGMA=1 STATWT=1 IA=5.2531 IB=32.0453  
 IC=36.7802 Ir(CH3)=0.5167 V(3)=2868 cm-1 ROSYM=3 Ir(C2H3)=3.0282 ROSYM=1  
 V(3)=3148 cm-1 estim. NU=3245,3175,3165,3160,3145,3133,3075,3034,1734,1681,  
 1521,1511,1491,1445,1413,1335,1304,1203,1074,1072,1046,994,973,923,899,808,645,  
 619,390,359,222 HF298=84.157 kJ HF0=105.77 kJ REF=Burcat G3B3 calc.  
 {HF298=18.2 KCAL REF=Weissman & Benson} Max Lst Sq Error Cp @ 1300 K 0.66%.

C5H8 1,3 Pentadi	A12/04C	5.H	8.	0.	0.G	200.000	6000.000	B	68.11702	1
1.06253702E+01	2.34322094E-02	-8.61216410E-06	1.40664328E-09	-8.47997015E-14						2
4.64864607E+03	-3.18725934E+01	3.47443097E+00	1.48104285E-02	6.38218646E-05						3
-9.32324174E-08	3.78929523E-11	8.03001422E+03	1.19810267E+01	1.01217000E+04						4

78-79-5

C5H8 ISOPRENE, 2-METHYL 1,3-BUTADIENE SIGMA=3 REF=Stull Westrum & Sinke  
 EXTRAPOLATED TO 5000 K USING WILHOIT'S POLYNOMIALS HF298=18.1 KCAL Max Lst Sq  
 Error H-Href @ 300 K 0.82%

C5H8 ISOPRENE	T 5/96C	5H	8	0	0G	298.150	5000.000	B	68.11852	1
0.10991663E+02	0.22439484E-01	-0.81159626E-05	0.13948336E-08	-0.92194080E-13						2
0.40581428E+04	-0.32980170E+02	-0.36106649E+01	0.74856698E-01	-0.83303221E-04						3
0.52256651E-07	-0.13581639E-10	0.74967178E+04	0.39483975E+02	0.91082217E+04						4

142-29-0

C5H8 CYCLOPENTENE REF=DOROFEEVA GURVICH & JORISH JPCRD 15 (1986) 437. DATA  
 EXTRAPOLATED USING WILHOIT POLYNOMIALS. HF298= 33.9 KJ REF=TRC Oct 1992.  
 Max

Lst Sq Error Cp @ 200 K \*\*\* 1.3%\*\*\* @ 2400 K 0.59%.

C5H8,cyclo-	g 1/93C	5.H	8.	0.	0.G	200.000	6000.000	B	68.11702	1
9.64282423E+00	2.42562834E-02	-8.72089503E-06	1.41190868E-09	-8.47267848E-14						2
-1.29253168E+03	-3.01225606E+01	2.68980514E+00	2.09635533E-03	1.13034459E-04						3
-1.54077581E-07	6.27623564E-11	2.45828931E+03	1.53075040E+01	4.07720960E+03						4

Table 4 (continued)

N/A

C5H8CL 5-CHLOROPENTENE-1YL-3 (\*CH2CH2CH=CHCH2CL) SIGMA=1 STATWT=2 IA=10.7042  
 IB=76.8105 IC=79.7213 Ir(CH2Cl)=12.8876 ROSYM=1 V3=1200 cm-1 est.  
 Ir(CH2\*)=0.2902 ROSYM=1 V(3)=1800. cm-1 est. Ir(\*CH2CH2-)=5.1900 ROSYM=1  
 V(3)=700. est NU=3273,3187,3174,3170,3154,3113,3036,2983,1731,1520,1491,1484,  
 1444,1346,1313,1296,1239,1188,1107,1084,1051,1017,951,932,800,794,668,551,491,  
 451,344,285,181 HF298=37.81 kcal REF=Burcat G3B3 calc {HF298=18.9 kcal Weissman  
 & Benson Prog. Energy Comb. 15,1989,273} Max Lst Sq Error Cp @ 6000 K 0.50%.  
 C5H8CL A04/05C 5.H 8.CL 1. 0.G 200.000 6000.000 B 103.56972 1  
 1.43282670E+01 2.08391545E-02-7.49363944E-06 1.20797259E-09-7.21763267E-14 2  
 1.27012428E+04-4.22055222E+01 3.44156454E+00 3.48300144E-02 2.10910844E-05 3  
 -5.81094559E-08 2.75563709E-11 1.63679217E+04 1.75792716E+01 1.90266221E+04 4

78-11-5

C5H8N4O12 PENTA ERITHRITOL TETRA NITRATE PETN C(CH2ONO2)4 Solid Cp 293-333  
 REF= Yin,Ziru,Ganghe,Chengyun 17th Internat. Pyrotech. Seminar 1991 Vol 1,  
 515-521 S298=24.37 cal Graphic Integ HF298(solid)=-128.7+/-0.2 Kcal  
 REF=NIST 98 (Ornelas et al Rev. Sci. Instrum. 37,(1966) 907-912 Max Lst Sq  
 Error Cp @ 293 K 0.05 %  
 PETN Solid T 4/99C 5.H 8.N 4.O 12.S 293.000 550.000 D 316.13828 1  
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2  
 0.00000000E+00 0.00000000E+00 2.77774680E+02-1.73349082E+00 3.09926721E-03 3  
 8.72626335E-07-2.15382459E-09-9.86240953E+04-1.19475100E+03-6.47639849E+04 4

78-11-5

C5H8N4O12 PENTA ERITHRITOL TETRA NITRATE PETN C(CH2ONO2)4 SIGMA=4 IA=172.42  
 IB=461.12 IC=462.62 (IR(NO2)=5.96 ROSYM=2 V(2)=9.1 kcal/mole )x4 rotors  
 NU=3029,3028,3006,2999,2972,2971,2936,2929,1735,1730,1711,1710,1494,1485,1473,  
 1469,1445,1435,1424,1417,1390,1380,1363,1362,1334,1325,1288,1256,1199,1198,  
 1128,1098,1079,1072,1055,1022,988,974,969,962,923,918,865,810.3(2),807(2),773,  
 764,724,696,694,667,663,645,590,541,462,409,408,372,284,274,249,222,218,199,184,  
 166,139,114,112.5,75.4,67.8,65.1,60,57 REF=C. MELIUS DATABASE BACMP22 #86 AA9A  
 HF298=-92.5 kcal REF=Cox & Pilcher 1970 Max Lst Sq Error Cp @ 1300 k 0.67%  
 C5H8N4O12 PETN T11/97C 5.H 8.N 4.O 12.G 200.000 6000.000 316.13828 1  
 4.20349983E+01 4.16412378E-02-1.62923542E-05 2.75856914E-09-1.70123449E-13 2  
 -6.48342117E+04-1.86444303E+02 1.01315796E+01 7.43819642E-02 7.88205030E-05 3  
 -1.68073189E-07 7.47114699E-11-5.32738211E+04-8.13692751E+00-4.65475416E+04 4

120-92-3

C5H8O CYCLOPENTANONE SIGMA=2 STATWT=1 A=0.221 B=0.112 C=0.080 cm-1  
 NU=3063(2), [2994], 2979, [2936,2931], 2894,2824,1776,1461,1418, [1409(2),1301,1298],  
 12277(2), [1212,1179], 1146, [1127,1119], 1033,967,953, [892,875], 826,718, [686], 577,  
 [541], 487,455, [225,93] REF=NIST 2000 IR + B3PW91/6-31G\* calc []. HF298=-197.4+/-  
 1.3 kJ REF=Wiberg, Crocker & Morgan JACS 113, (1991), 3447-3450. {HF298=-194.8+/-  
 1.7 Wolf, Helv.Chim.Acta 55, (1972), 1446-1459} Max Lst Sq Error Cp @ 200 K 0.92%  
 C5H8O T 7/01C 5.H 8.O 1. 0.G 200.000 6000.000 B 84.11642 1  
 1.18281325E+01 2.54559875E-02-9.23804811E-06 1.50152136E-09-9.03124493E-14 2  
 -2.99197006E+04-4.10040646E+01 2.19956938E+00 1.63298815E-02 8.59366418E-05 3  
 -1.28808609E-07 5.37997972E-11-2.56534705E+04 1.70106368E+01-2.37417623E+04 4



Table 4 (continued)

3212-60-0

C5H8O 1-5, Cyclopenten-2-ol C5H7-OH SIGMA=1 STATWT=1 IA=12.1906 IB=25.6872  
 IC=34.8070 Ir=0.14244 ROSYM=1 V3=1100+/-100 cm-1 (as in toluene). Nu=3741,3226,  
 3197,3114,3071,3062,3024,2956,1703,1530,1512,1451,1379,1365,1330,1306,1244,1238,  
 1189,1147,1098,1074,1021,991,972,928,879,864,772,755,592,526,386,311,281  
 HF298=-30.253 kcal {HF298=-31.32 kcal REF=THERM; HF298=-26.99 kcal REF=THERGAS  
 ; PM3 HF298=-36.42 kcal; AM1 HF298=-39.33 kcal} Max Lst Sq Error Cp @ 200 K  
 0.89%.

C5H8O CYC5H7-3-OH A 4/05C 5.H 8.0 1. 0.G 200.000 6000.000 B 84.11642 1  
 1.17779469E+01 2.43872329E-02-8.70273899E-06 1.39911956E-09-8.35284139E-14 2  
 -2.12332683E+04-3.95038282E+01 1.35585303E+00 2.20789635E-02 7.15429574E-05 3  
 -1.15934617E-07 4.97348755E-11-1.70358517E+04 2.13315119E+01-1.52238138E+04 4

3889-74-5

C5H9 CYCLOPENTYL RADICAL SIGMA=2 STATWT=2 IA=11.9909 IB=12.7666 IC=21.9880  
 NU=3213,3106,3098,3052(2),3030.4(2),2951(2),1537,1521,1504,1502,1386,1370,1349,  
 1317,1305,1249,1237,1198,1106,1055,1040,1023,939,918,903(2),857,829,664,572,337,  
 238,172.6 REF=Burcat G3B3 calc HF298=111.131 kJ HF0=138.404 kJ {HF298=115.06  
 kJ REF=NIST 1991.; HF298=81.59 kJ REF=Zhang JOC 63, (1998),1872-1877;  
 HF298=105.9+/-4.2 kJ REF=Luo CRC tables 2006} Max Lst Sq Error Cp @ 200 K  
 \*\*1.12%\*\* @ 6000 K 0.62%

C5H9 CyPentyl Rad A12/04C 5.H 9. 0. 0.G 200.000 6000.000 B 69.12496 1  
 9.62172581E+00 2.69929422E-02-9.68947889E-06 1.56341602E-09-9.35571341E-14 2  
 7.88729754E+03-2.98816293E+01 3.95252891E+00-2.62301053E-03 1.27596618E-04 3  
 -1.67919906E-07 6.73888175E-11 1.14767941E+04 9.87654675E+00 1.33659379E+04 4

41182-83-6

C5H9 2-PENTEN-5-YL CH3CH=CHCH2CH2\* SIGMA=1 STATWT=2 IA=4.5337 IB=39.0496  
 IC=40.1264 Ir(CH3)=0.5096 ROSYM=3 V(3)=685. cm-1 est. Ir(\*CH2)=0.2896  
 ROSYM=1 V(3)=1049. cm-1 est Ir(\*CH2CH2-)=3.0164 V(3)=1049. cm-1 est.  
 Nu=3266,3165,3143,3135,3113,3075.3030,3026,2952,1755,1523,1511,1489,1483,1443,  
 1367,1348,1331,1227,1133,1103,1082,1077,1014,1002,943,810,770,501,467,404,275,  
 218 HF298=41.734 kcal REF=Burcat G3B3 calc {HF298=38.0 kcal REF= Weismann &  
 Benson Prog. Energy Comb 15, (1989),273} Max Lst Sq Error Cp @ 6000 K 0.53%.

C5H9 2-penten-5- A 4/05C 5.H 9. 0. 0.G 200.000 6000.000 B 69.12496 1  
 1.09473230E+01 2.40008026E-02-8.50241891E-06 1.35542731E-09-8.03514292E-14 2  
 1.58040665E+04-2.82498345E+01 4.24938050E+00 2.67855567E-02 2.60883319E-05 3  
 -5.24680141E-08 2.30655275E-11 1.84060663E+04 1.00924612E+01 2.10012443E+04 4

130825-72-8

C5H9 2-PENTEN-1-YL \*CH2CH=CHCH2CH3 SIGMA=1 STATWT=2 IA=4.5849 IB=38.7290  
 IC=39.7034 Ir(CH3)=0.43455 ROSYM=3 V(3)=1150. cm-1 est. Ir(\*CH2)=0.34784  
 ROSYM=1 V(3)=1049. cm-1 est Ir(CH3CH2-)=3.15466 V(3)=1049. cm-1 est.  
 Nu=3259,3168,3145,3134,3122,3114,3063,3047,2999,1544,1537,1527,1520,1508,1433,  
 1393,1335,1302,1278,1223,1171,1078,1035,1003,984,888,798,777,749,548,490,393,303  
 HF298=27.892 kcal REF=Burcat C3B3 calc. {HF298=27. kcal Weismann & Benson  
 Energy Comb 15, (1989),273} Max Lst Sq Error Cp @ 6000 K 0.53%.

C5H9 2-en-1-yl A 4/05C 5.H 9. 0. 0.G 200.000 6000.000 B 69.12496 1  
 1.11277742E+01 2.38252436E-02-8.44023460E-06 1.34549364E-09-7.97578298E-14 2  
 8.68711411E+03-3.07833429E+01 2.34425040E+00 3.21504141E-02 2.45295981E-05 3  
 -5.81110933E-08 2.68653496E-11 1.17932336E+04 1.81635883E+01 1.40357192E+04 4

Table 4 (continued)

29791-12-6

C5H9 3-METHYL-1-BUTEN-3-YL H2C=CH-C\*(CH3)-CH3 SIGMA=1 STATWT=2 IA=10.3103  
 IB=22.2834 IC=31.5588 Ir(CH3)=1.53186 ROSYM=3 V(3)=2175. cm-1 est  
 Ir(CH3)=0.51074 ROSYM=3 V(3)=2175. cm-1 est Ir(H2C=CH-)=2.2382 ROSYM=2  
 V(3)=1049. cm-1 est. Nu=3226,3279,3143,3138,3117,3052,3042,3018,3007,1555,1544,  
 1515,1510,1498,1488,1445,1438,1383,1265,1242,1083,1082,1019,1009,979,947,767,  
 760,569,537,381,348,302 HF298=24.493 kcal REF=Burcat G3B3 calc {HF298=19.3  
 kcal REF=NIST-94} Max Lst Sq Error Cp @ 1300 K 0.5543%.

C5H9 A 4/05C 5.H 9. 0. 0.G 200.000 6000.000 B 69.12496 1  
 1.22463353E+01 2.32449977E-02-8.31633552E-06 1.33604189E-09-7.97458897E-14 2  
 6.42198786E+03-3.90954303E+01 3.71721393E+00 2.27270396E-02 4.82587229E-05 3  
 -7.99696495E-08 3.36979666E-11 9.92261584E+03 1.07095507E+01 1.23252858E+04 4

17439-95-1

C5H9 3-METHYL-1-BUTEN-1-YL \*HC=CH-CH(CH3)-CH3 SIGMA=1 STATWT=2 IA=11.4848  
 IB=20.3148 IC=28.0345 Ir(CH3)=0.51377 ROSYM=3 V(3)=2175 cm-1 Ir(CH3)=0.51495  
 ROSYM=3 V(3)=2175 cm-1 Ir(\*CH=CH-)=2.4640 ROSYM=1 V(3)=1049 cm-1 Nu=3261,3119,  
 3116,3112,3109,3092,3048,3042,3000,1682,1539,1532,1522,1519,1446,1427,1375,1333,  
 1281,1207,1138,1110,978,957,938,891,883,776,684,510,391,355,278 HF298=52.36  
 kcal REF=Burcat G3B3 calc {HF298=50.7 kcal REF=NIST 94} Max Lst Sq Error  
 Cp @ 6000 K 0.55%.

C5H9 1buten3mlyl A 4/05C 5.H 9. 0. 0.G 200.000 6000.000 B 69.12496 1  
 1.21319422E+01 2.34015078E-02-8.38992636E-06 1.34966598E-09-8.05758742E-14 2  
 2.04546205E+04-3.83660754E+01 3.17441228E+00 2.42140870E-02 4.71419240E-05 3  
 -8.02730499E-08 3.41552403E-11 2.40537598E+04 1.35804628E+01 2.63504375E+04 4

58175-93-2

C5H9 3-METHYL-1-BUTEN-4-YL H2C=CH-CH(CH3)-CH2\* SIGMA=1 STATWT=2 IA=11.0932  
 IB=21.1870 IC=28.2139 Ir(CH3)=0.51893 ROSYM=3 V(3)=2175 cm-1 est  
 Ir=(CH2\*)=0.28970 ROSYM=1 V(3)=2175 est Ir(H2C=CH-)=5.9663 ROSYM=1  
 V(3)=1049 cm-1 est Nu=3266,3241,3168,3164,3137,3125,3116,3048,2898,1727,1531,  
 1527,1489,1460,1430,1356,1330,1313,1174,1157,1072,1043,1025,970,941,909,801,601,  
 590,469,381,341,286 HF298=43.106 kcal REF=Burcat G3B3 calc. {HF298=42.3 kcal  
 REF=NIST 94} Max Lst Sq Error Cp @ 6000 K 0.55%.

C5H9 A 4/05C 5.H 9. 0. 0.G 200.000 6000.000 B 69.12496 1  
 1.27590656E+01 2.27460421E-02-8.21059083E-06 1.32807060E-09-7.95689217E-14 2  
 1.56429535E+04-4.01708255E+01 2.39680272E+00 3.13084410E-02 3.22477423E-05 3  
 -6.76807483E-08 3.02707808E-11 1.94200406E+04 1.80329371E+01 2.16916576E+04 4

694-05-3

C5H9N 1,2,3,6-TERAHYDRO-PYRIDINE SIGMA=1. IA=2.57 IB=2.86 IC=0.43 NU=3420,  
 3050,3040,2929,2925,2860,2850(2),2840,1600,1455,1454,1448,1438,1425,1369,1357,  
 1278,1250,1220,1215,1150,1124,1084,1054,965,950,890,885,815,811,770,700,630,521,  
 474,399,285,186 REF=Sidhu et. al., 1991 HF298=18.+/-2 KCAL ESTIMATED USING  
 BENSON'S GROUP ADDITIVITY. Max Lst Sq Error Cp @ 200 K 0.96%

C5H9N T 2/92C 5H 9N 1 0G 200.000 6000.000 B 83.13320 1  
 0.11833534E+02 0.28098151E-01-0.10182947E-04 0.16536607E-08-0.99405120E-13 2  
 0.26418000E+04-0.46192454E+02 0.17693067E+01 0.16923937E-01 0.94000576E-04 3  
 -0.13916857E-06 0.57777745E-10 0.71954216E+04 0.14882677E+02 0.90579000E+04 4

109-67-1

C5H10 1-PENTENE EXTRAPOLATED FROM TRC 4/87 1500 K USING WILHOIT'S POLYNOMIALS  
 HF298=-21.28 kJ Max Lst Sq Error Cp @ 200 K 0.64%

C5H10,1-pentene n 4/87C 5.H 10. 0. 0.G 200.000 6000.000 C 70.13290 1  
 1.19501622E+01 2.52159997E-02-8.85685260E-06 1.42602177E-09-8.54794944E-14 2  
 -8.52115733E+03-3.65337724E+01 5.88359146E+00 5.10403590E-03 9.78286629E-05 3  
 -1.32389833E-07 5.32233940E-11-5.16825430E+03 3.41988594E+00-2.55938113E+03 4

Table 4 (continued)

646-04-8

C5H10 2-PENTENE-Trans(E) EXTRAPOLATED FROM API PROJECT #44 DATA USING WILHOIT'S POLYNOMIALS HF298=-7.59 KCAL Max Lst Sq Error Cp @ 1200 K 0.35%

C5H10 2-PENTENE 2-P12/52C	5H	10	0	OG	298.150	5000.000	C	70.13440	1
0.94842492E+01	0.29600248E-01	0.11393033E-04	0.20468617E-08	0.13936013E-12					2
-0.89116325E+04	-0.23775434E+02	0.18750517E+01	0.37994733E-01	0.57083514E-05					3
-0.29082134E-07	0.13102964E-10	-0.60663547E+04	0.18907614E+02	-0.38194145E+04					4

563-46-2

C5H10 2METHYL-1-BUTENE EXTRAPOLATED FROM STULL WESTRUM & SINKE USING WILHOIT'S POLYNOMIALS HF298=-8.68 KCAL Max Lst Sq Error H @ 300 K 0.5%.

C5H10 2MB-1ene	T11/95C	5H	10	0	OG	298.150	5000.000	B	70.13440	1
0.10169614E+02	0.29142736E-01	0.11304015E-04	0.20426202E-08	0.13964602E-12						2
-0.97185802E+04	-0.27826511E+02	0.15343285E+01	0.40535723E-01	0.26841152E-05						3
-0.27784359E-07	0.12941501E-10	-0.66019829E+04	0.20108917E+02	-0.43679207E+04						4

513-35-9

C5H10 2METHYL-2-BUTENE EXTRAPOLATED FROM STULL WESTRUM & SINKE USING WILHOIT'S POLYNOMIALS HF298=-10.17 KCAL Max Lst Sq Error Cp @ 1200 K 0.35%.

C5H10 2MB-2ene	T11/95C	5H	10	0	OG	298.150	5000.000	B	70.13440	1
0.86980441E+01	0.30551374E-01	0.11746424E-04	0.21071085E-08	0.14329275E-12						2
-0.99867755E+04	-0.19723898E+02	0.12618252E+01	0.39178857E-01	0.31182431E-05						3
-0.25702067E-07	0.11609951E-10	-0.72175421E+04	0.21915280E+02	-0.51177135E+04						4

563-45-1

C5H10 2METHYL-3-BUTENE EXTRAPOLATED FROM STULL WESTRUM & SINKE USING WILHOIT'S POLYNOMIALS HF298=-6.92 KCAL Max Lst Sq Error H @ 300 K 0.8%.

C5H10 2MB-3ene	T 5/96C	5H	10	0	OG	298.150	5000.000	B	70.13440	1
0.10712560E+02	0.28487570E-01	0.10916621E-04	0.19543209E-08	0.13271736E-12						2
-0.87445219E+04	-0.30984943E+02	0.13221471E+00	0.61756848E-01	0.53167981E-04						3
0.29073931E-07	-0.74254711E-11	-0.57719514E+04	0.24567827E+02	-0.34822593E+04						4

287-92-3

C5H10 CYCLOPENTANE SIGMA=1 STATWT=1 IAIBIC=3875. Ir=1.11 ROSYM=10. V0=0. Nu=2960(5),2880(5),1480(3),1455(2),1310(2),1285(2),1250(2),1210(2),1160(2),1035(2),1022,985,949,896,886,858,827,770,617,545,283, REF=DOROFEEVA GURVICH & JORISH JPCRD 15 (1986) 437 HF298=-77.1 KJ REF=TRC Oct. 1990 Max Lst Sq Error Cp @ 6000 K 0.68 % @ 200 K \*\*\*1.6%\*\*\*.

C5H10,cyclo-	g 2/01C	5.H	10.	0.	0.G	200.000	6000.000	B	70.13290	1
9.13283832E+00	3.01131089E-02	-1.09169275E-05	1.77298877E-09	-1.06575265E-13						2
-1.50033856E+04	-2.92612779E+01	3.70339048E+00	-1.15575222E-02	1.64113330E-04						3
-2.09369707E-07	8.31059426E-11	-1.09388708E+04	1.19772908E+01	-9.27294573E+03						4

142-68-7

C5H100 TETRAHYDRO-PYRAN (CYCLO) SIGMA=2 STATWT=1 IA=18.0504 IB=18.7502 IC=32.4924 Nu=3105,3102,3088,3082,3076,3041(2),3026,2969,2962,1538,1522(2),1512,1504,1443,1413,1401,1397,1371,1341,1315,1298,1237,1206,1191,1124,1069,1060,1024,994,892,888,872,829(2),569,467,440,402,253,244 HF298=-53.605 kcal REF=Burcat G3B3 calc {HF298=-53.5 +/- 0.2 KCAL REF=STULL WESTRUM & SINKE 1969} Max Lst Sq Error Cp @ 200 K 0.94% @ 1300 K 0.66%.

C5H100 CYCLO	T A 4/05C	5.H	10.O	1.	0.G	200.000	6000.000	B	86.13230	1
1.02912978E+01	3.19376979E-02	-1.15141841E-05	1.86329429E-09	-1.11732195E-13						2
-3.31402099E+04	-3.53317739E+01	3.76713473E+00	-9.00843898E-04	1.38345597E-04						3
-1.79983389E-07	7.12378755E-11	-2.89582868E+04	1.04223588E+01	-2.69749294E+04						4

Table 4 (continued)

2672-01-7

N-C5H11 N-PENTYL RADICAL EXTRAPOLATED FROM TRC 10/84 1600 K TO 5000 K WITH WILHOIT'S POLYNOMIALS. HF298=45.81 kJ {HF298=13.29 kcal REF=N.Cohen JPC,96 (1992),9052} MAX LST SQ ERROR Cp @ 200 K 0.60%.

C5H11,pentyl	n10/84C	5.H	11.	0.	0.G	200.000	6000.000	C	71.14084	1
1.13174245E+01	2.96389697E-02	-1.08646942E-05	1.78411592E-09	-1.07914240E-13						2
-2.39944362E+02	-3.11204282E+01	7.17404710E+00	3.80923329E-03	1.04379542E-04						3
-1.39634688E-07	5.60397678E-11	2.52872058E+03	-1.18869179E+00	5.50964519E+03						4

2492-34-4

S-C5H11 S-PENTYL RADICAL REF=N.Cohen JPC,96 (1992),9052 EXTRAPOLATED USING WILHOIT'S POLYNOMIALS. HF298= 10.89 Kcal Max Lst Sq Error Cp @ 1500 K 0.43%

S-C5H11 1m-butyl	T03/97C	5.H	11.	0.	0.G	298.150	5000.000	D	71.14234	1
1.05838403E+01	3.11018862E-02	-1.17149660E-05	2.05728548E-09	-1.37198647E-13						2
-1.80355565E+02	-2.72603116E+01	7.53834570E+00	7.11191190E-03	7.97981697E-05						3
-1.00325084E-07	3.76603045E-11	2.39183947E+03	-3.31129273E+00	5.48002949E+03						4

4348-35-0

C5H11 T-C5H11 RADICAL 1,1-dimethyl-propyl SIGMA=1 STATWT=2 IAIBIC=8590.E-117 (Ir(CH3)=0.48 ROSYM=3 V(3)=0)x2 Ir(CH2)=0.48 ROSYM=3 V(3)=1254 cm-1 IB=2.1 ROSYM=1, V(3)=0 NU=2931(9),2825(2),1455(8),1370(3),1279,1252(2),1189(2),1126,992(3),733,541(2),380,200,990(2) HF298=32.6+/-4 kJ REF=WING TSANG JACS (1985) p.2872 Max Lst Sq Error Cp @ 200 K 0.72%.

C5H11,t-pentyl	g 1/93C	5.H	11.	0.	0.G	200.000	6000.000	B	71.14084	1
9.23108985E+00	3.11689026E-02	-1.12478717E-05	1.82090758E-09	-1.09205406E-13						2
-1.60063335E+03	-2.06135904E+01	6.44628584E+00	-9.54231607E-03	1.37892083E-04						3
-1.69241994E-07	6.53097634E-11	1.50839319E+03	5.43062020E+00	3.92085643E+03						4

3744-21-6

C5H11 2,2,M,M-PROPYL (NEOPENTYL) RADICAL SIGMA=54 REF=N.Cohen JPC,96 (1992),9052 EXTRAPOLATED USING WILHOIT POLYNOMIALS. HF298=8.22 KCAL Max Lst Sq Error Cp @ 1500 K \*\*1.12%.\*\*

C5H11 neopentyl	T03/97C	5.H	11.	0.	0.G	298.150	5000.000	D	71.14234	1
2.60303371E+01	-3.89073388E-03	1.18835338E-05	-2.05929731E-09	1.06754076E-13						2
-5.66523187E+03	-1.12796509E+02	-4.46503561E+00	9.32367831E-02	-1.41121240E-04						3
1.52613544E-07	-6.83999414E-11	2.30110241E+03	4.28019931E+01	4.13644099E+03						4

628-05-7

C5H11NO2 1-Nitro-Pentane STATWT=1 SYMNO=2 IA=21.264770 IB = 85.889716 IC = 100.4047696 Ir (NO2) = 5.96 ROSYM =2 V(2) = 0.08 kcal/mole Ir(CH3)= 0.51666 ROSYM =3 V(3) = 3.5 kcal Ir(C2H5) = 2.104 ROSYM =2 V(2) = 9.0 kcal Ir(C3H7) = 2.22 ROSYM = 2 V(2) =13.64 kcal NU = 3183,3088,3069,3034,3027,3024,2992,2955,2949,2947,2893,1901,1611,1474,1421,1410,1403,1402,1398,1386,1367,1341,1300,1253,1173,1167,1153,1146,1129,1121,1081,1039,1020,990,965,926,866,830,805,691,615, 480,470,394,315,295,214 REF = NIST 97 WEBBOOK HF298 =-39.3 kcal REF =BURCAT TAE # 824 (1998). Max Lst Sq Error Cp @ 200 & 6000 K 0.68%

NITRO-PENTANE	T06/98C	5.H	11.N	1.O	2.G	200.000	6000.000	B	117.14788	1
1.59382106E+01	3.48884183E-02	-1.29633850E-05	2.12755256E-09	-1.28618354E-13						2
-2.80406921E+04	-5.83080492E+01	4.00703926E+00	2.29727394E-02	1.04023119E-04						3
-1.55573589E-07	6.44328697E-11	-2.26341947E+04	1.39586649E+01	-1.97764150E+04						4

Table 4 (continued)

109-66-0

C5H12 N-PENTANE SIGMA=18 TRC Oct 1985 DATA To 1500 K EXTRAPOLATED THROUGH WILHOIT'S POLYNOMIALS. HF298=-146.76 kJ MAX LST SQ ERROR Cp @ 1200 K 0.80 %.

C5H12,n-pentane	n10/85C	5.H	12.	0.	0.G	200.000	6000.000	C	72.14878	1
1.67372700E+01	2.23922034E-02	-6.17705543E-06	1.02144924E-09	-6.65183115E-14						2
-2.57616661E+04	-6.45619087E+01	8.54851659E+00	-8.88170492E-03	1.43083890E-04						3
-1.78592329E-07	6.97489761E-11	-2.07492614E+04	-8.93518255E+00	-1.76510702E+04						4

78-78-4

I-C5H12 ISOPENTANE TRC 10/85 DATA EXTRAPOLATED THROUGH WILHOIT'S POLYNOMIALS. HF298=-153.7 kJ Max Lst Sq Error Cp @ 1300 K 0.74%

C5H12,i-pentane	P10/85C	5.H	12.	0.	0.G	200.000	6000.000	C	72.14878	1
1.04816310E+01	3.42018698E-02	-1.20571041E-05	1.91951808E-09	-1.13803609E-13						2
-2.43557061E+04	-3.10177093E+01	2.19440218E+00	3.61717165E-02	3.01586516E-05						3
-5.87986428E-08	2.47059837E-11	-2.09097364E+04	1.71851550E+01	-1.84857556E+04						4

463-82-1

C5H12 2,2-dimethylbutane NEOPENTANE TRC 10/85 DATA EXTRAPOLATED USING WILHOIT'S POLYNOMIALS. HF298=-167.92 kJ HF0=-135.02 kJ Max Lst Sq Error Cp @ 1400 K 0.95% @ 200 K \*\*\*3.3%\*\*\*

CH3C(CH3)2CH3	P10/85C	5.H	12.	0.	0.G	200.000	6000.000	C	72.14878	1
8.20556617E+00	3.91429094E-02	-1.34755411E-05	2.09281432E-09	-1.21719082E-13						2
-2.52830248E+04	-2.33002317E+01	-1.14339730E-01	5.26841774E-02	-6.21509048E-06						3
-2.28700893E-08	1.23593718E-11	-2.24093954E+04	2.22008439E+01	-2.01960188E+04						4

625-44-5

C5H12O(L) t-C4H9-O-CH3 Tertiary butyl-methyl ether LIQUID calculated from thermal measurements. REF=TRC 1983 HF298=-313.6 kJ

C5H12O tC4H9OCH3	T08/00C	5.H	12.O	1.	0.L	200.000	310.000	A	88.14968	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
0.00000000E+00	0.00000000E+00	1.81730017E+01	-1.70292004E-02	1.27817452E-04						3
-5.81277666E-08	-4.62085850E-11	-4.33711851E+04	-7.15912586E+01	-3.77171956E+04						4

625-44-5

C5H12O t-C4H9-O-CH3 Tertiary butyl-methyl ether SIGMA=1 IA=20.675347 IB=30.958288 IC=30.991722 3x(Ir=0.47 V3=2.4 kcal ROSYM=3) Nu=[3089](2), 3006,3003(2),3000,[2986,2945],2940,2935,[2837,2730],1492,1483,[1475],1472,1461,1459,1457,1443(2),1391,[1372],1365,1249,[1205],1198,1172,1143,[1093,1021],1007,930,892,[855],831,[724],488,440,394,350,324,275.9,272.7,246.5 REF= NIST 2000, Webbook, IR in parenthesis and Gaussian 98 B3LYP/6-31G\* calc of Jan 1999. HF298=-283.2 kJ REF=TRC-83 {HF298=-293.8 kJ REF=NIST 94; HF298=-283.7+/-0.8 kJ REF=Pedly & Rylance 1977} Max Lst Sq Error Cp @ 1300 K 0.61%

C5H12O tC4H9OCH3	T08/00C	5.H	12.O	1.	0.G	200.000	6000.000	B	88.14968	1
1.33868819E+01	3.29283214E-02	-1.18027402E-05	1.90207547E-09	-1.13712190E-13						2
-4.07919507E+04	-4.60060101E+01	4.24395629E+00	3.82110434E-02	2.49992458E-05						3
-5.45089669E-08	2.33555478E-11	-3.71488062E+04	6.40373322E+00	-3.40609368E+04						4

129066-00-8

C6 linear SIGMA=2 STATWT=3. B0=0.048479 Nu=2061,1694,637,1960,1197,665(2), 246(2),434(2),90(2) HF298=314. HF0=311.26 +/-16.7 kJ REF=Van-Orden & Saykally Chem REV 98,(1998),2313 Max Lst Sq Error Cp @ 1300 K 0.46%

C6 linear	A09/04C	6.	0.	0.	0.G	200.000	6000.000	B	72.06420	1
1.09690747E+01	5.40080233E-03	-2.05587055E-06	3.44673440E-10	-2.11743818E-14						2
1.54041379E+05	-2.89517984E+01	3.01754669E+00	3.79181685E-02	-6.06833596E-05						3
5.23078196E-08	-1.79226696E-11	1.55866233E+05	9.92611478E+00	1.58010033E+05						4

Table 4 (continued)

118-74-1

C6CL6 HEXACHLOROBENZENE DATA FROM STULL WESTRUM &amp; SINKE EXTRAPOLATED USING WILHOIT'S POLYNOMIALS HF298=-8.10 KCAL Max Lst Sq Error Cp @ 1300 K 0.4%

C6CL6	T 1/92C	6CL	6	0	OG	298.150	6000.000	B	284.78220	1
0.25828477E+02	0.83148412E-02	-0.33076208E-05	0.57000698E-09	-0.35641306E-13						2
-0.13505569E+05	-0.99653026E+02	0.46643307E+01	0.79424296E-01	-0.98554390E-04						3
0.61217228E-07	-0.15381401E-10	-0.82398803E+04	0.66783480E+01	-0.40760550E+04						4

34346-16-2

C6D5 PHENYL-D5 RAD SIGMA=2 STATWT=2 IA=33.7696 IB=17.9469 IC=15.8227  
 NU=2293,943,1037,497,2292,969,827,601,1286,824,662(2),2287,1335(2),814,2265(2),  
 1552(2),867(2),577(2),795,352(2) REF=BURCAT,ZELEZNIK & MCBRIDE HF298=315.7 kJ.  
 HF0=327.5 kJ. MAX LST SQ ERROR CP @ 1300 K 0.65 % .

C6D5,phenyl	g 1/01C	6.D	5.	0.	OG	200.000	6000.000	B	82.13471	1
1.42048142E+01	1.62416818E-02	-6.14709484E-06	1.02680905E-09	-6.29242933E-14						2
3.15140960E+04	-5.29078812E+01	-2.42438172E+00	5.49431516E-02	-2.56858433E-05						3
-1.26752764E-08	1.11056357E-11	3.64972825E+04	3.48056612E+01	3.79697661E+04						4

1076-43-3

C6D6 BENZENE-D6 IA=35.8938 IB=IC=17.9469 SIGMA=12 NU=2293,943,1037,497,  
 2292,969,827,601,1286,824,662(2),2287(2),1335(2),814(2),2265(2),1552(2),867(2),  
 577(2),795(2),352(2) REF=SHIMANOUCI HF298=58.18 kJ REF=BURCAT, ZELEZNIK &  
 McBRIDE MAX LST SQ ERROR CP @ 1300 K 0.86 % .

C6D6	L12/84C	6.D	6.	0.	OG	300.000	5000.000	B	84.15061	1
0.15619864E 02	0.17123934E-01	-0.62012759E-05	0.98493058E-09	-0.56891557E-13						2
-0.14433052E 03	-0.63901352E 02	-0.20701218E 01	0.52938197E-01	-0.96074828E-05						3
-0.32802372E-07	0.19012528E-10	0.54068984E 04	0.30680710E 02	0.69971633E 04						4

392-56-3

C6F6 HEXAFLOROBENZENE SIGMA=12 IA=IB=79.9862 IC=159.979 NU=1660(2),1534(2),  
 1498,1327,1156(2),1077,992(2),765,623(2),602,572,546,431(2),389.5(2),304(2),  
 262.2,256.6(2),218,181,135.7(2) REF=Melius Database Q9X HF298=-228.64 Kcal  
 REF=STULL WESTRUM & SINKE Max Lst Sq Error Cp @ 1300 K 0.48%

C6F6	T03/97C	6.F	6.	0.	OG	200.000	6000.000	B	186.05642	1
2.33186087E+01	1.07562779E-02	-4.17044638E-06	7.07443606E-10	-4.38074922E-14						2
-1.23931487E+05	-9.30677826E+01	1.97866627E+00	8.21868402E-02	-1.03031945E-04						3
6.88636763E-08	-1.94291617E-11	-1.18514980E+05	1.44710988E+01	-1.15055458E+05						4

355-42-0

C6F14 PERFLUOROHEXANE (FC-5-1-14) SIGMA=18 CALCULATED and EXTRAPOLATED USING  
 NIST 94 AND BOZZELLI & RITTER'S PROGRAM. HF298=-704.87 KCAL Max Lst Sq Error Cp  
 @ 1000 K 0.07% .

C6F14	FC 51-14	T12/94C	6F	14	0	OG	298.150	5000.000	E	338.04364	1
0.44067386E+02	0.12770763E-01	-0.53399367E-05	0.95791650E-09	-0.61923975E-13						2	
-0.37074786E+06	-0.18473799E+03	-0.14298519E+02	0.24055087E+00	-0.34353654E-03						3	
0.22553364E-06	-0.55889775E-10	-0.35851817E+06	0.98855981E+02	-0.35470535E+06						4	

88053-50-3

C6H RAD T0=0 STATWT=4 IB=60.398 NU=3329,3313,2201,1115,625(3),1570,491(2),  
 258(2),433(2),105(2) T0=3000. STATWT=2 REF= BAUER & DUFF and BURCAT (unpub).  
 HF298=248.0 KCAL REF= Kiefer, Sidhu, Kern, Xie, Chen, Harding 1992. Max Lst Sq  
 Error Cp @ 6000 K 0.34%

C6H	T 3/92C	6H	1	0	OG	200.000	6000.000	C	73.07394	1
0.11361786E+02	0.75157820E-02	-0.27216114E-05	0.43917513E-09	-0.26217995E-13						2
0.12080112E+06	-0.29989833E+02	0.10110111E+01	0.59781961E-01	-0.10773934E-03						3
0.96196601E-07	-0.32681317E-10	0.12261638E+06	0.17998104E+02	0.12479773E+06						4

Table 4 (continued)

3161-99-7

C6H2 HEXATRIYNE STATWT=1. SIGMA=2. IB=63.5805 NU=3313,2201,2019,625,3328,2125,1115,625(2),491(2),258(2),622(2),433(2),105(2) Ref=Bjarnov, Christiansen & Nielsen Spectrochim Acta 20A (1974), 1255. HF298=167.5 KCAL REF= Kiefer, Sidhu, Kern, Xie, Chen, Harding 1992 {HF0=168.6 kcal REF=Bauer & Duff JCP 36,(1962), 1754} Max Lst Sq Error @ 1300 K 0.38%

C6H2	T 3/92C	6H	2	0	OG	200.000	6000.000	B	74.08188	1
	0.12532801E+02	0.87766321E-02	-0.31329616E-05	0.50371820E-09	-0.30071921E-13					2
	0.79784338E+05	-0.38858580E+02	-0.54109216E+00	0.74532628E-01	-0.13578252E-03					3
	0.12226630E-06	-0.41825207E-10	0.82115132E+05	0.21882710E+02	0.84288792E+05					4

63520-46-7

C6H2Cl3O\* 2,4,6 Tri-Chloro-Phenoxy Radical SIGMA=2 STATWT=2 IA=100.4975  
IB=114.5959 IC=215.0933 NU=3241,3240,1595,1539,1474,1427,1369,1275,  
1182,1135,1080,883,883,864,805,754,747,603,562,484,425,377,375,334,304,197,  
193,192,135,85 HF298=-27.48 kJ HF0=-20.29 kJ REF=Janoschek G3MP2B3  
calculations Max Lst Sq Error Cp @ 1300 K 0.44%

C6H2Cl3O	RADICAL	T 6/03C	6.H	2.O	1.CL 3.G	200.000	6000.000	B	196.43758	1
	2.02798797E+01	1.29194844E-02	-4.81871155E-06	7.97954205E-10	-4.86299607E-14					2
	-1.12907568E+04	-7.45021576E+01	2.39930652E+00	6.22028801E-02	-4.88719347E-05					3
	1.03520477E-08	3.04767726E-12	-6.37525850E+03	1.77969078E+01	-3.30506548E+03					4

591755-75-8

C6H2Cl3O 2,4,6-Trichlorophenol-3-yl Radical STATWT=2 SIGMA=1 IA=211.8900  
IB=255.2599 IC=467.1499 IR= Ir=0.1424 ROSYM=1 V(3)=1116.8 cm-1 NU=3692,  
3230,1641,1575,1482,1391,1367,1303,1206,1173,1100,869,847,792,734,697,579,562,  
506,427,413,375,372,330,294,216,192,177,134. HF298=101.51 kJ HF0=107.37 kJ  
REF=Janoschek G3MP2B3 calc. Max Lst Sq Error Cp @ 1300 K 0.41%.

C6HCL3OH	TCP-3-yl	T 6/03C	6.H	2.O	1.CL 3.G	200.000	6000.000	B	196.43758	1
	2.07200382E+01	1.18233128E-02	-4.36636375E-06	7.18769650E-10	-4.36384388E-14					2
	4.25092666E+03	-7.50784561E+01	3.12110317E-01	8.16782350E-02	-9.99655571E-05					3
	6.30326984E-08	-1.62053682E-11	9.25165496E+03	2.71083126E+01	1.22087772E+04					4

591755-76-9

C6H2Cl3O3 2,4,6-Tri-ChloroBiCyclo-2,5-Hexadiene-1,4 Peroxy-1-Phenoxy Radical  
Symetric SIGMA=1 STATWT=2 IA=110.4572 IB=142.0755 IC=207.5354 NU=3258,3257,  
1684,1662,1279,1223,1194,1158,1072,994,920,918,856,844,809,785,765,749,663,  
594,541,530,510,469,424,411,392,344,340,250,244,226,176,175,136,79 HF298=30.7  
kJ HF0=142.99 kJ REF=Janoschek G3MP2B3 Max lst sq Error Cp @ 1300 K 0.39%.

C6H2Cl3O3	Sym BiCyT07/03C	6.H	2.CL	3.O	3.G	200.000	6000.000	B	228.43638	1
	2.61260505E+01	1.31211452E-02	-4.90861350E-06	8.14544010E-10	-4.97157498E-14					2
	5.82258664E+03	-1.04714077E+02	-1.20971521E+00	1.06353628E-01	-1.27674801E-04					3
	7.40376577E-08	-1.64033592E-11	1.24291237E+04	3.19460204E+01	1.58061028E+04					4

591755-77-0

C6H2Cl3O3 2,4,6-Tri-ChloroBiCyclo-2-Hexene-1-One-4,6-Peroxy-5-yl Radical  
SIGMA=1 STATWT=2 IA=118.3628 IB=131.9052 IC=224.3314 Nu=3284,3235,1844,1630,  
1324,1292,1183,1130,1094,1052,1027,939,889,875,870,836,802,774,750,684,612,496,  
490,420,388,381,363,335,302,285,238,202,175,159,134,70 HF298=28.95 kJ  
HF0=40.41 kJ REF=Janoschek J. Mol.Struct 661-2,(2003),635 Max Lst Sq Error  
Cp @ 1300 K 0.39%.

C6H2Cl3O3	BiCy	T07/03C	6.H	2.CL	3.O	3.G	200.000	6000.000	B	228.43638	1
	2.54863454E+01	1.37336374E-02	-5.13874263E-06	8.52778911E-10	-5.20494616E-14					2	
	-6.36349755E+03	-1.00915829E+02	8.25960455E-01	8.97046703E-02	-8.89846443E-05					3	
	3.66349413E-08	-3.29895819E-12	-3.61540530E+01	2.42683330E+01	3.48186484E+03					4	

Table 4 (continued)

182180-13-8

C6H3 RAD CH2=C\*-CC-CCH STATWT=2. SIGMA=2. IA=.278 IB=66.1121 IC=66.3901  
 NU=3012,629,450,3102,870,230,1410,1580,530,1090,1100,147,935,1950,490,3305,2100,  
 290,615,107,480 HF0=158.3 kcal HF298=163. kcal REF=DUFF & BAUER MAX LST SQ  
 ERROR CP @ 1300K 0.44%

C6H3	T 2/90C	6H	3	0	OG	200.000	6000.000	C	75.08982	1
0.12196528E+02	0.11454228E-01	0.41312980E-05	0.66884722E-09	0.40122816E-13						2
0.77275592E+05	0.35794114E+02	0.17798531E+01	0.50337619E-01	0.65263026E-04						3
0.47594586E-07	0.14300850E-10	0.79748524E+05	0.15767468E+02	0.82027246E+05						4

182180-09-2

o-C6H3 1,2-Benzyne-3-yl Radical SIGMA=1 STATWT=2 IA=12.1510 IB=13.2660  
 Ic=25.41705 Nu=3213,3207,3184,1565,1540,1438,1432,1318,1186,1129,1128,1033,  
 948,872,838,769,568,553,476,443,398 HF298=728.91 kJ HF0=733.879 kJ  
 REF=Burcat G3B3 calc. {HF298=468.6 kJ REF=Xu,Wang et al 6th Internat Conf Chem  
 Kinet NIST 2005, p56 C6H3a config} Max Lst Sq Error Cp @ 1300 K 0.52%

o-C6H3 Radical Cy A02/05C	6.H	3.	0.	0.G	200.000	6000.000	B	75.08802	1
1.07791236E+01	1.29752918E-02	4.74348788E-06	7.75171464E-10	4.68121821E-14					2
8.28078760E+04	3.23817342E+01	8.25343066E-01	2.54304386E-02	2.14951562E-05					3
-5.23692607E-08	2.43576096E-11	8.61930921E+04	2.24157823E+01	8.76673882E+04					4

88-06-2

C6H3Cl3O 2,4,6-Tri-Chloro-Phenol SIGMA=2 IA=98.8686 IB=118.4291  
 IC=217.2977 Ir=0.14239 ROSYM=1 V(3)=1116.8 cm-1 Nu=3857,3569,3095,1724,1713,  
 1572,1468,1397,1321,1261,1223,1168,1109,1076,1067,918,847,809,733,564,[571,508,  
 433,417,383,374,350,301,213,198,188,141] REF=NIST Webbook 2000 IR data  
 +B3LYP/6-31G(d) calculation. HF298=-189.07 kJ HF0=-176.92 kJ REF=Janoschek  
 J. Mol.Struct 661-2,(2003),635 {HF298=-34.28 kcal REF=W.Shaub Thermochemica  
 Acta 58,(1982),11} Max Lst Sq Error Cp @ 1300 K 0.43%.

TRICHLOROPHENOL	T 6/03C	6.H	3.0	1.CL	3.G	200.000	6000.000	B	197.44552	1
2.00548095E+01	1.48689736E-02	5.41339688E-06	8.82942340E-10	5.32711832E-14						2
-3.07414767E+04	7.38666469E+01	1.04736140E+00	7.13669355E-02	6.63730092E-05						3
2.75555456E-08	3.25677598E-12	2.56905886E+04	2.33240058E+01	2.27397646E+04						4

N/A

C6H3Cl3O 1,3,5-trichloro-hexa-triene-6-one CHCl=CH-CCL=CH-CCL=C=O SIGMA=1  
 STATWT=1 Very Rough Estimation by THERGAS 298-1000 K Extrapolated to 3000 using  
 Wilhoit's polynomials. HF298=-4.74 kcal

C6H3Cl3O linear	S03/01C	6.H	3.CL	3.O	1.G	298.150	3000.000	F	197.44732	1
6.44233770E+00	5.41042263E-02	2.06267600E-05	3.49123249E-09	2.24394761E-13						2
-7.07280084E+03	2.19999991E+00	5.90519827E+00	5.06643694E-02	1.50612584E-05						3
2.45538664E-09	9.38609447E-13	6.26909577E+03	7.09136936E+00	2.38524700E+03						4

591755-78-1

C6H3Cl3O2 Cyclo-2,4,6 tri-chloro-3,5-hexadiene-1-quinone-2-ol  
 cy/CO-CCL(OH)-CH=CCL-CH=CCL-/ SIGMA=1 STATWT=1 IA=108.7606 IB=133.0775  
 Ic=202.6839 Ir(OH)=0.1434 V(3)=1213. cm-1 ROSYM=1 NU=3585,3248,3235,1788,  
 1685,1611,1456,1371,1357,1251,1197,1138,1059,940,922,865,825,787,749,642,606,  
 579,552,482,410,374,349,343,329,293,247,185,181,153,96 HF298=-266.02 kJ  
 HF0=-263.99 kJ REF=Janoschek J. Mol.Struct 661-2,(2003),635 Max Lst Sq Error  
 Cp @ 1300 K 0.47%

C6H2Cl3OOH Cy	T 7/03C	6.H	3.CL	3.O	2.G	200.000	6000.000	B	213.44492	1
2.30154197E+01	1.51042221E-02	5.54122582E-06	9.08005114E-10	5.49482329E-14						2
-4.23211655E+04	8.83191815E+01	8.72968514E-02	9.12361582E-02	1.04155296E-04						3
5.98780411E-08	1.36147269E-11	3.66182071E+04	2.69710455E+01	3.33453204E+04						4



Table 4 (continued)

731798-94-0

o-C6H3I 1,2-Benzyne-3-Iodo SIGMA=1 STATWT=1 IA=11.93932 IB=115.32193  
 IC=127.261238 Nu=3213,3194,3168,2000,1468,1459,1425,1292,1187,1147,1100,1035,  
 943,881,850,767,667,584,492,442,441,265,212,143.2 REF=Burcat B3LYP/6-311G\*  
 HF298=534.7+/-12 kJ REF=Wang et al 6th Int. Conf Chem Kin. NIST 2005 p.56  
 {HF298=546.01+/-50. kJ REF= PM3 calc.} Max Lst Sq Error Cp @ 1300 K 0.48%  
 o-C6H3I Cy A08/05C 6.H 3.I 1. 0.G 200.000 6000.000 B 201.99249 1  
 1.33050435E+01 1.34129920E-02-4.90406618E-06 8.01426651E-10-4.83968269E-14 2  
 5.86748176E+04-4.12260115E+01 1.77626967E+00 3.57073993E-02-1.00289131E-06 3  
 -3.05265417E-08 1.66127632E-11 6.22557563E+04 2.04443084E+01 6.43110899E+04 4

99-35-4

C6H3(NO2)3 1,3,5-Tri-Nitro-Benzene SYMNO = 6 STATWT = 1 IA = 111.42859  
 IB = 172.18627 IC = 252.862147 Ir(NO2)=5.96 ROSYM = 2 V(2) = 3.11 kcal  
 NU = 3071,3038,2993,1923,1913,1742,1720,1671,1594,1580,1431,1368,1321,1209,1183,  
 1121,1113,1018,1000,970,952,939,843,778,751,748,688,680,644,591,568,522,504,448,  
 393,350,335,323,294,256,251,147,129,87.5,66. REF =BURCAT, TAE Report # 824 1998  
 HF298=14.9 kcal REF = Pedley, Naylor & Kirby 1986 Max Lst Sq Error Cp @  
 1300 K 0.53%  
 TRI-NITRO BENZEN T 5/98C 6.H 3.N 3.O 6.G 200.000 6000.000 C 213.10644 1  
 2.87195273E+01 2.08056280E-02-8.03680268E-06 1.35348056E-09-8.32405765E-14 2  
 -3.92148064E+03-1.15710853E+02 2.18818193E+00 1.02515207E-01-1.05642628E-04 3  
 5.50716150E-08-1.13737832E-11 3.11892525E+03 1.95711122E+01 7.49792832E+03 4

462-80-6

C6H4 o-BENZYNE SIGMA=2 STATWT=1 IA=11.9698 IB=14.7194 IC=267.6891  
 Nu=3220,3216,3194,3178,2026,1503,1487,1440,1329,1286,1173,1117,1088,1008,963,  
 914,871,844,755,623,596,438,406,396 HF298=110.21 kcal REF=Burcat G3B3 calc  
 {HF298=106.6 kcal REF=Xu,Wang et al 6th Internat Conf Chem Kinet NIST 2005,p56;  
 HF298=115. kcal REF=Pollack & Hehre TETRAHEDRON LETT. 21,(1980),2483;  
 HF298=105.1+/-3.2 kcal REF=Squires et al JACS 113,(1991),7414; HF298=124. kcal  
 REF=Bauer's estimate JCP 36,(1962),1743} Max Lst Sq Error Cp @ 200 K 0.73%  
 1,2-C6H4 BENZYNE A02/05C 6.H 4. 0. 0.G 200.000 6000.000 B 76.09596 1  
 1.05707063E+01 1.56860613E-02-5.68267148E-06 9.22956737E-10-5.54966417E-14 2  
 5.04976657E+04-3.32563927E+01 7.21604591E-01 2.47976151E-02 3.16372209E-05 3  
 -6.53230986E-08 2.96082142E-11 5.39797980E+04 2.16733825E+01 5.54615216E+04 4

1828-89-3

m-C6H4 1,3-Benzyne SIGMA=2 STATWT=1 IA=9.5976 IB=16.6885 IC=26.2861  
 Nu=3234,3230,3183,3178,1856,1585,1436,1407,1315,1173,1095,1087,1084,981,914,829,  
 818,806,765,618,586,570,403,317 HF298=125.165 kcal REF=Burcat G3B3 calc.  
 {HF298=122.0 kcal REF=Xu,Wang et al 6th Internat Conf Chem Kinet NIST 2005,p56;  
 HF298=121.9+/-3.1 kcal REF=Squires et al JACS 113,(1991),7414} Max Lst Sq.  
 Error Cp @ 200 K 0.78%  
 1,3-C6H4 BENZYNE A02/05C 6.H 4. 0. 0.G 200.000 6000.000 B 76.09596 1  
 1.10822567E+01 1.52050006E-02-5.50413279E-06 8.93543569E-10-5.37122075E-14 2  
 5.78788327E+04-3.59993464E+01 1.90321135E-01 2.91815358E-02 2.38253207E-05 3  
 -5.98452144E-08 2.82709926E-11 6.15257646E+04 2.37632933E+01 6.29851140E+04 4

Table 4 (continued)

3355-34-8

p-C6H4 1,4-Benzyne SIGMA=4 STATWT=1 IA=12.7346 IB=14.5334 IC=27.2680  
 Nu=3245,3244,3229,3225,1720,1492,1329,1253,1179,1109,1091,953,897,856,825,739,  
 722,707,556,494,480,458,292 HF298=137.25 kcal REF=Burcat G3B3 calc  
 {HF298=137.3 kcal REF=Xu,Wang et al 6th Internat Conf Chem Kinet NIST 2005,p56;  
 HF298=137.8+/-2.9 kcal REF=Squires et al JACS 113,(1991),7414} Max Lst Sq.  
 Error Cp @ 200 K 0.62%.

1,4-C6H4 BENZYNE A02/05C 6.H 4. 0. 0.G 200.000 6000.000 B 76.09596	1
1.18961684E+01 1.43787478E-02-5.18375433E-06 8.39304747E-10-5.03613102E-14	2
6.37981144E+04-4.05006008E+01-5.78996617E-01 3.95315415E-02-1.83312631E-06	3
-3.45973149E-08 1.93580017E-11 6.75574889E+04 2.58067944E+01 6.90664874E+04	4

16668-68-1

C6H4 trans-1,5-HEXADIYNE-3-ENE SIGMA=2 STATWT=1 IA=1.7718 IB=58.0179  
 IC=59.7897 Nu=3494(2),3181,3174,2229,2206,1662,1333,1307,1055,1041,977,865,  
 635(2),587,579,547,529,520,381,255,132,125 HF298=523.1 kJ HF0=527.03 kJ  
 REF=Burcat G3B3 calc {HF298=125.8 KCAL REF=NIST 91; HF298=129.5 kcal REF=Xu,  
 Wang et al 6th Internat Conf Chem Kinet NIST 2005,p56; HF298=128.6 kcal  
 REF=Roth et al Chem. Ber. 124(1991),2499} Max Lst Sq Error Cp @ 6000 K 0.44%

C6H4 1,5- trans A02/05C 6.H 4. 0. 0.G 200.000 6000.000 B 76.09596	1
1.22328906E+01 1.36328237E-02-4.80871703E-06 7.66968774E-10-4.55328106E-14	2
5.80208413E+04-3.69903232E+01 2.21633052E-01 5.81529280E-02-7.13934059E-05	3
4.76725943E-08-1.28753162E-11 6.08064933E+04 2.23249817E+01 6.29146636E+04	4

16668-67-0

C6H4 cis-1,5-HEXADIYNE-3-ENE (Z) SIGMA=2 STATWT=1 IA=11.5068 IB=34.0212  
 IC=45.5280 Nu=3495(2),3185,3169,2228,2209,1650,1437,1258,1049,963,900,782,744,  
 631,627,618,592,567,449,381,263,236,108 HF298=524.22 kJ HF0=528.6 kJ REF=Burcat  
 G3B3 calc {HF298=123 KCAL REF=NIST 91; HF298=129.49 kcal REF=Roth et al Chem.  
 Ber. 124,(1991),2499} Max Lst Sq Error Cp @ 6000 K 0.42%.

1,5-C6H4 1,5 cis A02/05C 6.H 4. 0. 0.G 200.000 6000.000 B 76.09596	1
1.22388926E+01 1.36279082E-02-4.80715345E-06 7.66746640E-10-4.55210640E-14	2
5.81401255E+04-3.70117245E+01-4.36293187E-01 6.12732353E-02-7.68492543E-05	3
5.18458875E-08-1.40527024E-11 6.10383325E+04 2.53964956E+01 6.30485193E+04	4

121058-10-4

C6H4 HexaPentaene H2C=C=C=C=CH2 SIGMA=4 STATWT=1 IA=0.5752 IB=67.7896  
 IC=68.3649 Nu=3212(2),3140(2),2222,2126,1724,1496,1454,1203,1032.5(2),863.5(2),  
 667,650,643,592,558,373,294,273,117,114 HF298=568.26 kJ HF0=572.16 kJ  
 REF=Burcat G3B3 Calc. {HF298=129.37 kcal REF=THERM, Bozzelli @ Ritter} Max  
 Lst Sq Error Cp @ 6000 K 0.47%

C6H4 PENTAENE A02/05C 6.H 4. 0. 0.G 200.000 6000.000 B 76.09596	1
1.15160949E+01 1.45816929E-02-5.21944977E-06 8.40605048E-10-5.02392470E-14	2
6.35897979E+04-3.41128898E+01 1.72575865E+00 4.58663914E-02-4.46314139E-05	3
2.38247581E-08-5.11679045E-12 6.61423782E+04 1.55428939E+01 6.83458811E+04	4

121076-12-8

C6H4 Hexa-1,2,3-triene-5-yne H2C=C=C=CH-CCH SIGMA=1 STATWT=1 IA=4.3607  
 IB=55.1036 IC=59.4643 Nu=3495,3225,3150,3134,2232,2191,1687,1474,1333,1064,  
 1045,888,874,855,628.5(2),578,564,553,379,327,271,223,99.5 HF298=559.71 kJ  
 HF0=563.79 kJ REF=Burcat G3B3 calc. {HF298=327.9 KJ REF=THERM approximation}  
 Max Lst Sq Error Cp @ 6000 K 0.44%

1,2,3-Hexatriene A03/05C 6.H 4. 0. 0.G 200.000 6000.000 B 76.09596	1
1.19575424E+01 1.40266572E-02-4.98340919E-06 7.98638006E-10-4.75692474E-14	2
6.24778222E+04-3.45944009E+01 6.27067962E-01 5.48105471E-02-6.45567865E-05	3
4.20781203E-08-1.12070896E-11 6.51861777E+04 2.17065953E+01 6.73168030E+04	4

Table 4 (continued)

3474-42-8

C6H4Cl o-CHLOROPHENYL RADICAL SIGMA=1 STATWT=2 IA=13.899634 IB=53.9800  
 IC=67.879698 Nu=3034,3026,3017,3005,1478,1458,1393,1370,1244,1172,1111,1055,  
 1031,955,914,911,874,788,693,663,620,579,436,391,377,273,166 T0=36470 cm-1  
 HF298=72.46+/-6.9 kcal REF=Melius Database A72N Max Lst Sq Error Cp @  
 200 K 0.57%.  
 C6H4CL ortho S 6/01C 6.H 4.CL 1. 0.G 200.000 6000.000 B 111.55046 1  
 1.44384386E+01 1.52000987E-02-5.57438606E-06 9.12463189E-10-5.51404855E-14 2  
 3.02001028E+04-4.99704496E+01 1.61880112E-01 4.30726825E-02 4.84191280E-07 3  
 -4.13968410E-08 2.25995610E-11 3.45672294E+04 2.61860763E+01 3.64630796E+04 4

3474-40-6

C6H4Cl m-CHLOROPHENYL RADICAL SIGMA=1 STATWT=2 IA=13.85346 IB=52.96167  
 IC=66.815131 Nu=3037,3036,3025,3009,1481,1437,1407,1335,1245,1207,1109,1040,  
 1008,954,922,907,825,791,713,660,599,576,441,391,376,285,172 T0=33990 cm-1  
 HF298=70.99+/-6.7 kcal REF=Melius Database A72O Max Lst Sq Error Cp @  
 200 K 0.57%.  
 C6H4CL meta S 6/01C 6.H 4.CL 1. 0.G 200.000 6000.000 B 111.55046 1  
 1.45027534E+01 1.51288383E-02-5.54539620E-06 9.07354105E-10-5.48075943E-14 2  
 2.94485822E+04-5.03741566E+01-4.60582399E-02 4.47703825E-02-3.43359616E-06 3  
 -3.76582691E-08 2.13062831E-11 3.38418761E+04 2.69429649E+01 3.57233511E+04 4

2396-00-1

C6H4Cl p-CHLOROPHENYL RADICAL SIGMA=2 STATWT=2 IA=15.06576 IB=51.0399  
 IC=66.10564 Nu=3036(2),3018,3017,1461,1459,1412,1312,1247,1214,1104,1035,  
 1022,970,[900],887,873,749,735,653,616,577,427,394,361,285,[175] T0=18425,  
 34920 cm-1 HF298=71.43+/-6.7 kcal REF=Melius Database A72M; [] Jacox  
 Max Lst Sq Error Cp @ 200 K 0.57%.  
 C6H4CL para S 6/01C 6.H 4.CL 1. 0.G 200.000 6000.000 B 111.55046 1  
 1.44772310E+01 1.51913741E-02-5.59219624E-06 9.20192422E-10-5.57428868E-14 2  
 2.96797652E+04-5.01940297E+01 4.13120770E-02 4.42723819E-02-2.32486285E-06 3  
 -3.87394504E-08 2.16914777E-11 3.40515357E+04 2.65941669E+01 3.59447664E+04 4

63125-12-2

C6H4ClO o-Chloro-Phenoxy Radical STATWT=2 SIGMA=1 IA=27.3738 IB=54.7074  
 IC=82.0813 Nu=3227,3222,3210,3197,1603,1556,1502,1441,1422,1313,1247,1177,  
 1142,1050,1035,986,948,864,846,783,705,657,559,527,504,426,379,246,243,132  
 HF298=30.60 kJ HF0=43.48 kJ REF=R. Janoschek J. Mol. Struct 661-2, (2003), 635  
 Max Lst Sq Error Cp @ 1300 K 0.50%  
 C6H4ClO Radical T06/03C 6.H 4.CL 1.O 1.G 200.000 6000.000 B 127.54806 1  
 1.53867708E+01 1.69350990E-02-6.18032414E-06 1.00884274E-09-6.08772262E-14 2  
 -3.05114157E+03-5.43107079E+01 9.57405366E-01 4.20335440E-02 8.56567765E-06 3  
 -4.98052355E-08 2.53381197E-11 1.53738766E+03 2.34806486E+01 3.68031309E+03 4

N/A

C6H4ClO 2,5-CYCLOHEXADIENE-2-CHLORO-1-ONE-4-yl. This radical does not exist as  
 a separate specie since it is in resonance with o-Chloro-Phenoxy Radical and  
 therefore the values of the later are the same as this radical.

Table 4 (continued)

591755-79-2

C6H4ClO 2,4-CYCLOHEXADIENE-6-CHLORO-1-ONE-2-yl STATWT=2 SIMNO=1 IA=33.8249  
 IB=49.29192 IC=72.7614 NU=3216,3198,3177,3118,1771,1706,1612,1416,1322,  
 1308,1213,1205,1107,1012,988,974,928,899,802,765,729,607,753,510,443,422,322,  
 206,176,47 HF298=225.91 kJ HF0=237.50 REF= R. Janoschek J. Mol. Struct  
 661-2, (2003), 635 Max Lst Sq Error Cp @ 1300 K 0.50%.  
 C6H4ClO Radical T06/03C 6.H 4.CL 1.O 1.G 200.000 6000.000 B 127.54806 1  
 1.53946748E+01 1.69393034E-02-6.18312270E-06 1.00932824E-09-6.09043545E-14 2  
 2.05053855E+04-5.24329138E+01 1.65158004E+00 4.13983180E-02 5.69311208E-06 3  
 -4.47238205E-08 2.30800897E-11 2.48653163E+04 2.15630236E+01 2.71705729E+04 4

120-83-2

C6H4CL2O 2-4 Dichloro-Phenol STATWT=1 SIGMA=1 IA=38.80849 IB=115.5815  
 IC=154.3899 Ir=0.1364 ROSYM=1 V(3)=1116.8 cm-1 NU=3651,3582,3302,3078,  
 1876,1736,1628,1582,1481,1408,1331,1282,1191,1097,1079,1058,939,866,813,772,726,  
 656,551,509, [448,413,398,380,341,282,198,175] REF=NIST Webbook 2000 IR+B3LYP  
 HF298=-167.01 kJ HF0=-151.82 kJ REF=Janoschek J. Mol. Struct 661-2,  
 (2003), 635 Max Lst Sq Error Cp @ 1300 K 0.47%.  
 C6H4CL2O 2-4 T 6/03C 6.H 4.O 1.CL 2.G 200.000 6000.000 B 163.00076 1  
 1.73875692E+01 1.70836492E-02-6.16851985E-06 1.00019896E-09-6.00885445E-14 2  
 -2.73287945E+04-6.24163609E+01-4.19895656E-01 6.90164830E-02-6.00079651E-05 3  
 2.21556939E-08-1.50150715E-12-2.25418548E+04 2.88886606E+01-2.00865715E+04 4

29382-90-9

o-C6H4I 2-Iodobenzene-1yl Radical (2-Iodophenyl Radical) SIGMA=1 STATWT=2  
 IA=13.80067 IB=114.83418 IC=128.6348 Nu=3195,3185,3177,3165,1619,1573,1461,  
 1437,1321,1250,1181,1121,1072,1032,975,973,930,839,739,669,652,619,467,411,260,  
 201,144 T0=33360. REF=Burcat B3LYP/6-31G\* calc HF298=427.186 kJ HF0=439.0 kJ  
 REF=Wang et al 6th Int. Conf Chem Kin. NIST 2005 p.56 {HF298=413.38 kJ  
 REF=NIST 94 HF298=411.1 kJ REF=Orlov Zaripov Lebedev Russ Chem Bul 47, (1998),  
 621} Max Lst Sq Error Cp @ 1300 K 0.55%.  
 o-C6H4I A08/05C 6.H 4.I 1. 0.G 200.000 6000.000 B 203.00043 1  
 1.35035874E+01 1.58549160E-02-5.76920884E-06 9.39544809E-10-5.65700366E-14 2  
 4.54058274E+04-4.27139862E+01 2.03414502E+00 2.89038569E-02 2.97018989E-05 3  
 -6.71751371E-08 3.10075057E-11 4.93429522E+04 2.06684955E+01 5.13784216E+04 4

615-42-9

o-C6H4I2 1,2-Diiodobenzene SIGMA=1 STATWT=1 IA=103.2547 IB=163.1162  
 IC=266.37095 NU=3115,3065,2975,2335,1950,1911,1828,1794,1677,1571,1438,1326,  
 1254,1159,1087,1009,947,847,786,747,680,630,580, [436,320,315,207,191,101.6,96.3]  
 REF=IR Webbook 2005 + [B3LYP/6-311G\*] HF298=248.95 kJ HF0=263.625 kJ REF=Wang  
 et al 6th Int. Conf Chem Kin. NIST 2005 p.56 {HF298=252.+/-5.9 kJ REF=Cox &  
 Pilcher Thermochim. Org and Organomet. Compds. Academic Press 1970.} Max Lst  
 Sq Error Cp @ 1300 K 0.62%.  
 o-C6H4I2 A08/05C 6.H 4.I 2. 0.G 200.000 6000.000 B 329.90490 1  
 1.37138831E+01 1.88326408E-02-6.95336680E-06 1.14317842E-09-6.93053737E-14 2  
 2.38458232E+04-3.96814444E+01 3.81101190E+00 3.44177711E-02 6.56146547E-07 3  
 -2.35164054E-08 1.12985060E-11 2.73109585E+04 1.47131881E+01 2.99416322E+04 4

Table 4 (continued)

626-00-6

m-C6H4I2 1,3-Diiodobenzene SIGMA=2 STATWT=1 IA=45.30 IB=403.7569  
 IC=449.1559 Nu=3218,3212,3207,3178,1601,1599,1491,1432,1339,1293,1204,1123,  
 1101,1060,1004,975,903,886,776,703,682,652,496,429,320,275,234,169,125.8,95.8  
 REF=B3LYP/6-311G\* calc HF298=243.5 kJ REF=NIST94 \*\*\*NIST94 gives the same  
 value for m- & p- isomers \*\*\* Max Lst Sq Error Cp @ 1300 K 0.47%.  
 m-C6H4I2 A08/05C 6.H 4.I 2. 0.G 200.000 6000.000 B 329.90490 1  
 1.60908067E+01 1.62362626E-02-5.91117203E-06 9.63342746E-10-5.80651596E-14 2  
 2.24832562E+04-5.30465845E+01 3.46942264E+00 3.48832342E-02 1.81905849E-05 3  
 -5.63874729E-08 2.71654060E-11 2.66402451E+04 1.57520683E+01 2.92872099E+04 4

624-38-4

p-C6H4I2 1,4-Diiodobenzene SIGMA=4 STATWT=1 IA=13.80067 IB=114.83418  
 IC=128.6348 Nu=3086,2790,2557,2364,1893,1768,1620,1472,1382,[1332],1211,[1217,  
 1133],1109,1069,995,950,[950,825],802,[692,637,472],456,[365,283,236,157,130,  
 58.] REF=IR Webbook + [B3LYP/6-311G\*] HF298=242.7 kJ REF=Liebman JPCRD Suppl.  
 1988 {HF298=243.5 kJ REF=NIST 94 \*\*\*NIST94 gives the same value for m- &  
 p-isomers \*\*\* ; HF298=276.9 kJ REF=PM3} Max Lst Sq Error Cp @ 1300 K 0.60%  
 p-C6H4I2 A08/05C 6.H 4.I 2. 0.G 200.000 6000.000 B 329.90490 1  
 1.52787357E+01 1.76683769E-02-6.59041284E-06 1.09072046E-09-6.64257232E-14 2  
 2.24710423E+04-5.12934236E+01 4.13755327E+00 2.89111692E-02 2.65768114E-05 3  
 -5.79087837E-08 2.56642444E-11 2.65388293E+04 1.10745679E+01 2.91899342E+04 4

106-51-4

C6H4O2 1,4 BENZOQUINONE O=C6H4=O SIGMA=4 IA=10.07447 IB=20.4035 IC=28.5342  
 NU\*=3339,3278,3073,(2348),1874,1754,1681,1535,1517,1357,1299,(1218,1262,1151),  
 1077,1055,(962),951,881,(828),763,(714,609,475,430,365,291,187,112,28.5)  
 REF=IR SPECTRUM NIST WEBBOOK 1997, \*(in parenthesis) MOPAC6-AM1 HF298=-122.9 kJ  
 REF=PEDLEY & NYLOR Max Lst Sq Error Cp @ 1300 K 0.58%  
 C6H4O2 O=C6H4=O T10/97C 6.H 4.O 2.00 0.G 200.000 6000.000 B 108.09656 1  
 1.43886174E+01 1.81624210E-02-6.69934678E-06 1.10097880E-09-6.67372266E-14 2  
 -2.12444054E+04-5.02572901E+01 3.79867882E+00 2.51676569E-02 3.79846917E-05 3  
 -7.06777516E-08 3.06126573E-11-1.72429606E+04 9.80455363E+00-1.47813881E-04 4

1516-60-5

C6H4N4O2 4-NitroPhenyl Azide O2N-C6H4-N3 SIGMA=1 STATWT=1 IA=24.4370  
 IB=194.4254 IC=218.81986 Ir(NO2)=4.722026 ROSYM=2 (V3=1088 cm-1 from Melius  
 C6H5-NO2) Ir=(N3)=7.29329 ROSYM=2 V3=1750. cm-1 estim. NU=3042(2),3012,3009,  
 2408,1869,1784,1754,1596,1578,1547,1428,1346,1291,1247,1199,1188,1167,1162,1015,  
 988,947,894,846,798,777,676,643,638,550,531,489,424,378,353,334,278,232,114,111  
 REF=Burcat PM3 MOPAC 2000 calc. HF298=389.7+/-5.2 kJ (HF298(s)=308.7+/-4.3)  
 REF=Finch, Gardner, Head, Xiaoping Thermochim. Acta 298,(1997),191-4. HF0=410.7  
 kJ {HF298=383.6 kJ REF=PM3 MOPAC 2000} Max Lst Sq Error Cp @ 1300 K 0.56%.  
 C6H4N4O2 4-Nitro A12/04C 6.H 4.N 4.O 2.G 200.000 6000.000 B 164.12172 1  
 2.18951683E+01 2.16718761E-02-8.19157895E-06 1.36294486E-09-8.31998956E-14 2  
 3.75490205E+04-8.46634576E+01 2.14105578E+00 6.48319303E-02-2.22920220E-05 3  
 -2.47066996E-08 1.66809458E-11 4.35878355E+04 2.01821296E+01 4.68698697E+04 4

193197-13-6

C6H5 CHAIN HEXA-1,3-DIEN-5-YN-1-YL RADICAL STATWT=1 SIGMA=1 IA=11.77 IB=35.66  
 IC=47.43 NU=72,111,252,253,424,415,593,616,677,692,710,760,796,1089,1131,1184,  
 1352,1584,1720,2311,3275,3421,3440,3640,3795 REF=DEWAR, GARDINER, FRENKLACH &  
 OREF JACS 109 (1987) 4456. HF298=127 KCAL  
 C6H5 CHAIN T09/90C 6H 5 0 0G 200.000 6000.000 B 77.10570 1  
 0.13411768E+02 0.14720221E-01-0.50817705E-05 0.79886354E-09-0.46950844E-13 2  
 0.58503716E+05-0.41652032E+02 0.77929707E+00 0.54372126E-01-0.47873814E-04 3  
 0.16187164E-07 0.33735744E-12 0.61650312E+05 0.22128592E+02 0.63908517E+05 4

Table 4 (continued)

2396-01-2

C6H5 PHENYL RAD. SIGMA=2 STATWT=2 IA=13.3874 IB=14.9862 IC=28.3737 NU=3085, 3073, 3071, 3060, 3052, 1593, 1499, 1441, 1433, 1344, 1226, [1140], 1086, 1080, 1067, 1027, 1011, 976, 971, [948], 878, 707, 656, [645], 605, 586, 416 REF=NIST Webbook 2002 (JACOX) [ ] scaled calculated G3(MP2)/B3LYP vib. See IUPAC Radical DataSheets Max Lst Sq ERROR CP @ 200 K \*\*1.25 %\*\*\* . HF298=339.7+/-2. kJ REF=Davico et al JACS (1995) 117 p.2590.

C6H5 PHENYL RAD	T04/02C	6.H	5.	0.	0.G	200.000	6000.000	B	77.10570	1	
						1.08444762E+01	1.73212473E-02	-6.29233249E-06	1.02369961E-09	-6.16216828E-14	2
						3.55598475E+04	-3.53735134E+01	2.10306633E-01	2.04745507E-02	5.89743006E-05	3
						-1.01534255E-07	4.47105660E-11	3.95468722E+04	2.52910455E+01	4.08610970E+04	4

304524-27-6

C6H5 6- FULVENYL RADICAL (5-METHYLENYL-Cy-1,3-PENTADIENE-6-YL) SIGMA=2 STATWT=2 IA=10.0654 IB=20.9480 IC=31.0134 NU=3264, 3260, 3257, 3235, 3222, 1669, 1631, 1544, 1399, 1320, 1178, 1119, 1115, 1014, 938, 924, 908, 858, 803, 789, 740, 697, 678, 631, 517, 329, 208 HF298=111,691 kcal REF=Burcat G3B3 calc {HF298=206 kcal REF=THERM approx Max Lst Sq Error Cp @ 200 K 0.89%.

C6H5 FULVENYL RA	A03/05C	6.H	5.	0.	0.G	200.000	6000.000	B	77.10390	1	
						1.18218485E+01	1.69728200E-02	-6.08273807E-06	9.80872464E-10	-5.86876305E-14	2
						5.07444189E+04	-3.91774906E+01	4.38207659E-02	3.20479966E-02	2.74260552E-05	3
						-6.83854398E-08	3.25016824E-11	5.46447646E+04	2.53346807E+01	5.62047726E+04	4

97937-92-3 ??

C6H5 FULVENYL RADICAL METHYLENE-CYCLOPENTA-2,4-DIENE-2-YL -C(=CH2)C\*=CHCH=CH- SIGMA=1 STATWT=2 IA=9.09378 IB=22.7103 IC=31.8041 NU=3059, 3057, 3043, 3028, 2979, 1509, 1405, 1367, 1321, 1230, 1182, 1139, 997, 952, 911, 870, 853, 826, 746, 734, 691, 654, 590, 580, 461, 330, 200.5 HF298=117.2 +/- 12.3 kcal REF=C.Melius Database BACMP4 #2538 A72B Max Lst Sq Error Cp @ 200 K 0.79%

C6H5 FULVENYL M	T05/97C	6.H	5.	0.	0.G	200.000	6000.000	B	77.10570	1	
						1.29807636E+01	1.62661044E-02	-5.90215593E-06	9.59452737E-10	-5.77215384E-14	2
						5.31703711E+04	-4.45338857E+01	-8.96711182E-01	4.31740526E-02	2.41329970E-06	3
						-4.48391263E-08	2.43949284E-11	5.73811680E+04	2.94156683E+01	5.89769932E+04	4

108-86-1

C6H5Br BROMOBENZENE DATA FROM STULL WESTRUM & SINKE EXTRAPOLATED USING WILHOIT POLYNOMIALS Max Lst Sq Error H-H298 @ 300 K 0.76% HF298=25.10 KCAL

C6H5BR	T 1/92C	6H	5BR	1	OG	298.150	6000.000	B	157.00970	1	
						0.14996437E+02	0.14432860E-01	-0.34629621E-05	0.42896352E-09	-0.22127110E-13	2
						0.60318879E+04	-0.54089098E+02	-0.27725929E+01	0.59329702E-01	-0.36394766E-04	3
						0.10605809E-08	0.51502469E-11	0.11137385E+05	0.38720437E+02	0.12630738E+05	4

95-56-7

C6H5BrO 2-Bromophenol 2-C6H4BrOH SIGMA=1 STATWT=1 IA=29.0366 IB=77.0248 IC=114.8138 IR=0.135228 V(3)=1117 cm-1 ROSYM=1 Nu=[218, 263, 295, 444, 457], 465, 552, [557], 659, 746, [766], 838, [869], 935, [983], 1032, [1064], 1114, [1146], 1197, 1249, 1286, 1337, 1386, 1478, 1595, [1640], 1677, 3049, 3088(2), 3350, 3559 REF=vib=IR; [vib]+ moments=B3LYP/6=31G(d) HF298=-15.25+/-4. kcal REF=Thergas Max Lst Sq Error Cp @ 1300 K 0.50%

C6H5BrO	T05/04C	6.H	5.O	1.BR	1.G	200.000	6000.000	B	173.00730	1	
						1.61693771E+01	1.91950646E-02	-6.95651049E-06	1.13037861E-09	-6.79985809E-14	2
						-1.48213261E+04	-5.86952647E+01	-6.71675969E-01	5.44902837E-02	-9.39381158E-06	3
						-3.62908524E-08	2.13363675E-11	-9.74101440E+03	3.06846921E+01	-7.66398982E+03	4

Table 4 (continued)

108-90-7

C6H5Cl CHLOROBENZENE DATA FROM STULL WESTRUM & SINKE EXTRAPOLATED USING WILHOIT POLYNOMIALS Max Lst Sq Error Cp @ 1200 K 0.37% HF298=12.39 KCAL.

C6H5Cl	T 1/92C	6H	5CL	1	OG	298.150	6000.000	B 112.55840	1
0.14388354E+02	0.15909241E-01	-0.44684021E-05	0.61870168E-09	-0.33950580E-13					2
-0.15529718E+03	-0.52147823E+02	-0.35215940E+01	0.64559671E-01	-0.47928160E-04					3
0.11765905E-07	0.15381225E-11	0.48148068E+04	0.40540413E+02	0.62348545E+04					4

95-57-8

C6H5ClO o-CHLOROPHENOL SIGMA=1 IA=28.3432 IB=54.8521 IC=83.1953 Ir=0.1364 ROSYM=1 V(3)=1116.8 cm-1 Nu=3650,3569,3326,3084,3052,1767,1669,1588,[1509], 1479,1381,1326,1288,1245,1196,1125,1054,1027,924,[859],842,746,706,680,553,494,[496,448,415,376,266,256] REF= NIST Webbook 2000 Ir spectra + [] Janoschek HF298=-138.38 kJ HF0=-121.06 kJ REF=Janoschek J. Mol. Struct. 2003 Max Lst Sq Error Cp @ 1300 K 0.49%

C6H5ClO	T 6/03C	6.H	5.CL	1.O	1.G	200.000	6000.000	B 128.55600	1
1.53214996E+01	1.87944129E-02	-6.75243790E-06	1.09107503E-09	-6.53851559E-14					2
-2.33861708E+04	-5.45126543E+01	-9.90706299E-01	5.84862054E-02	-2.88225011E-05					3
-1.14267446E-08	1.11429110E-11	-1.86753778E+04	3.08818436E+01	-1.66431936E+04					4

542813-69-4

C6H5ClO 2,4 Cyclohexadiene-6-chloro-1-one SIGMA=1 STATWT=1 IA=34.2897 IB=50.0466 IC=73.8397 NU=3224,3215,3199,3187,3123,1775,1712,1631,1456,1411, 1344,1261,1215,1202,1167,1034,1022,995,973,956,874,786,771,750,592,569,521,455, 452,344,204,183,50 HF298=-35.75 kJ HF0=-19.81 kJ REF=Janoschek G3MP2B3 J. Mol. Struct. 2003 Max Lst Sq Error Cp @ 200 K & 6000 K 0.52%

C6H5ClO	2,4-cyc	T06/03C	6.H	5.CL	1.O	1.G	200.000	6000.000	B 128.55600	1
1.51795595E+01	1.96991331E-02	-7.15108952E-06	1.16305239E-09	-7.00008591E-14					2	
-1.11242043E+04	-5.30610437E+01	1.69565645E+00	3.78571909E-02	2.39639291E-05					3	
-6.58152265E-08	3.11191047E-11	-6.58425435E+03	2.08957084E+01	-4.29971219E+03					4	

N/A

C6H5ClO 2,5-Cyclohexadiene-6-Chloro-1-one SIGMA=1 STATWT=1 IA=28.2675 IB=56.8559 IC=84.6176 NU=3214,3201,3180,3015,3002,1772,1713,1673,1461,1425, 1390,1368,1247,1210,1154,1043,1021,1020,971,912,847,830,816,649,636,535,528,397, 374,317,242,221,101 HF298=-55.87 kJ HF0=-39.79 kJ REF=Janoschek J. Mol. Struct 661-2, (2003), 635 Max Lst Sq Error Cp @ 1300 K 0.54%.

C6H5ClO	2,5-cyc	T06/03C	6.H	5.CL	1.O	1.G	200.000	6000.000	B 128.55600	1
1.50103213E+01	1.99756951E-02	-7.27896337E-06	1.18670757E-09	-7.15400891E-14					2	
-1.34849672E+04	-5.27889463E+01	1.78698412E+00	3.92434580E-02	1.66121496E-05					3	
-5.53241392E-08	2.65037680E-11	-9.04656573E+03	1.95344336E+01	-6.71957818E+03					4	

462-06-6

C6H5F FLUOROBENZENE DATA FROM STULL WESTRUM & SINKE EXTRAPOLATED USING WILHOIT POLYNOMIALS Max Lst Sq Error Cp @ 1200 K 0.48% HF298=-27.86 KCAL

C6H5F	T 1/92C	6H	5F	1	OG	298.150	6000.000	B 96.10410	1
0.13603270E+02	0.17680782E-01	-0.56138646E-05	0.84146369E-09	-0.48322310E-13					2
-0.20280095E+05	-0.49526306E+02	-0.44173359E+01	0.66471817E-01	-0.49219304E-04					3
0.12039107E-07	0.15890440E-11	-0.15246744E+05	0.43825425E+02	-0.14019616E+05					4

Table 4 (continued)

591-50-4

C6H5I Iodobenzene SIGMA=2 STATWT=1 IA=14.73838 IB=114.05969 IC=128.7981  
 Nu=3145,3080(2),3019,2998,1628,1576,1533,1472,1442,1321,1260,1183,1092,1062,  
 1018,[1013],997,923,902,833,729,686,655,612,[458,411,256,220.6,149.4  
 REF=IR (Webbook 2005) [] B3LYP/6-311G\* HF298=165+/-6. kJ HF0=181.04 kJ  
 REF=Cox & Pilcher 1970 {HF298=39.0 kcal REF=NIST 94 HF298=35.4 kcal REF=PM3}  
 Max Lst Sq Error Cp @ 200 K 0.69%.

C6H5I	A08/05C	6.H	5.I	1.	0.G	200.000	6000.000	B	204.00837	1
1.33706566E+01	1.87659285E-02	-6.84320341E-06	1.11613300E-09	-6.73026482E-14						2
1.36758829E+04	-4.44311783E+01	1.88711965E+00	2.81975868E-02	3.97228339E-05						3
-7.87332375E-08	3.52679092E-11	1.78168785E+04	1.99622616E+01	1.98448255E+04						4

586-96-9

C6H5NO NITROSO-PHENYL or NITROSO-BENZENE CALCULATED BY BOZZELLI USING GROUP  
 ESTIMATES. EXTRAPOLATED TO 6000 K USING WILHOIT'S POLYNOMIALS. HF298=48.0 KCAL  
 REF=Choo, Golden & Benson, Int. J. Chem Kinet 7,(1975),713. Max Lst Sq Error  
 Cp @ 1500 K 0.36%.

C6H5NO	T 7/95C	6H	5N	1O	1G	298.150	5000.000	F	107.11184	1
0.15129273E+02	0.20169394E-01	-0.79009702E-05	0.14240839E-08	-0.96649392E-13						2
0.17118219E+05	-0.56899184E+02	0.20849489E+01	0.34489960E-01	0.27707248E-04						3
-0.65460444E-07	0.29821820E-10	0.21870293E+05	0.15898367E+02	0.24154400E+05						4

98-95-3

C6H5NO2 Nitro-Benzene SYMNO = 2 STATWT = 1 IA = 20.6002 IB = 63.9627  
 IC = 84.5628 Ir(NO2)= 5.96 ROSYM = 2 V(2) = 2.8 kcal/mole Nu= 3084,2935,  
 2888,2700,1966,1912,1797,1609,1541,1481,1353,1312,1245,1171,1103,1070,1020,  
 (1019,1004,999,977),928,(860),854,787,692,(674,665,599,510,436,409,388,254.49,  
 171.09) REF =NIST 97 Webbook & Melius Database 1988 R5M HF298=16.38 kcal  
 REF = Pedley Naylor & Kirby 1986 Max Lst Sq Error Cp @ 1300 K 61%.

NITRO-BENZENE	T11/97C	6.H	5.N	1.O	2.G	200.000	6000.000	B	123.11124	1
1.71572651E+01	2.10600071E-02	-7.92285643E-06	1.31641516E-09	-8.03337816E-14						2
4.22627769E+02	-6.59268666E+01	3.22564706E-01	4.78049433E-02	1.44052454E-05						3
-6.09010999E-08	2.98988437E-11	6.00070276E+03	2.56985144E+01	8.24268899E+03						4

2122-46-5

C6H5O PHENOXY RADICAL SIGMA=2 STATWT=2 IA=15.2355 IB=30.2176 IC=45.4531  
 NU=3078,3076,3066,3051,3044,1531,1494,1432,1392,1369,12911231,1123,1122,1049,  
 972,950,942,931,880,775,772,760,628,571,507,464,424,364,187 REF=IUPAC 2002  
 data HF298=54+/-10 KJ REF=TSANG 1996 MAX LST SQ ERROR CP @ 200 K 0.72 % .

C6H5O Phenoxy R	T05/02C	6.H	5.O	1.	0.G	200.000	6000.000	B	93.10510	1
1.37221720E+01	1.74688771E-02	-6.35504520E-06	1.03492308E-09	-6.23410504E-14						2
2.87274751E+02	-4.88181680E+01	-4.66204455E-01	4.13443975E-02	1.32412991E-05						3
-5.72872769E-08	2.89763707E-11	4.77858391E+03	2.76990274E+01	6.49467016E+03						4

189628-71-5 ?

C6H5O 2,4-Cyclohexadiene-1-one-2-yl Radical cy)-CO-CH\*-CH=CH-CH=CH-(-  
 SIGMA=1 STATWT=2 IA=15.1548 IB=31.8141 IC=46.4611 Nu=44,270,402,435,474,  
 555,576,699,749,879,925,939,958,981,1000,1112,1195,1203,1321,1331,1420,1435,  
 1606,1707,1761,3030,3058,3167,3180,3206 HF298=246.58 kJ HF0=260.42 kJ  
 REF= Janoschek J. Mol.Struct 661-2,(2003),635 Max Lst Sq Error Cp @ 200 &  
 1300 K 0.56%.

C6H5O 2,4-cyclo	T06/03C	6.H	5.O	1.	0.G	200.000	6000.000	B	93.10330	1
1.29030189E+01	1.90770078E-02	-6.93077391E-06	1.12768340E-09	-6.78871785E-14						2
2.36556456E+04	-4.19987250E+01	1.42119736E+00	3.09988829E-02	3.06365948E-05						3
-6.78383584E-08	3.08907323E-11	2.77038599E+04	2.18583542E+01	2.96565883E+04						4



Table 4 (continued)

91422-02-5

C6H5OO PEROXYPHENYL SIGMA=1 STATWT=2 IA=16.0594 IB=51.5184 IC=67.5778  
 NU=3061,3032,3024,3014,3004,1526,1515,1461,1425,1303,1246,1223,1124,1115,1106,  
 1032,977,936,924,917,860,788,759,712,629,593,587,457,427,382.5,257.4,216.5,59.5  
 HF298=39.59 KCAL REF=C. Melius Database AA3V Max Lst Sq Error Cp @ 200 K 0.65%  
 C6H5OO T03/97C 6.H 5.O 2. 0.G 200.000 6000.000 B 109.10450 1  
 1.61783950E+01 1.80959380E-02-6.61459065E-06 1.08059157E-09-6.52339007E-14 2  
 1.28261324E+04-5.89741433E+01 1.99359550E-01 4.70697558E-02 8.34324919E-06 3  
 -5.63540961E-08 2.94168315E-11 1.77945712E+04 2.67267648E+01 1.99223478E+04 4

71-43-2

BENZENE Liquid, REF=TRC 4/83 TABLES. HF298(L)=49.08 kJ {HF298=49.036+/-0.26 kJ  
 REF=ATcT A} Max lst sq Error Cp @ 440 K 0.03%  
 C6H6(L) P10/86C 6.H 6. 0. 0.L 278.680 500.000 78.11184 1  
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2  
 0.00000000E+00 0.00000000E+00 6.36157438E+01-5.99984368E-01 2.66582586E-03 3  
 -5.05955979E-06 3.63735942E-09-1.66678000E+03-2.43685622E+02 5.90293355E+03 4

71-43-2

C6H6 BENZENE SIGMA=12 IA=IB=14.8396 IC=29.6792 NU=3062,992,1326,673,3068,  
 1010,995,703,1310,1150,849(2),3048(2),1484(2),1038(2),3047(2),1596(2),1178(2),  
 606(2),975(2),410(2) DJ=3.934E-08 DJK=-6.90E-08 DK=3.21E-08 REF=SHIMANOUCI and  
 Pliva et al J. Molec. Spetros 107,(1984),209 HF298=82.88 kJ REF=TRC Oct 1986  
 {HF298=82.884+/-0.26 kJ REF=ATcT A} MAX LST SQ ERROR CP @ 200 K \*\*\*1.2%\*\*\*  
 @ 6000 K 0.59%.  
 C6H6 g 6/01C 6.H 6. 0. 0.G 200.000 6000.000 B 78.11184 1  
 1.10809576E+01 2.07176746E-02-7.52145991E-06 1.22320984E-09-7.36091279E-14 2  
 4.30641035E+03-4.00413310E+01 5.04818632E-01 1.85020642E-02 7.38345881E-05 3  
 -1.18135741E-07 5.07210429E-11 8.55247913E+03 2.16412893E+01 9.96811598E+03 4

497-20-1

C6H6 FULVENE (5-METHYLENE-1,3-CYCLOPENTADIENE) SIGMA=2 IA=10.1825 IB=21.7319  
 IC=31.9144 NU=3059,3053,3051,3036,3028,2980,1677,1604,1524,1423,1341,1318,1227,  
 1081,1078,976,956,946,943,932,863,785,782,770,692,644,606,483,328,199.8  
 HF298=56.60+/-2.3 KCAL REF=C.MELIUS DATABASE A70D Max Lst Sq Error Cp @  
 200 K 0.95%  
 C6H6 FULVENE T03/97C 6.H 6. 0. 0.G 200.000 6000.000 B 78.11364 1  
 1.19233607E+01 1.98993861E-02-7.21223888E-06 1.17141499E-09-7.04278845E-14 2  
 2.27199368E+04-4.13488172E+01 1.25853571E-01 3.04056534E-02 4.01806332E-05 3  
 -8.27651456E-08 3.77645005E-11 2.68838408E+04 2.44628931E+01 2.84820633E+04 4

695-85-8

C6H6 Benzvalene (Cyclopentene with CH conected to carbons 5, 1 and 2) SIGMA=1  
 A=0.253 B=0.177 C=0.131 NU=498.9,525,652,695,756,762,788,795,826,889,897,931,  
 952,956,1006,1090,1114,1123,1165,1196,1260,1318,1386,1601,3007.5(2),3035,3041,  
 3051,3065 scaled 0.8929 HF298=92+/-2 kcal REF=Wang & Law JPC 1001 (1997),3400.  
 Gaussian94 HF/6-31G(d) calc + private communication. Max Lst Sq Error Cp @  
 400 K \*\*\*1.0%. WARNING 1.6% Error at 200 K \*\*\*\*  
 C6H6 Benzvalen T02/04C 6.H 6. 0. 0.G 298.150 6000.000 C 78.11184 1  
 1.18859885E+01 1.87773298E-02-6.69841929E-06 1.08549169E-09-6.53737102E-14 2  
 4.04476817E+04-4.23000157E+01-8.95191536E-01 2.53574082E-02 6.41883041E-05 3  
 -1.15420436E-07 5.17549322E-11 4.50723354E+04 2.98460408E+01 4.62959333E+04 4

Table 4 (continued)

4447-21-6

C6H6 1,3-Hexadiyne HCC-CC-CH<sub>2</sub>CH<sub>3</sub> SIGMA=1 STATWT=1 IA=3.8553 IB=63.3025  
 IC=66.1170 Ir(CH<sub>3</sub>)=0.52427 ROSYM=3 [V(3)=1162.cm<sup>-1</sup> REF=East Radom JCP, 106,  
 (1997), 6655] Nu=3496, 3141, 3134, 3062, 3059, 3030, 2357, 2181, 1534, 1524, 1501, 1436,  
 1367, 1298, 1185, 1115, 1086, 962, 794, 694, 685, 669, 576, 571, 482, 360, 254, 239, 137  
 HF298=93.777 kcal REF=Burcat G3B3 calc {HF298=90.8+/-5. kcal NIST94;  
 HF298=95.0 kcal REF=Rosenstock et al Radiat. Phys. Chem. 20, (1982), 7.}

Max Lst Sq Error Cp @ 5000 K 0.50%

C6H6 1,3-Hexadiyn A03/05C 6.H 6. 0. 0.G 200.000 6000.000 B 78.11184	1
1.16492306E+01 1.91179786E-02-6.79248428E-06 1.08835980E-09-6.48105723E-14	2
4.20820448E+04-3.42312621E+01 1.49404579E+00 4.73666457E-02-3.35829125E-05	3
8.79564694E-09 9.24848243E-13 4.49182853E+04 1.82483063E+01 4.71901493E+04	4

2809-69-0

C6H6 2,4 Hexadiyne CH<sub>3</sub>-CC-CC-CH<sub>3</sub> SIGMA=2 STATWT=1 IA=1.0501 IB+IC=75.8356  
 Ir(CH<sub>3</sub>)=0.26257 ROSYM=3 V(3)=25. cm<sup>-1</sup> REF=G3B3 One rotation only Nu=3096(4),  
 3034(2), 2382, 2280, 1503(4), 1445, 1438, 1303, 1066(2), 1059(2), 962, 673(2), 564, 373(2),  
 242(2), 106(2) HF298=88.217 kcal REF=Burcat G3B3 calc {HF298=85.9+/-4. kcal  
 REF=NIST 94; HF298=90.2 kcal REF=Luk'yanova et al Russ JPC 66, (1992), 1083.;  
 HF298=90. kcal REF=Rosenstock et al Radiat. Phys. Chem. 20, (1982), 7.}

Max Lst Sq Error Cp @ 1300 K 0.57%

C6H6 2,4-Hexadiy A03/05C 6.H 6. 0. 0.G 200.000 6000.000 B 78.11184	1
1.02546916E+01 2.06082372E-02-7.38382179E-06 1.18968316E-09-7.11140162E-14	2
3.96350323E+04-2.57727679E+01 5.34555093E+00 1.96720327E-02 2.42747636E-05	3
-4.20607694E-08 1.73660983E-11 4.17845840E+04 3.30280048E+00 4.43922646E+04	4

628-16-0

C6H6 1,5-Hexadiyne HCC-CH<sub>2</sub>CH<sub>2</sub>-CCH SIGMA=2 IA=3.3213 IB=58.0865 IC=60.3753  
 Ir=9.12833 ROSYM=2 V(3)=1140 cm<sup>-1</sup> NU=3495(2), 3096, 3075, 3055, 3046, 2242(2),  
 1514, 1505, 1392, 1326, 1303, 1218, 1054, 1025, 984, 956, 778, 627(2), 604(2), 503, 495, 383,  
 340, 219, 125 HF298=99.705 kcal REF=Burcat G3B3 calc {HF298=99.5+/-4. kcal  
 REF=NIST 94; HF298=103.37+/-4.6 kcal Melius database P4A; HF298=99.0 kcal  
 REF=Rosenstock et al Radiat. Phys. Chem. 20, (1982), 7.} Max Lst Sq Error Cp  
 @ 6000 K 0.52%

C6H6 1,5-Hexadi A03/05C 6.H 6. 0. 0.G 200.000 6000.000 B 78.11184	1
1.27627347E+01 1.77516318E-02-6.31267704E-06 1.01181415E-09-6.02595474E-14	2
4.47746179E+04-3.91868742E+01 1.05462594E+00 5.30359803E-02-4.42294933E-05	3
1.60203849E-08-7.28253865E-13 4.78609473E+04 2.05280769E+01 5.01732177E+04	4

29776-96-3

C6H6 1,2,4,5-Hexatetraene H<sub>2</sub>C=C=CH-CH=C=CH<sub>2</sub> SIGMA=2 STATWT=1 IA=2.5855  
 IB=61.9688 IC=63.4654 Ir=7.2925 ROSYM=1 {V3=259.cm<sup>-1</sup> REF=Bronstein Exper  
 Tables Rot Barr. Group II Mol & Rad Vol 24 Subvol C Springer 2002 #67 p.233}  
 NU=3198(2), 3162, 3153, 3132(2), 2069, 2043, 1526, 1487, 1421, 1290, 1184, 1123, 1050, 1032,  
 1030, 934, 898, 879(2), 678, 555, 541, 492, 370, 334, 240, 125 HF298=94.701 kcal  
 REF=Burcat G3B3 calc {HF298=94.5+/-3.5 kcal REF=Melius BAC/MP2 A72A+ NIST 94  
 HF298=98.0 kcal REF=Rosenstock et al Radiat. Phys. Chem. 20, (1982), 7.}

Max Lst Sq Error Cp @ 6000 K 0.53%

C6H6 1,2,4,5 A03/05C 6.H 6. 0. 0.G 200.000 6000.000 B 78.11184	1
1.18041233E+01 1.90294928E-02-6.86057265E-06 1.10920501E-09-6.64442984E-14	2
4.23294268E+04-3.35946492E+01 3.10289191E+00 2.90180407E-02 1.88556724E-05	3
-4.87757671E-08 2.28149663E-11 4.53592635E+04 1.45726287E+01 4.76551215E+04	4

Table 4 (continued)

33142-15-3

C6H6 1,2-Hexadiene-5-yne H2C=C=C-CH2CCH SIGMA=1 IA=5.7718 IB=54.03  
 IC=55.8843 NU=55.9,164,214,332,354,455,533,585,709,724,853,900,904,920,1005(2),  
 1104,1194,1286,1358,1444,1455,1990,2156,2868,2919,2969,3039,3272  
 HF298=98.6+/-5.6 kcal REF= Melius P13S 1988.{HF298=82.7 kcal REF=NIST 94;  
 HF298=87 kcal REF=Rosenstock et al Radiat. Phys. Chem. 20,(1982),7.} Max Lst  
 Sq Error Cp @ 6000 K 0.52%  
 C6H6 1,2-Hexad T12/98C 6.H 6. 0. 0.G 200.000 6000.000 B 78.11364 1  
 1.25675553E+01 1.91426138E-02-6.89392180E-06 1.11473036E-09-6.68050965E-14 2  
 4.40428652E+04-3.88525255E+01 1.93913583E+00 4.09525988E-02-7.95640732E-06 3  
 -2.25455163E-08 1.34743616E-11 4.73272824E+04 1.77887106E+01 4.96171632E+04 4

108-95-2

C6H5OH PHENOL IA=14.854 IB=32.045 IC=46.8942 Ir=0.1336 ROSYM=2 V(2)=1212.95  
 cm-1 NU=3087,3063,3027,1603,1501,1261,1168,1025,999,823,526,958,817,409,973,  
 881,751,686,503,225,3070,3049,1610,1472,1343,1277,1150,1070,619,403,3656,1176.  
 HF298= -96.4 KJ. HF0=-77.83 kJ REF=BURCAT,ZELEZNIK & MCBRIDE NASA TM-83800  
 1985 MAX LST SQ ERROR Cp @ 200 K 0.76%  
 C6H5OH,phenol g 8/00C 6.H 6.O 1. 0.G 200.000 6000.000 B 94.11124 1  
 1.41552427E+01 1.99350340E-02-7.18219540E-06 1.16229002E-09-6.97147483E-14 2  
 -1.81287441E+04-5.17984911E+01-2.90978575E-01 4.08562397E-02 2.42829425E-05 3  
 -7.14477617E-08 3.46002146E-11-1.34129780E+04 2.68745637E+01-1.15940687E+04 4

24599-57-3

C6H6O 2,4-cyclohexadiene 1-one. SIGMA=1. STATWT=1 IA=16.2138 IB=31.3541  
 IC=47.0631 NU=69,271,447,454,494,544,579,725,750,820,950,954,961,992,1007,1023,  
 1170,1203,1204,1259,1351,1415,1438,1462,1626,1711,1765,3029,3051,3175,3180,3206,  
 3217 HF298=-21.63 kJ HF0=-3.31 kJ REF=R. Janoschek J.Mol.Struct 661-2,(2003)  
 ,635 Max Lst Sq Error Cp @ 200 K 0.67%  
 C6H6O 2,4-cyclo T06/03C 6.H 6.O 1. 0.G 200.000 6000.000 B 94.11124 1  
 1.26746353E+01 2.18954738E-02-7.93048713E-06 1.28766673E-09-7.74049768E-14 2  
 -8.76791877E+03-4.29349247E+01 1.42905833E+00 2.75022373E-02 4.89356224E-05 3  
 -8.89267073E-08 3.89096730E-11-4.52491549E+03 2.10316391E+01-2.60147621E+03 4

207803-58-5

C6H7 1,4-CYCLO-RADICAL STATWT=2 SIGMA=2 IA=15.707 IB=16.0895 IC=31.2965  
 NU=3017,3002,2998,2984,2983,2799.5,2796,1469.5,1456,1435,1405,1379,1332,1258,  
 1160,1117,1112,1058.5,953,916,909,898,881.5,876,806,710,657,589.5,552,528,473,  
 335.5,159 HF298=47.942+/-8.31 KCAL REF= C. Melius BAC/MP4 Database Max Lst  
 Sq Error Cp @ 200 K 0.9%.  
 C6H7 1,4 CYCLO T 6/93C 6H 7 0 OG 200.000 6000.000 B 79.12158 1  
 0.12801758E+02 0.21924749E-01-0.79713001E-05 0.12972935E-08-0.78100416E-13 2  
 0.17889539E+05-0.45804341E+02-0.10303140E+00 0.34393354E-01 0.39788466E-04 3  
 -0.85116612E-07 0.39012224E-10 0.22425515E+05 0.26022350E+02 0.24125213E+05 4

465500-32-7

C6H7 1,3,5-HEXATRIENE-6-YL RADICAL SIGMA=1 STATWT=2 Ia=3.0728 Ib=60.6518  
 Ic=63.7246 Ir(CH2=CH)=2.9265 ROSYM=1 [V(3)=994. cm-1 REF=Xuedong IJQC 69,(1998),  
 659 as in 1,3 pentadiene] Ir(\*CH=CH-)=2.8708 ROSYM=1 V(3)=994. cm-1  
 Nu=3255,3249,3166(2),3155,3147,3113,1706,1668,1630,1472,1345,1337,1316,1260,  
 1204,1129,1053,989,973,923,914,880,871,684,636,523,446,339,263,222 HF298=431.39  
 kJ HF0=446.41 kJ REF=Burcat G3B3 calc with QCISD/SCF=QC {HF298 =389.15 KJ  
 REF=THERM from 1,3,5-Hexatriene} Max Lst Sq Error Cp @ 6000 K 0.49%.  
 C6H7 1,3,5 Hexat A03/05C 6.H 7. 0. 0.G 200.000 6000.000 B 79.11978 1  
 1.26756164E+01 2.04172005E-02-7.25924649E-06 1.15611123E-09-6.84356944E-14 2  
 4.62236276E+04-3.66322038E+01 2.82605342E+00 3.48404920E-02 1.31406933E-05 3  
 -4.68820461E-08 2.29960533E-11 4.94582065E+04 1.70295025E+01 5.18836511E+04 4

Table 4 (continued)

136202-28-3

C6H7-1 CY-C5H5-CH2\* 1-Methenyl-2,4-Cyclopentadiene -CH(-CH2\*)CH=CH-CH=CH- cyclo  
 SIGMA=1 STATWT=2 IA=11.6840 IB=22.3382 IC=30.5303 Ir=0.2886 ROSYM=2  
 V(3)=280 cm-1 (as in C4H7) Nu=3051,3049,3044,3027,3018,2957,2838,1623,1558,  
 1423,1370,1289,1269,1211,1108,1087,1055,1008,969,963,952,938,827,771,762,737,  
 694,551,525,473,281,165 HF298=79.85+/-1.5 kcal REF=C. Melius BAC/MP4 P72JB  
 Max Lst Sq Error Cp @ 200 K 0.90%

C6H7	C5H5-1-CH2	A03/05C	6.H	7.	0.	0.G	200.000	6000.000	B	79.11978	1	
							1.27079227E+01	2.13529273E-02	-7.71585835E-06	1.25058460E-09	-7.50743824E-14	2
							3.41136541E+04	-4.24117660E+01	1.64289716E+00	2.65257755E-02	5.29482958E-05	3
							-9.65595872E-08	4.29631206E-11	3.82157747E+04	2.03616391E+01	4.01818508E+04	4

189101-98-2

C6H7-3 CY-C5H5-3-CH2\* 3-Methenyl-2,4-Cyclopentadiene SIGMA=1 STATWT=2  
 IA=10.4426 IB=24.0148 IC=33.9472 Ir=0.2750 ROSYM=2 V(3)=280 cm-1 as in C4H7  
 Nu=3052,3037,3027,3018,2972,2865,2845,1462,1440,1415,1391,1303,1293,1238,1188,  
 1109,1044,966,906,901,879,875,873,741,687,667,610,553,527,483,328,321  
 HF298=59.11+/-4.6 kcal REF=C. Melius P72JA {HF298=54.10 kcal REF=THERGAS;  
 HF298=54.34 kcal PM3 HF298=59.17 kcal AM1 REF=Chem-3D} Max Lst Sq Error Cp  
 @ 200 K 0.78%.

C6H7	C5H5-3-CH2	A03/05C	6.H	7.	0.	0.G	200.000	6000.000	B	79.11978	1	
							1.31180563E+01	2.10247437E-02	-7.60660029E-06	1.23388906E-09	-7.41144871E-14	2
							2.35701438E+04	-4.51867987E+01	-4.65377649E-02	3.96188470E-02	2.21522238E-05	3
							-6.60053606E-08	3.19768019E-11	2.79177074E+04	2.66778342E+01	2.97451371E+04	4

137363-30-5

C6H7-1 Cy-C5H4-1\*-CH3 1-Methyl-2,4-Cyclopentadiene-1-yl SIGMA=2 STATWT=2  
 IA=10.2931 IB=24.4197 IC=34.2002 Ir=0.4892 ROSYM=3 [V(3)=700 cm-1  
 REF=Sebbbar & Bozzelli JPC A 108, (2004), 8353 supplement] Nu=3055,3045,3033,3028,  
 2926,2893,2850,1467,1452,1436,1410,1397,1383,1252,1213,1167,1049,1003,977,919,  
 899,858,856,835,685,671,650,586,548,481,309,206 HF298=54.20+/-3. kcal  
 REF=C. Melius Bac/MP4 P72JC Max Lst Sq Error Cp @ 200 K 0.63%.

C6H7	C5H4-1-CH3	A03/05C	6.H	7.	0.	0.G	200.000	6000.000	B	79.11978	1	
							1.28996538E+01	2.12183240E-02	-7.67565006E-06	1.24495899E-09	-7.47731827E-14	2
							2.12053775E+04	-4.47534535E+01	5.64034275E-01	3.84201803E-02	1.94958520E-05	3
							-5.95545053E-08	2.86869522E-11	2.53304225E+04	2.27464371E+01	2.72743433E+04	4

62-53-3

C6H5NH2 liquid ANILINE DATA TAKEN FROM TRC 6/90 HF298=7.529 kcal Max Lst Sq  
 Error Cp @ 420 K 0.43%

C6H5NH2(L)	anilin	P 6/95C	6.H	7.N	1.	0.C	267.130	460.000	B	93.12652	1	
							0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	2
							0.00000000E+00	0.00000000E+00	4.76544974E+01	-3.11868497E-01	1.30585811E-03	3
							-2.19040282E-06	1.31395681E-09	-4.38670916E+03	-1.96839076E+02	3.78855759E+03	4

62-53-3

C6H5NH2 ANILINE SIGMA=2 REF=STULL, WESTRUM & SINKE EXTRAPOLATED TO 5000 K USING  
 BOZZELLI & RITTER'S PROGRAM HF298=87.03 KJ

C6H7N	ANILINE	T 2/92C	6H	7N	1	0G	298.150	5000.000	B	93.12832	1	
							0.13217261E+02	0.24501606E-01	-0.93690211E-05	0.16310315E-08	-0.10639893E-12	2
							0.40229641E+04	-0.47212282E+02	-0.23879495E+01	0.62140204E-01	-0.35907649E-04	3
							0.22025563E-08	0.38067823E-11	0.87295677E+04	0.35046606E+02	0.10468446E+05	4

Table 4 (continued)

287-12-7

C6H8 DIHYDROBENZVALENE SIGMA=1 STATWT=1 A=221 B=0.165 C=0.122 Nu=3080, 3066, 2994, 2993, 2914, 2894, 2993, 2914, 2894, 2880, 2866, 1485, 1461, 1416, 1317, 1300, 1272, 1223, 1222, 1191, 1148, 1121, 1105, 1060, 994, 982, 972, 940, 884, 879, 827, 821, 790, 758, 743, 707, 633, 437, 227.6 scaled 0.8929 HF298=55+/-2 kcal REF=Gaussian 94 HF/3-21-G Wang & Law JPC 101 (1997), 3400/3 + private communication Max Lst Sq Error Cp @ 400 K \*\*\*1.06% WARNING 1.7% Error at 200 K\*\*\*

C6H8	T02/04C	6.H	8.	0.	0.G	298.150	6000.000	C	80.12772	1
1.28729403E+01	2.38087609E-02	-8.69023186E-06	1.41812611E-09	-8.55395874E-14						2
2.09789566E+04	-4.90200962E+01	6.73185642E-01	1.27777539E-02	1.15643866E-04						3
-1.73057475E-07	7.32867255E-11	2.61939628E+04	2.39322490E+01	2.76769166E+04						4

96-38-8

C6H8 1-Methyl-2,4-CYCLOPENTADIENE 2,4-C5H5-1-CH3 SIGMA=1 STATWT=1 IA=11.9702 IB=23.7336 IC=32.1443 Ir=0.5268 ROSYM=3 V3=525. cm-1 REF=CH3-CH... Bozzelli JPC A 108, (2004), 8353 suppl. NU=3239, 3231, 3215, 3206, 3129, 3115, 3050, 2993, 1663, 1578, 1530 (2), 1438, 1417, 1333, 1300, 1278, 1153, 1124, 1105, 1088, 1032, 1004, 960, 952 (2), 874, 810, 785, 721, 717, 561, 542, 293, 268 HF298=112.2 kJ HF0=135.27 kJ REF=Burcat G3B3 calc {HF298=103.3 kJ REF=NIST 94} Max Lst Sq Error Cp @ 200 K 0.94%

C6H8	2,4-C5H5-1CH3A03/05C	6.H	8.	0.	0.G	200.000	6000.000	B	80.12772	1
1.12002638E+01	2.50104924E-02	-8.94914815E-06	1.44109704E-09	-8.61256818E-14						2
7.66096956E+03	-3.68265351E+01	2.93206487E+00	1.12663266E-02	9.41193663E-05						3
-1.36178031E-07	5.64768524E-11	1.15372662E+04	1.42303662E+01	1.35013031E+04						4

3727-31-9

C6H8 3-METHYL CYCLOPENTADIENE (CH3-C5H5) ESTIMATED USING NIST 94 PROGRAM FROM 2x[CD-(C)(H)]; [CD-(C)(CD)]; [CD-(CD)(H)]; [C-(CD)2(H)2]; [C-(H)3] ROSYM=3 RING CORRECTION HF=25.1 KJ S=117.2 J HF298=102.0 KJ Max Lst Sq Error H-H298 @ 500 K 0.68%

C6H8	CY CH3-C5H5	T10/94C	6H	8	0	0G	298.150	5000.000	E	80.12952	1
0.16399698E+02	0.18988824E-01	-0.60996114E-05	0.95861755E-09	-0.59364731E-13						2	
0.48834021E+04	-0.65341031E+02	-0.35829269E+01	0.78077845E-01	-0.73143499E-04						3	
0.33645368E-07	-0.48086229E-11	0.10447644E+05	0.37418709E+02	0.12267710E+05						4	

2235-12-3 and 821-07-8 and 2612-46-6

1,3,5-C6H8 1,3,5 HEXATRIENE EQUILIBRIUM MIXTURE OF THREE ISOMERS TTT, TTC and CTC REF=PRIVATE COMMUNICATION FROM J.D. VAUGHAN. CFF/PI CALCULATIONS WERE USED FOR VIBRATIONS AND MMP2 CALCULATIONS WERE USED FOR HF298. HF298=152.58 KJ VAL FOR TTT NU=3098.3, 3091.4, 3082.2, 3078.8, 3063.2 (2), 2988 (2), 1664.2, 1645.5, 1594.85, 1445.4, 1419.4, 1350, 1310, 1306, 1289, 1206.4, 1172.9, 1082.25, 1051, 990.43, 952.4, 949.25, 946.5, 858.82, 643.67, 611.92, 589.23, 461, 393.4, 242, 214.4, 179.7, 101.53, 941 IAIBIC=13505.E-117 SIGMA=2 VAL FOR TTC T0=1232.18 NU=3096.3, 3084.6, 3083.8, 3078.8, 3063.2, 3062.6, 2988 (2), 1668.6, 1640.2, 1607.7, 1448.22, 1437, 1341.8, 1321.45, 1299.5, 1288.5, 1200, 1089.37, 1070, 1041.3, 1001.34, 982.44, 953.2, 950, 940.4, 864, 649.2, 647, 601.84, 492.1, 383.1, 279.23, 187.85, 171.2, 136 IAIBIC=19687.E-117 SIGMA=1 VAL FOR CTC T0=1376.0 NU=3089.7, 3084.2, 3083.5, 3078.82, 3062 (2), 2988.3 (2), 1669.7, 1645.28, 1614.83, 1452, 1444.36, 1345.43, 1337.46, 1290, 1284.7, 1142, 1042.65, 1041, 1018.4, 1017.9, 955.3, 954, 950, 868.2, 658.3, 650.2, 593.2 (2), 324.3, 257.5, 243.73, 221.73, 93.59 IAIBIC=17093.E-117 SIGMA=2 Max Lst Sq Error Cp @ 6000 K 0.57%.

C6H8	L 8/89C	6H	8	0	0G	200.000	6000.000	B	80.12952	1
0.13184588E+02	0.24023820E-01	-0.86729021E-05	0.14049681E-08	-0.84315805E-13						2
0.11858656E+05	-0.45629943E+02	0.38587790E+01	0.15885821E-01	0.81120967E-04						3
-0.12184205E-06	0.50832636E-10	0.15950538E+05	0.10384627E+02	0.18307022E+05						4

Table 4 (continued)

592-57-4

C6H8 1,3-CYCLOHEXADIENE SIGMA=2 OPT. ISOM=2 STATWT=1 IAIBIC=8.517E-114  
 NU=3050(4),2939,2838(2),1577,1444,1330,1243,1223,1178(2),1150,1059,994,945,850,  
 753,559,506,201,2884,1602,1435,1377,1165,1100,1040,1016,927,745,658,468,298  
 REF=DOROFEEVA GURVICH & JORISH JPCRD 15 (1986) 437 HF298=106.3 KJ Max Lst Sq  
 Error Cp @ 6000 K .62%  
 H8C6 (1,3-CYCLO) T 2/90H 8C 6 0 OG 200.000 6000.000 B 80.12952 1  
 0.11779870E+02 0.25519980E-01-0.92666947E-05 0.15068122E-08-0.90658701E-13 2  
 0.65486686E+04-0.41618805E+02 0.17265319E+01 0.14887612E-01 0.94809230E-04 3  
 -0.14083394E-06 0.58859873E-10 0.11021297E+05 0.19130886E+02 0.12784878E+05 4

628-41-1

C6H8 1,4-CYCLOHEXADIENE SIGMA=4 STATWT=1 IAIBIC=9.26E-114 NU=3032,2822,1680,  
 1426,1197,854,530,1250,970,370,1240,706,3032,1377,1280,1035,574,2875,1010,985,  
 403,3042,2840,1439,1405,962,888,2889,962,625,108,3042,1642,1362,1159,887  
 REF=DOROFEEVA GURVICH & JORISH JPCRD 15 (1986) 437 HF298=109.0 KJ Max Lst Sq  
 Error Cp @ 6000 K 0.62%.  
 C6H8 (1,4-CYCLO) T 2/90C 6H 8 0 OG 200.000 6000.000 B 80.12952 1  
 0.11453943E+02 0.25861139E-01-0.94007909E-05 0.15296731E-08-0.92076611E-13 2  
 0.69849680E+04-0.40634874E+02 0.19018200E+01 0.14819394E-01 0.91312194E-04 3  
 -0.13458949E-06 0.55907972E-10 0.11316750E+05 0.17407151E+02 0.13109612E+05 4

12550-20-8

C6H9 1,3-HEXADIENE-5-YL CH2=CHCH=CHCH\*CH3 SIGMA=1 STATWT=2 IA=3.3965  
 IB=66.7153 IC=69.594 Ir(CH3)=0.5155 ROSYM=3 [V3=760 cm-1 est]  
 Ir(CH3-CH\*-)=3.0908 ROSYM=1 [V(3)=1049. cm-1 est] Ir(CH2=CH-)=1.24245  
 ROSYM=1 [V(3)=1049 cm-1 est.] Nu=3255,3167,3158,3151,3142,3133,3113,3058,3019,  
 1624,1551,1517,1504,1501,1440,1400,1324,1307,1284,1246,1185,1112,1052,1029,978,  
 975,943,855,829,780,610,543,441,340,294,245 HF298=41.465 kcal HF0=46.77 kcal  
 REF=Burcat G3B3 calc {HF298=44. kcal REF=Weissman & Benson Prog Energy Comb.  
 Sci 15, (1989), 273} Max Lst Sq Error Cp @ 6000 K 0.55%  
 C6H9 A05/05C 6.H 9. 0. 0.G 200.000 6000.000 B 81.13566 1  
 1.28337418E+01 2.50402195E-02-8.89066578E-06 1.41988377E-09-8.43184829E-14 2  
 1.48497750E+04-3.82494268E+01 3.73081988E+00 3.16118987E-02 3.09371935E-05 3  
 -6.53851492E-08 2.94240980E-11 1.81904792E+04 1.30369615E+01 2.08658790E+04 4

52840-34-3

C6H9 1,3-HEXADIENE-6-YL CH2=CHCH=CHCH2CH2\* SIGMA=1 STATWT=2 IA=5.0924  
 IB=63.2282 IC=63.8121 Ir(CH2\*)=0.29037 ROSYM=1 [V(3)=272. cm-1 est.]  
 Ir(CH2\*CH2-)=4.1637 ROSYM=1 [V(3)=1049. cm-1 est] Ir(CH2=CH-)=1.26611  
 ROSYM=1 [V(3)=2575 cm-1 est] Nu=3270,3246,3168,3164,3154,3146,3129,3025,2957,  
 1734,1686,1488,1483.1475,1360,1341,1338,1314,1239,1178,1105,1075,1055,1009,991,  
 964,921,871,795,665,512,456,443,385.216,188 HF298=63.464 kcal HF0=68.59 kcal  
 REF=Burcat G3B3 calc {HF298=60. kcal REF=Weissman & Benson Prog Energy Comb.  
 Sci 15, (1989), 273} Max Lst Sq Error Cp @ 6000 K 0.56%  
 C6H9 A05/05C 6.H 9. 0. 0.G 200.000 6000.000 B 81.13566 1  
 1.29128125E+01 2.49789213E-02-8.89951453E-06 1.42497072E-09-8.47614769E-14 2  
 2.59056103E+04-3.64451228E+01 4.61356093E+00 2.58846293E-02 4.54508557E-05 3  
 -8.10845041E-08 3.54678866E-11 2.91520568E+04 1.14181789E+01 3.19361425E+04 4

Table 4 (continued)

7493-04-1

C6H9 CYCLOHEXENYL-3 SIGMA=1 STATWT=2 IA=17.4563 IB=17.4772 IC=32.3194  
 Nu=3196,3187,3160,3087,3060,3052,3041,2976,2974,1533,1522,1506,1503,1467,1419,  
 1389,1371,1362,1283,1233,1173,1154,1147,1074,1064,1019,963,957,898,869,840,731,  
 685,602,515,503,431,256,187. HF298=31.422 kcal HF0=38.0 kcal REF=Burcat  
 G3B3 calc. {HF298=28.6 kcal REF=Luo CRC BDE book 2006 edition; HF298=30. kcal  
 REF=Weissman & Benson Prog Energy Comb. Sci 15, (1989), 273} Max Lst Sq Error  
 Cp @ 200 K 0.95%

C6H9 1-CycloHexe	A05/05C	6.H	9.	0.	0.G	200.000	6000.000	B	81.13566	1
1.13323277E+01	2.81990701E-02	-1.01386508E-05	1.63781300E-09	-9.80945860E-14						2
9.61555288E+03	-3.85483471E+01	2.16099562E+00	1.36943982E-02	9.99484967E-05						3
-1.44517419E-07	5.96459936E-11	1.39334953E+04	1.80484569E+01	1.58120741E+04						4

C6H9 Cyclo-1-penten-4methyl-4-yl Cy C5H6-CH3 SIGMA=2 STATWT=2 IA=11.8557  
 IB=26.4881 IC=36.7726 Ir=0.5004 ROSYM=3 V(3)=2000. cm-1 Nu=3217,3193,3091,  
 3047,2963,2958,2955,2943,2940,1699,1517,1508,1499,1494,1438,1390,1388,1300,1266,  
 1219,1152,1139,1138,1029,990,974,968,938,933,919,806,791,685,574,391,308,224,111  
 HF298=188.468 kJ HF0=214.32 kJ REF=Burcat G3B3 calc Max Lst Sq Error Cp @  
 200 K 0.86 %

C6H9 Cy C5H6-CH3	A09/04C	6.H	9.	0.	0.G	200.000	6000.000	B	81.13566	1
1.23587689E+01	2.70420128E-02	-9.77062449E-06	1.58360669E-09	-9.50683666E-14						2
1.61870653E+04	-4.32405993E+01	3.86577624E+00	7.70961470E-03	1.11177443E-04						3
-1.54635897E-07	6.30017592E-11	2.04657451E+04	1.05842411E+01	2.26673947E+04						4

119225-15-9

C6H9 4-Methenyl-1-Cyclopentene CY-C5H7-CH2\* ch(#1)/ch2/ch(/ch2(.))/ch2/ch//1  
 SIGMA=2 STATWT=2 IA=12.3043 IB=25.1118 IC=34.8771 Ir=048178 ROSYM=2  
 V(3)=1500 cm-1 Nu=3254,3212,3188,3158,3066,3063,3016(2),2930,1702,1525,1518,  
 1486,1386,1369,1323,1309,1297,1198,1167,1147,1141,1114,1036,992,983,971,931,890,  
 833,771,712,579,514,404,394,320,103.3 HF298=215.731 HF0=241.534 kJ REF=Burcat  
 G3B3 calc {HF298=47.58 kcal REF=Thergas; HF298=49.95 kcal REF=THERM} Max Lst  
 Sq Error Cp @ 200 K 0.87%

C6H9 Cy C5H7-CH2	A09/04C	6.H	9.	0.	0.G	200.000	6000.000	B	81.13566	1
1.28004531E+01	2.62432567E-02	-9.38824650E-06	1.51151443E-09	-9.03196262E-14						2
1.94773825E+04	-4.50030753E+01	2.25978996E+00	2.10480383E-02	8.16756034E-05						3
-1.28838961E-07	5.49321877E-11	2.38441556E+04	1.71670712E+01	2.59463545E+04						4

N/A

C6H9 1-Cyclopentene-3-Methenyl 1-C5H7-3-CH2\* SIGMA=1 STATWT=2 IA=12.3328  
 IB=25.5338 IC=34.4046 Ir=0.2867 ROSYM=2. V3=280. cm-1 (as in C4H7) Nu=3262,  
 3215,3190,3160,3116,3071,3057,3016,2998,1694,1529,1512,1487,1392,1357,1329,1327,  
 1291,1234,1183,1150,1118,1077,1051,987,968,950,926,861,822,758,742,589,499,494,  
 330,283,122 HF298=212.46 kJ HF0=237.97 kJ REF=Burcat G3B3 calc Max Lst Sq  
 Error Cp @ 200 K 0.90%.

C6H9 1-C5H7-3-CH2	A04/05C	6.H	9.	0.	0.G	200.000	6000.000	B	81.13566	1
1.18634484E+01	2.70294846E-02	-9.65911211E-06	1.55394507E-09	-9.28041069E-14						2
1.93825470E+04	-3.85521731E+01	3.57987649E+00	1.12979205E-02	1.00236207E-04						3
-1.44017416E-07	5.95983742E-11	2.33547327E+04	1.30536118E+01	2.55533423E+04						4

N/A

C6H9 1-Methenyl-1-Cyclopentene CY-C5H7-CH2\* CALCULATED USING THERGAS  
 ch2(#1)/ch2/c(/ch2(.))/ch/ch2/1 HF298=29.85 kcal {THERM HF298=35.17 kcal}  
 All attempts to use G3B3 ended up in transition species.

C6H9-1	S 8/01C	6H	9	0	OG	300.000	5000.000	F	81.13746	1
0.13077980E+02	0.24417660E-01	-0.76107300E-05	0.11419440E-08	-0.67470450E-13						2
0.81911070E+04	-0.46905720E+02	-0.59623810E+01	0.70753750E-01	-0.46027670E-04						3
0.13313790E-07	-0.11235350E-11	0.14037320E+05	0.53699530E+02	1.50210143E+04						4

Table 4 (continued)

95896-89-2

C6H9I 3-Iodo-1-Cyclohexene SIGMA=1 STATWT=1 IA=19.24485 IB=120.81473  
 IC=133.6664 Nu=3176,3144,3106,3087,3071,3049,3045,3024,2999,1695,1513,1507,  
 1492,1426,1384,1381,1377,1348,1294,1262,1224,1184,1150,1106,1066,1053,1001,995,  
 930,906,878,829,739,717,577,524,458,324,268,200,190,86.2 REF=B3LYP/6-311G\*  
 HF298=16.5+/-5. kcal REF=Burcat Very Rough Estimate {HF298=16.13 kcal REF=PM3;  
 HF298=16.68 REF=THERGAS-Benson est} Max Lst Sq Error Cp @ 200 K 0.78%  
 C6H9I CyHexene3-I A08/05C 6.H 9.I 1. 0.G 200.000 6000.000 B 208.04013 1  
 1.37186171E+01 2.88259443E-02-1.03831858E-05 1.67941393E-09-1.00674506E-13 2  
 1.28492265E+03-4.68652571E+01 3.97475016E+00 1.42793424E-02 1.03555742E-04 3  
 -1.49989737E-07 6.19200179E-11 5.83559728E+03 1.30713396E+01 8.30307499E+03 4

14596-92-0

C6H10 1,3-HEXADIENE SIGMA=1 STATWT=1 IA=5.4844 IB=65.1013 IC=65.7673  
 Ir(CH3)=0.52230 ROSYM=3 [V(3)=1025 cm-1 Bronstein 2002] Ir(CH2=CH-)=2.98935  
 ROSYM=1 [V(3)=994 cm-1 REF=Xuedong IJQC 69, (1998)] Ir(C2H5)=4.59592 ROSYM=1  
 V(3)=980. cm-1 Nu=3245,3163,3151,3139,3131,3122,3114,3069,3047,3016,1737,1689,  
 1537,1527,1510,1476,1436,1377,1345,1340,1318,1283,1222,1135,1098,1055,1038,990,  
 959,919,917,872,793,664,500,448,384,262,195 HF298=58.377+/-8 kJ HF0=84.568 kJ.  
 REF=Burcat G3B3 calc. {HF298=13.4 KCAL REF=Weismann & Benson Prog Energy Comb.  
 Sci 15, (1989), 273} Max Lst Sq Error Cp @ 6000 K 0.56%  
 C6H10 1,3-HexadienA09/05C 6.H 10. 0. 0.G 200.000 6000.000 B 82.14360 1  
 1.22036500E+01 2.83718594E-02-1.01536016E-05 1.62760437E-09-9.68053329E-14 2  
 9.92055464E+02-3.55142375E+01 4.33043903E+00 2.50924406E-02 5.32462166E-05 3  
 -8.82977395E-08 3.75813502E-11 4.31740800E+03 1.10070626E+01 7.03748507E+03 4

110-83-8

C6H10 CYCLOHEXENE SIGMA=2 OPT.ISO=2 so STATWT=2. IAIBIC=10.71E-114 NU=3040  
 2940,2916,2865,2839,1660,1460,1445,1353,1343(2),1240,1222,1140(2),1095,1068,966,  
 905,812,657,520,392,276,3078,2960,2890,2878,2858,1455,1450,1325,1269,1215,1039,  
 1009,919,877,719,638,450,165 REF DOROFEEVA GURVICH & JORISH JPCRD 15 (1986) 437.  
 HF298=-4.6 KJ. Max Lst Sq Error Cp @ 1300 K 0.65%; @200 K \*\*\*1.06%\*\*\*.  
 C6H10,cyclo- g 1/93C 6.H 10. 0. 0.G 200.000 6000.000 B 82.14360 1  
 1.17732584E+01 3.09483545E-02-1.12347470E-05 1.82632297E-09-1.09855802E-13 2  
 -7.20259047E+03-4.26551390E+01 2.36636823E+00 1.06805227E-02 1.18223934E-04 3  
 -1.65681286E-07 6.76137946E-11-2.48250573E+03 1.67688051E+01-5.53249680E+02 4

1759-81-5

C6H10 4-Methyl-1-Cyclopentene CH3-C5H7 SIGMA=1 STATWT=1 Ia=12.5123 Ib=26.4939  
 Ic=35.8841 Ir=0.512363 V(3)=2400 cm-1 ROSYM=3 Nu=3212.5,3187.3103.6(2),3065,  
 3059,3038,3030,3001(2),1702,1532,1528,1524,1517,1440,1392(2),1350,1325,1312,  
 1251,1179,1159,1142,1119,1074,999,983,972,944,931,913,822,777,708,576,425,396,  
 315,254 HF298=2.022 kcal REF= Burcat G3B3 calc {HF298=2.27 kcal REF=Thergas}  
 {NIST Webbook ~ HF298=3.58 kcal} Max Lst Sq Error Cp @ 200 K 0.91%  
 C6H10 Cy C5H7-CH A09/04C 6.H 10. 0. 0.G 200.000 6000.000 B 82.14360 1  
 1.17597909E+01 3.02653241E-02-1.09337044E-05 1.77193386E-09-1.06366036E-13 2  
 -5.56308227E+03-4.24415838E+01 2.77310355E+00 9.17838384E-03 1.17713565E-04 3  
 -1.62911323E-07 6.60032485E-11-9.66456768E+02 1.47665739E+01 1.01750410E+03 4



Table 4 (continued)

16183-00-9

C6H11 1-Hexene-6-yl CH<sub>2</sub>=CHCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>\* SIGMA=1 STATWT=2 IA=13.7894  
 IB=58.7630 IC=60.6715 Ir(CH<sub>2</sub>\*)=0.2900 ROSYM=1 V(3)=257. est  
 Ir(CH<sub>2</sub>=CH-)=2.8357 ROSYM=1 V(3)=1200 cm<sup>-1</sup> est. Ir(\*CH<sub>2</sub>CH<sub>2</sub>-)=5.0872 ROSYM=1  
 V(3)=1049. cm<sup>-1</sup> est Ir(CH<sub>2</sub>=CHCH<sub>2</sub>-)=6.62072 ROSYM=1 V(3)=1200. cm<sup>-1</sup> est.  
 Nu=3258,3233,3159,3155,3133,3081,3057,3044,3028,3017,2940,1733,1528,1511,1498,  
 1487,1476,1403,1384,1343,1330,1316,1247,1213,1191,1097,1053,1044,1035,972,939,  
 936,895,825,774,642,496,439,427,316,225 HF298=38.839+/-1.9 kcal HF0=45.62 kcal  
 REF=Burcat G3B3 calc {HF298=39.3 kcal NIST 94 est} Max Lst Sq Error Cp  
 @ 200 K 0.65%.

C6H11 lene-6-yl A07/05C 6.H 11. 0. 0.G 200.000 6000.000 B 83.15154 1  
 1.34689347E+01 2.93407723E-02-1.05597833E-05 1.69865803E-09-1.01266746E-13 2  
 1.29566669E+04-3.78640667E+01 5.35649510E+00 1.95201537E-02 7.89832938E-05 3  
 -1.21172346E-07 5.11597188E-11 1.65972774E+04 1.13655159E+01 1.95444321E+04 4

60288-55-3

C6H11 2-Hexene-6-yl CH<sub>3</sub>CH=CHCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>\* SIGMA=1 STATWT=2 IA=5.3638 IB=67.8736  
 IC=68.8831 Ir(\*CH<sub>2</sub>-)=0.288 ROSYM=1 V(3)=257. est Ir(CH<sub>3</sub>)=0.51556 ROSYM=3  
 V(3)=780. cm<sup>-1</sup> est Ir(\*C<sub>2</sub>H<sub>4</sub>-)=4.809 ROSYM=1 V(3)=1200. cm<sup>-1</sup> est  
 Ir(CH<sub>3</sub>CH=CH-)=4.19524 ROSYM=1049. cm<sup>-1</sup> V(3)=1049. cm<sup>-1</sup> est Nu=3260,3162,3138,  
 3123,3112,3074.5(2),3050,3029,3010,2934,1760,1523,1516,1510,1500,1486,1442,1398,  
 1362,1346,1310,1303,1216,1143,1100,1093,1080,1073,1014,992,927,884,781,751,539,  
 456,389,314,284,215 HF298=36.774+/-1.9 kcal HF0=43.47 kcal REF=Burcat G3B3  
 calc {HF298=36.4 kcal REF=NIST 94} Max Lst Sq Error Cp @ 6000 K 0.58%.

C6H11 2-ene-6-yl A07/05C 6.H 11. 0. 0.G 200.000 6000.000 B 83.15154 1  
 1.27605793E+01 3.01168355E-02-1.08197236E-05 1.73977051E-09-1.03692791E-13 2  
 1.22100274E+04-3.54020393E+01 6.23788522E+00 1.86370994E-02 7.02342856E-05 3  
 -1.04621010E-07 4.32055091E-11 1.53829414E+04 5.23415999E+00 1.85052897E+04 4

188662-48-8

C6H11 RAD trans-3-HEXENE-6-YL CH<sub>3</sub>CH<sub>2</sub>CH=CHCH<sub>2</sub>CH<sub>2</sub>\* SIGMA=1 STATWT=2 IA=8.4509  
 IB=60.7525 IC=64.3746 Ir(CH<sub>3</sub>)=0.5226 ROSYM=3 V(3)=1773. cm<sup>-1</sup> Ir(CH<sub>2</sub>\*)=0.29068  
 ROSYM=1 V(3)=257. cm<sup>-1</sup> Ir(\*CH<sub>2</sub>-CH<sub>2</sub>-)=4.25007 ROSYM=1 V(3)=1049. cm<sup>-1</sup>  
 Ir(CH<sub>3</sub>CH<sub>2</sub>-)=4.62347 ROSYM=1 V(3)=1049. cm<sup>-1</sup> Nu=3267,3165,3140,3124,3120,3111,  
 3067,3046,3022,3018,2952,1761,1537,1528,1511,1488,1483,1436,1391,1362,1341,1330,  
 1292,1227,1148,1113,1097,1083,1033,1012,997,915,840,800,780,502,461,407.5,270,  
 202 HF298=36.936+/-1.9 kcal HF0=43.78 kcal REF=Burcat G3B3 calc {HF298=34.  
 kcal REF>Weisman & Benson Prog Energ Comb. Sci 15, (1989), 273.} Max Lst Sq  
 Error Cp @ 6000 K 0.57%.

C6H11 3-ene-6yl A07/05C 6.H 11. 0. 0.G 200.000 6000.000 B 83.15154 1  
 1.33625885E+01 2.96436808E-02-1.06633691E-05 1.71602022E-09-1.02335391E-13 2  
 1.20158790E+04-3.93326138E+01 5.59157708E+00 1.95048737E-02 7.53690243E-05 3  
 -1.14012165E-07 4.75032751E-11 1.55897538E+04 8.14490073E+00 1.85868108E+04 4

N/A

C6H11 2-METHYLENE-1-PENTEN RADICAL CH<sub>2</sub>=C(CH<sub>2</sub>\*)C<sub>3</sub>H<sub>7</sub> SIGMA=1 STATWT=2 IA=11.4324  
 IB=45.6146 IC=51.6488 Ir(CH<sub>3</sub>)=0.51462 ROSYM=3 V(3)=1773. cm<sup>-1</sup> Ir(CH<sub>2</sub>\*)=  
 0.28542 ROSYM=1 V(3)=257. cm<sup>-1</sup> Ir(C<sub>2</sub>H<sub>5</sub>-)=4.6966 ROSYM=1 V(3)=1049. cm<sup>-1</sup>  
 Ir(CH<sub>2</sub>=C(CH<sub>2</sub>\*)-)=5.22857 ROSYM=1 V(3)=1049. cm<sup>-1</sup> Nu=3255,3253,3169,3162,3112,  
 3108,30833061,3044,3040,3034,1556,1540,1529,1526,1515(2),1440,1405,1388,1377,  
 1331,1314,1258,1122,1099,1060,1049,994,924,886,869,794,759,753,592,556,546.5,  
 455,405.5,323 HF298=22.788+/-1.9 kcal HF0=29.95 kcal REF=Burcat G3B3 calc  
 {HF298=22.3 kcal REF=NIST 94} Max Lst Sq Error Cp @ 200 K & 6000 K 0.58%.

C6H11 1-ene2M-YL A07/05C 6.H 11. 0. 0.G 200.000 6000.000 B 83.15154 1  
 1.35236225E+01 2.93883533E-02-1.05716798E-05 1.70239749E-09-1.01591371E-13 2  
 4.80822757E+03-4.14343179E+01 3.00563392E+00 3.26389745E-02 5.08487031E-05 3  
 -9.38814873E-08 4.13292780E-11 8.83724196E+03 1.87641384E+01 1.14673014E+04 4

Table 4 (continued)

N/A

C6H11 2-METHYL-1-PENTENE-5-YL RADICAL CH<sub>2</sub>=C(CH<sub>3</sub>)C<sub>3</sub>H<sub>6</sub>\* ESTIMATED TO 1500 K  
 USING NIST 1994 S&P PROGRAM. EXTRAPOLATED USING WILHOIT'S POLYNOMIALS  
 HF298=35.8 KCAL {Warning! Attempts to calculate G3B3 values ended up in  
 transition states} Max Lst Sq Error Cp @ 500 K 0.38%.

C6H11 2M-1ENE-5YL T11/95C 6H 11 0 0G 298.150 5000.000 E 83.15334	1
0.14332084E+02 0.29125927E-01-0.10865216E-04 0.19028973E-08-0.12681084E-12	2
0.11021737E+05-0.46268468E+02 0.28792433E+01 0.40613348E-01 0.24127870E-04	3
-0.61187151E-07 0.27837372E-10 0.15246181E+05 0.17899962E+02 0.18015157E+05	4

120303-49-3

C6H11 2-METHYLENE-2-PENTENE trans RADICAL CH<sub>3</sub>C(CH<sub>2</sub>\*)=CHC<sub>2</sub>H<sub>5</sub> SIGMA=1 STATWT=2  
 IA=12.1120 IB=44.4186 IC=50.9203 Ir(CH<sub>3</sub>)=0.51453 ROSYM=3 V(3)=18. cm-1  
 Ir(CH<sub>3</sub>)=0.5217 ROSYM=3 V(3)=1129 cm-1 Ir(CH<sub>2</sub>\*)=0.28374 ROSYM=1 V(3)=257 cm-1  
 Ir(C<sub>2</sub>H<sub>5</sub>)=4.7706 ROSYM=1 [V3=1049. cm-1 est] Nu=3262,3178,3149,3126,3122,3114,  
 3104,3090,3046(2),3014,1561,1539,1527,1525,1523,1519,1493,1439,1432,1365,1355,  
 1308,1278,1152,1117,1074,1069,1021,996,921,863,773,764,737,552,514,488,430,361,  
 310 HF298=21.713+/-1.9 kcal HF0=28.95 kcal REF=Burcat G3B3 Vrot by Benson  
 {HF298=19.4 kcal REF=NIST 94} Max Lst Sq Error Cp @ 6000 K 0.57%

C6H11 2M-YL-2ENE A06/05C 6.H 11. 0. 0.G 200.000 6000.000 B 83.15154	1
1.22192185E+01 3.04565109E-02-1.08745741E-05 1.74508562E-09-1.03950204E-13	2
4.69640353E+03-3.50603370E+01 3.63027734E+00 2.78605250E-02 5.48191213E-05	3
-9.22108921E-08 3.93432592E-11 8.28499175E+03 1.54759619E+01 1.09263435E+04	4

N/A

C6H11 2-METHYL-2-PENTENE-5-YL RADICAL CH<sub>3</sub>C(CH<sub>3</sub>)=CHC<sub>2</sub>H<sub>4</sub>\* Estimated to 1500 K  
 USING NIST 1994 S&P PROGRAM. EXTRAPOLATED USING WILHOIT'S POLYNOMIALS  
 HF298=33.9 KCAL Max Lst Sq Error Cp @ 1500 K 0.36%. {WARNING attempts to  
 calculate G3B3 ended up in transition states species}

C6H11 2M-2ENE-5YL T11/95C 6H 11 0 0G 298.150 5000.000 E 83.15334	1
0.12977914E+02 0.30699396E-01-0.11544244E-04 0.20325566E-08-0.13596284E-12	2
0.10444175E+05-0.39319934E+02 0.50011464E+01 0.18999758E-01 0.79270344E-04	3
-0.11764308E-06 0.48290683E-10 0.14232811E+05 0.98591862E+01 0.17059045E+05	4

386702-48-3

C6H11 2-METHYL-2-PENTENE-4-YL RADICAL (CH<sub>3</sub>)<sub>2</sub>C=CHCH\*CH<sub>3</sub> SIGMA=1 STATWT=2  
 IA=11.2847 IB=46.9367 IC=56.6688 [Ir(CH<sub>3</sub>)=0.515754 ROSYM=3 V(3)=778 cm-1]x2  
 Ir(CH<sub>3</sub>)=0.513094 ROSYM=3 V(3)=419. cm-1 Nu=3174,3140,3124,3113,3107,3048,3045,  
 3037,3014,3010,3002,1558,1543,1516,1513,1508,1505,1497,1448,1443,1435,1428,1359,  
 1273,1233,1116,1081,1064,1039,1011,980,948,936,819,733,524,425,401,346,238,198  
 HF298=17.426+/-1.9 kcal HF0=24.27 kcal REF=Burcat G3B3 V(3) Benson's formula  
 {SIGMA(Total)=27 HF298=13.9 kcal REF=NIST 94} Max Lst Sq Error Cp @ 6000 K  
 0.64%.

C6H11 2M-2ene4yl A06/05C 6.H 11. 0. 0.G 200.000 6000.000 B 83.15154	1
1.15464940E+01 3.22525680E-02-1.17193892E-05 1.89817435E-09-1.13683723E-13	2
2.75708577E+03-3.24744443E+01 7.15573896E+00 1.34674499E-02 7.38540091E-05	3
-9.94466642E-08 3.88336296E-11 5.56268067E+03-2.10097996E+00 8.76905362E+03	4

Table 4 (continued)

N/A

C6H11 2-METHYL-4-PENTENE-3-YL RADICAL (CH<sub>3</sub>)<sub>2</sub>CHCH\*CH=CH<sub>2</sub> SIGMA=1 STATWT=2  
 IA=14.2398 IB=41.2367 IC=45.2456 [Ir(CH<sub>3</sub>)=0.5194 ROSYM=3 V(3)=1006. cm<sup>-1</sup>]  
 Ir(CH<sub>2</sub>=CH)=2.9734 ROSYM=1 V(3)=2000. cm<sup>-1</sup> Ir(CH<sub>2</sub>=CH-CH\*-)=7.729127 ROSYM=1  
 V(3)=1868. cm<sup>-1</sup> HF298=21.805+/-1.9 kcal HF0=28.66 kcal REF=Burcat G3B3 calc  
 V(3) Benson's formula {SIGMA(Total)=9 HF298=18.1 kcal REF=NIST 94} Max Lst  
 Sq Error Cp @ 6000 0.54%.

C6H11	2M-4en3yl	A06/05C	6.H	11.	0.	0.G	200.000	6000.000	B	83.15154	1	
							1.56644556E+01	2.83277423E-02	-1.01656596E-05	1.63515295E-09	-9.75533048E-14	2
							3.58552903E+03	-5.45844939E+01	3.41120809E+00	3.77072862E-02	4.07702069E-05	3
							-8.40649398E-08	3.75403765E-11	8.06781961E+03	1.43676791E+01	1.09726394E+04	4

N/A

C6H11 2-METHYL-1-PENTENE-4-YL RADICAL CH<sub>2</sub>=C(CH<sub>3</sub>)CH<sub>2</sub>CH\*CH<sub>3</sub> SIGMA=1 STATWT=2  
 IA=11.9228 IB=45.0639 IC=52.0795 Ir(CH<sub>3</sub>)=0.51259 ROSYM=3 V(3)=318. cm<sup>-1</sup>  
 Ir(CH<sub>3</sub>)=0.52065 ROSYM=3 V(3)=879 cm<sup>-1</sup> Ir(CH<sub>3</sub>CH\*-)=4.53597 ROSYM=2  
 V(3)=1049. cm<sup>-1</sup> Ir(CH<sub>2</sub>=C(CH<sub>3</sub>)-)=5.2778 ROSYM=1 V(3)=7320. cm<sup>-1</sup> Nu=3231,3172,  
 3155,3127,3081,3048,3032,3003,2958,2949,1738,1527,1516,1508,1504,1492,1470,  
 1437.5(2),1414,1324,1304,1207,1149,1129,1075,1051,1003,993,926,918,899,824,725,  
 538,459,447,385,330,206 HF298=32.723+/-1.9 kcal HF0=39.63 kcal REF=Burcat G3B3  
 calc V(3) Benson's formula {SIGMA(Total)=9 HF298=32.4 kcal REF=NIST 94} Max  
 Lst Sq Error Cp @ 6000 K 0.58%

C6H11	1en-2M4yl	A06/05C	6.H	11.	0.	0.G	200.000	6000.000	B	83.15154	1	
							1.21446028E+01	3.14688351E-02	-1.13442729E-05	1.82084771E-09	-1.08228214E-13	2
							1.02900824E+04	-3.43984793E+01	5.47596358E+00	2.16998362E-02	6.37297729E-05	3
							-9.68447154E-08	3.99209272E-11	1.34790988E+04	6.78005637E+00	1.64667590E+04	4

3170-58-9

C6H11 Cyclohexyl Radical SIGMA=2 STATWT=2 IA=18.6303 IB=19.4845 IC=34.0506  
 Nu=3181,3078,3073,3069,3063(2),3032(2),3017,2920,2914,1532,1519,1517,1502,1498,  
 1412,1407,1399,1377,1363,1357,1307,1296,1268,1166,1138,1123,1106,1064,1039,1023,  
 935,881,878,861,812,789,611,459,437,385,331,215,177 HF298=18.126+/-1.9 kcal  
 REF=Burcat G3B3 calc {HF298=18.0 kcal REF=Tsang "Shock Tubes in Chemistry edited  
 A. Lifshitz 1981; HF298=16.3+/-1.7 kcal REF=NIST 94} Max Lst Sq Error Cp @  
 200 K 0.90% and @ 1300 K ).64%.

C6H11	Cyclohexyl	A06/05C	6.H	11.	0.	0.G	200.000	6000.000	B	83.15154	1	
							1.12404984E+01	3.36561705E-02	-1.21056416E-05	1.95588984E-09	-1.17152247E-13	2
							2.56382321E+03	-3.94448686E+01	3.79371262E+00	4.21885696E-03	1.33519603E-04	3
							-1.78159024E-07	7.12566162E-11	6.94149226E+03	1.08152587E+01	9.12130528E+03	4

626-62-0

C6H11I Iodocyclohexane SIGMA=1 STATWT=1 Ia=19.71313 Ib=127.8641 Ic=142.37162  
 Nu=3103,3086,3079,3065,3060,3059,3037,3035,3017,3013,3009,1521,1508,1502(2),  
 1498,1393,1390,1384,1374,1369,1339,1304,1295,1290,1208.6(2),1123,1103,1088,1065,  
 1034,1003,932,892,891,852,808,798,649,488,440,416,311,229,210,190,112  
 HF298=-50.0 +/-4.7 kJ HF0=-11.926 kJ REF=Pedley Naylor & Kirby 1986  
 {HF298=-14.1 kcal REF=NIST 94.; HF298=-6.63 kcal REF=PM3} Max Lst Sq Error  
 Cp @ 200 K 0.79%.

C6H11I		A08/05C	6.H	11.I	1.	0.G	200.000	6000.000	B	210.05601	1	
							1.35564987E+01	3.43152462E-02	-1.23552838E-05	1.99766653E-09	-1.19717263E-13	2
							-1.34081288E+04	-4.75544759E+01	4.95588995E+00	6.24026007E-03	1.36950270E-04	3
							-1.85303576E-07	7.45515658E-11	-8.64749115E+03	9.04456000E+00	-6.01358348E+03	4

Table 4 (continued)

13269-52-8

C6H12 trans-HEXENE-3 C2H5CH=CHC2H5 SIGMA=2 STATWT=1 IA=6.2922 IB=67.4988  
 IC=69.3795 [Ir(CH3)=0.5218 ROSYM=3 V(3)=1200. cm-1]x2 [Ir(C2H5)=4.7098  
 ROSYM=2 V(3)=830. cm-1]x2 Nu=3126,3120(2),3118,3111(2),3066.6(2),3045(2),  
 3017(2),1754,1537(2),1527.5(2),1511.5(2),1434(2),1402,1354,1344,1337,1301,1280,  
 1198,1125,1097.5(2),1052,1016(2),913(2),841,802,761,484,470,328,321,240  
 HF298=-12.053 kcal REF=Burcat G3B3 calc. {HF298=-12.7 kcal REF=Weissman &  
 Benson 1989; HF298(sol)=19.72+/-0.3 kcal REF=Wiberg & Wasserman JACS 103,  
 (1981),6563}. Max Lst Sq Error Cp @ 6000 K 0.61%.

C6H12 trans 3-HE	A03/05C	6.H	12.	0.	0.G	200.000	6000.000	B	84.15948	1
1.22026584E+01	3.33112698E-02	-1.19842937E-05	1.92997393E-09	-1.15175007E-13						2
-1.24462369E+04	-3.80004425E+01	5.32120633E+00	2.06273139E-02	7.37584289E-05						3
-1.08945044E-07	4.45825285E-11	-9.02450060E+03	5.13145237E+00	-6.06376082E+03						4

592-41-6

C6H12 1-HEXENE TRC 4/87 DATA EXTRAPOLATED USING WILHOIT'S POLYNOMIALS.  
 HF298=-41.95 kJ HF0=-11.06 {HF298(liq)=-82.13+/-0.84 kJ REF=JACS 1981} Max Lst  
 Sq Error Cp @ 20 K 0.68%.

C6H12,1-hexene	P 4/87C	6.H	12.	0.	0.G	200.000	6000.000	C	84.15948	1
1.60616093E+01	2.75650562E-02	-9.32973368E-06	1.49349013E-09	-8.98810268E-14						2
-1.28042951E+04	-5.69925586E+01	7.31509054E+00	3.71150329E-03	1.27250318E-04						3
-1.71556964E-07	6.89805935E-11	-8.20916507E+03	-5.94354365E-01	-5.04539654E+03						4

763-29-1

C6H12 2-METHYL-1-PENTEN EXTRAPOLATED FROM STULL WESTRUM & SINKE 1987 CORRECTION  
 USING WILHOIT'S POLYNOMIALS HF298=-14.19 KCAL Max Lst Sq Error H @ 300 K 7.2%.

C6H12 2MP-1en	T11/95C	6H	12	0	OG	298.150	5000.000	B	84.16128	1
0.12620641E+02	0.34649597E-01	-0.13383899E-04	0.24131627E-08	-0.16477558E-12						2
-0.13612080E+05	-0.38598787E+02	0.10315879E+01	0.57920573E-01	-0.20275943E-04						3
-0.90784811E-08	0.65369897E-11	-0.98286087E+04	0.23785709E+02	-0.71406445E+04						4

625-27-4

C6H12 2-METHYL-2-PENTEN EXTRAPOLATED FROM STULL WESTRUM & SINKE 1987 CORRECTION  
 USING WILHOIT'S POLYNOMIALS HF298=-15.98 KCAL Max Lst Sq Error H @ 300 K 7.2%.

C6H12 2MP-2en	T11/95C	6H	12	0	OG	298.150	5000.000	B	84.16128	1
0.12088676E+02	0.34068725E-01	-0.12394277E-04	0.21676186E-08	-0.14583479E-12						2
-0.14418698E+05	-0.36076756E+02	-0.47423428E+00	0.58156280E-01	-0.13393809E-04						3
-0.20423535E-07	0.11920207E-10	-0.10331807E+05	0.31630843E+02	-0.80414023E+04						4

691-38-3

C6H12 4-METHYL-2-PENTEN cis(Z) EXTRAPOLATED FROM STULL WESTRUM & SINKE 1987  
 CORRECTION USING WILHOIT'S POLYNOMIALS HF298=-13.73 KCAL Max Lst Sq Error H  
 @ 300 K 8.6%.

C6H12 4MP-2en	T 5/96C	6H	12	0	OG	298.150	5000.000	B	84.16128	1
0.13429190E+02	0.33252141E-01	-0.12845171E-04	0.23193196E-08	-0.15851939E-12						2
-0.13800258E+05	-0.44366460E+02	0.39826011E+01	0.33553100E-01	0.43946883E-04						3
-0.79076359E-07	0.33590735E-10	-0.98357639E+04	0.10885860E+02	-0.69091648E+04						4

674-76-0

C6H12 4-METHYL-2-PENTEN TRANS EXTRAPOLATED FROM STULL WESTRUM & SINKE 1987  
 CORRECTION USING WILHOIT'S POLYNOMIALS HF298=-14.69 KCAL Max Lst Sq Error H  
 @ 300 K 4.3%.

C6H12 4MP-2en	T11/95C	6H	12	0	OG	298.150	5000.000	B	84.16128	1
0.12531029E+02	0.34618444E-01	-0.13221262E-04	0.23625501E-08	-0.16027053E-12						2
-0.13640433E+05	-0.39312583E+02	0.13269297E+01	0.63390645E-01	-0.39908762E-04						3
0.12904041E-07	-0.15823617E-11	-0.10277554E+05	0.19495838E+02	-0.73922528E+04						4

Table 4 (continued)

110-82-7

C6H12 CYCLOHEXANE SIGMA=6 IAIBIC=13350. Nu=2936,2853,1465,1158,802,384,1380,1150,1100,1350,1100,2914,2863,1457,1039,522,2924(2),2895(2),1445(2),1347(2),1268(2),1029(2),785(2),427(2),2934(2),2863(2),1457(2),1346(2),1260(2),906(2),862(2),241(2) (T0=1925. SIGMA=4 STATWT=1)x2 HF298=-123.3 kJ HF0=-83.7 kJ REF=DOROFEEVA GURVICH & JORISH JPCRD 15 (1986) 437{HF298=-122.383+/-0.67 kJ REF=ATcT A} Max Lst Sq Error Cp @ 200 K 0.98%.

C6H12,cyclo-	g 6/90C	6.H 12.	0.	0.G	200.000	6000.000	B	84.15948	1
1.32145970E+01	3.58243434E-02	-1.32110852E-05	2.17202521E-09	-1.31730622E-13					2
-2.28092102E+04	-5.53518322E+01	4.04357527E+00	-6.19608335E-03	1.76622274E-04					3
-2.22968474E-07	8.63668578E-11	-1.69203544E+04	8.52527441E+00	-1.48294969E+04					4

2679-29-0

N-C6H13 N-HEXYL RADICAL TRC 10/83 DATA TO 3000K EXTRAPOLATED USING WILHOIT'S POLYNOMIALS TO 5000K. HF298=25.1 kJ HF0=57.48 kJ MAX LST SQ ERROR Cp @ 400 K 0.67% .

C6H13 n-hexyl	P10/83C	6.H 13.	0.	0.G	200.000	6000.000	C	85.16742	1
1.39163141E+01	3.48510892E-02	-1.26898935E-05	2.07144196E-09	-1.24756674E-13					2
-4.01785625E+03	-4.33071846E+01	8.76348959E+00	2.16244832E-03	1.31674686E-04					3
-1.73828247E-07	6.92518175E-11	-5.42630596E+02	-5.91729689E+00	3.01881891E+03					4

2493-44-9

2-C6H13 2-HEXYL RADICAL CH3CH\*CH2CH2CH2CH3 SIGMA=1 STATWT=2 IA=5.3311 IB=74.0192 IC=74.4199 [Ir(CH3)=0.5191 ROSYM=3 V(3)=778 cm-1 est]x2 Ir(CH3CH\*-)=4.9974 ROSYM=1 V(3)=1200 cm-1 Ir(CH3CH2-)=4.44475 ROSYM=1 V(3)=1200 est Ir(CH3CH\*CH2-)=5.88152 ROSYM=1 V(3)=1200 cm-1 est HF298=6.73+/-1.9 kcal HF0=14.65 kcal REF=Burcat G3B3 calc {HF298=5.8 kcal REF=NIST 94; HF298=7.0 kcal REF=Liebmann JPCRD Supl. 1988} Max Lst Sq Error Cp @ 1500 K 0.4%.

C6H13 2-Hexyl	A07/05C	6.H 13.	0.	0.G	200.000	6000.000	B	85.16742	1
1.41986473E+01	3.46787125E-02	-1.25515738E-05	2.02767674E-09	-1.21224274E-13					2
-3.68102477E+03	-4.23012097E+01	7.58145549E+00	1.89615514E-02	8.16571755E-05					3
-1.18091545E-07	4.81236008E-11	-2.27328454E+02	5.28216352E-05	3.38664816E+03					4

85908-58-3

C6H13 2-METHYL-PENTANE-1YL RADICAL \*CH2CH(CH3)C3H7 SIGMA=1 STATWT=2 IA=15.0104 IB=42.0846 IC=46.7173 [Ir(CH3)=0.5283 ROSYM=3 V(3)=780. cm-1]x2 Ir(\*CH2-)=0.2881 ROSYM=1 V(3)=525. cm-1 est. Ir(C2H5-)=4.9539 ROSYM=1 V(3)=1200. est Ir(\*CH2CH(CH3)-)=7.5520 ROSYM=1 V(3)=1500. cm-1 est. Nu=3254,3157,3119,3113,3108(2),3068,3057,3046,3043,3036,3019,2923,1542,1534,1533,1527,1520,1510,1488,1443,1433,1403,1398,1359,1333,1291.5,1270,1199,1184,1114,1085,1062,1012,972,936,904,851,838,740,517,472,401,384.5,333,285 HF288=8.517+/-1.9 kcal HF0=16.92 kcal REF=Burcat G3B3 calc. {HF298=7.0 kcal REF=NIST 94} Max Lst Sq Error Cp @ 6000 K 0.59%

C6H13 2M-1yl	A07/05C	6.H 13.	0.	0.G	200.000	6000.000	B	85.16742	1
1.36085138E+01	3.39146566E-02	-1.21614746E-05	1.95675271E-09	-1.16757847E-13					2
-2.56836652E+03	-4.22106248E+01	6.32753023E+00	2.29432563E-02	7.00368709E-05					3
-1.05250882E-07	4.31449156E-11	9.48442814E+02	2.87731563E+00	4.28589634E+03					4

Table 4 (continued)

65596-90-9

C6H13 2-METHYL-PENTANE-5YL RADICAL CH<sub>3</sub>CH(CH<sub>3</sub>)C<sub>2</sub>H<sub>4</sub>CH<sub>2</sub>\* SIGMA=1 STATWT=2  
 IA=12.2796 IB=48.6781 IC=55.8408 [Ir(CH<sub>3</sub>)=0.5191 ROSYM=3 V(3)=780 cm<sup>-1</sup> est]  
 x2 Ir(CH<sub>2</sub>\*)=0.32193 ROSYM=1 V(3)=257. cm<sup>-1</sup> est. Ir(\*CH<sub>2</sub>CH<sub>2</sub>-)=4.4635 ROSYM=1  
 V(3)=1200. cm<sup>-1</sup> est. Ir(\*CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>-)=5.6854 ROSYM=1 V(3)=1200. cm<sup>-1</sup> est.  
 Nu=3258,3160,3117,3108,3104,3098,3063,3043,3041,3035,3019,3002,2923,1541,3019,  
 3002,2923,1541,1536,1528,1521,1516,1499,1488,1448,1429,1416,1389,1371,1326,1312,  
 1243,1207,1176,1129,1092,1059,999,975,940,936,896,818,750,477,445,434,379,323,  
 256 HF298=7.736+/-1.9 kcal HF0=16.115 kcal REF=Burcat G3B3 calc {HF298=7.8  
 kcal REF=NIST 94} Max Lst Sq Error Cp @ 6000 K 0.59%  
 C6H13 2M-5yl A07/05C 6.H 13. 0. 0.G 200.000 6000.000 B 85.16742 1  
 1.30255399E+01 3.46052579E-02-1.24155454E-05 1.99658702E-09-1.19050622E-13 2  
 -2.77515469E+03-3.72134757E+01 6.60629923E+00 1.98623693E-02 7.69757749E-05 3  
 -1.11917751E-07 4.55660959E-11 5.59978604E+02 3.72645563E+00 3.89288413E+03 4

N/A

C6H13 2-METHYL, 4-PENTYL (SECONDARY) RADICAL (CH<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>CH\*CH<sub>3</sub> SIGMA=1  
 STATWT=2 IA=12.2796 IB=48.6781 IC=55.8408 [Ir(CH<sub>3</sub>)=0.5191 ROSYM=3  
 [V(3)=778. cm<sup>-1</sup> est]]x3 Ir(CH<sub>3</sub>CH\*-)=4.9974 ROSYM=1 V(3)=1200 cm<sup>-1</sup> est.  
 Ir(CH<sub>3</sub>CH\*CH<sub>2</sub>-)=4.44475 ROSYM=1 V(3)=1200. cm<sup>-1</sup> est. Nu=3157,3116,3108,3102(2),  
 3097,3047,3039,3034,3013,2998,2955,2918,1539,1533,1525,1518,1516,1506,1494,1448,  
 1439,1429,1424,1382,1378,1305,1255,1204,1195,1149,1123,1068,1002,978,973,941,  
 906,870,815,457,441,430,370,321,256 HF298=4.8+/-1.9 kcal REF=Burcat G3B3 calc  
 {HF298=3.5 kcal REF=NIST 94} Max Lst Sq Error Cp @ 6000 K 0.60%.  
 C6H13 2M-4yl A07/05C 6.H 13. 0. 0.G 200.000 6000.000 B 85.16742 1  
 1.30098703E+01 3.47425832E-02-1.24788818E-05 2.00755656E-09-1.19720967E-13 2  
 -4.20396046E+03-3.83895964E+01 6.32479866E+00 2.55005418E-02 5.87383483E-05 3  
 -9.03289388E-08 3.69266574E-11-9.62096601E+02 2.93990634E+00 2.41493678E+03 4

21058-26-4

C6H13 2-METHYL, 2-PENTYL (TERTIARY) RADICAL (CH<sub>3</sub>)<sub>2</sub>C\*CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub> SIGMA(ext)=1  
 STATWT=2 IA=13.2158 IB=49.1410 IC=56.4702 [Ir(CH<sub>3</sub>)=0.51728 ROSYM=3  
 V(3)=780 cm<sup>-1</sup> est]x3 Ir(C<sub>2</sub>H<sub>5</sub>-)=5.2773 ROSYM=1 V(3)=1200. cm<sup>-1</sup>  
 Ir((CH<sub>3</sub>)<sub>2</sub>C-)=5.32464 ROSYM=1 V(3)=1200. cm<sup>-1</sup> est NU=3110,3106,3095,3093,3070,  
 3044,3040.5(3),3036,2989,2953,2946,1538,1527.5(2),1521,1515,1509,1505,1499,1445,  
 1438,1428,1391,1364,1336,1320,1290,1251,1104,1082,1047,1041,1011,992,958,885,  
 881,781,750,444,384,331.5,292.5,237 HF298=4.1+/-1.9 kcal HF0=12.47 kcal  
 REF=Burcat G3B3 calc. {HF298=2.2 kcal REF=NIST 94} Max Lst Sq Error Cp @  
 6000 K 0.61%  
 C6H13 2-M-2yl A07/05C 6.H 13. 0. 0.G 200.000 6000.000 B 85.16742 1  
 1.27183265E+01 3.50419951E-02-1.26214954E-05 2.03554638E-09-1.21626246E-13 2  
 -4.50680272E+03-3.66810455E+01 7.00863829E+00 1.91966023E-02 7.32824258E-05 3  
 -1.04058649E-07 4.16237288E-11-1.33458073E+03 5.81908346E-01 2.06973015E+03 4

110-54-3

C6H14 liquid n-HEXANE DATA TAKEN FROM TRC 4/85 HF298=-47.481 kcal  
 {HF298=-198.353+/-0.48 REF=ATcT A} Max Lst Sq Error Cp @ 230 K 0.06%  
 C6H14(L) n-hexa P 4/85C 6.H 14. 0. 0.C 177.860 300.000 B 86.17536 1  
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2  
 0.00000000E+00 0.00000000E+00 3.23581200E+01-1.55919703E-01 6.05367043E-04 3  
 -5.71237410E-07-1.30759900E-10-3.07686562E+04-1.23866466E+02-2.38931699E+04 4

Table 4 (continued)

110-54-3

C6H14 N-HEXANE SIGMA=18 TRC 1985 DATA EXTRAPOLATED THROUGH WILHOIT'S POLY-  
NOMIALS. HF298=-166.92 kJ HF0=-130.02 kJ {HF298=-166.805+/-0.48 kJ REF=ATcT A}  
Max Lst Sq Error Cp @ 200 K 0.69 %.

C6H14,n-hexane	g	6/01C	6.H	14.	0.	0.G	200.000	6000.000	C	86.17536	1
1.95158086E+01	2.67753942E-02	-7.49783741E-06	1.19510646E-09	-7.51957473E-14							2
-2.94362466E+04	-7.74895497E+01	9.87121167E+00	-9.36699002E-03	1.69887865E-04							3
-2.15019520E-07	8.45407091E-11	-2.37185495E+04	-1.24999353E+01	-2.00757471E+04							4

107-83-5

C6H14 2-METHYLPENTANE TRC 1985 DATA EXTRAPOLATED THROUGH WILHOIT'S POLYNOMIALS.  
MAX LST SQ ERROR CP @ 1400 K 0.58 % HF298=-174.55 KJ

H14C6	T12/91H	14C	6	0	0G	298.150	5000.000	C	86.17716	1
0.13108042E+02	0.39278025E-01	-0.14080404E-04	0.24208876E-08	-0.16060487E-12						2
-0.28005811E+05	-0.43334246E+02	-0.18831303E+00	0.62825959E-01	-0.96052544E-05						3
-0.26183767E-07	0.13717321E-10	-0.23599561E+05	0.28793617E+02	-0.20993420E+05						4

96-14-0

C6H14 3-METHYLPENTANE TRC 1985 DATA EXTRAPOLATED USING WILHOIT'S POLYNOMIALS.  
MAX LST SQ ERROR CP @ 1500 K 0.44% HF298=-171.97 KJ

C6H14	3MP	T12/91C	6H	14	0	0G	298.150	5000.000	C	86.17716	1
0.11469782E+02	0.42180865E-01	-0.15849621E-04	0.28068586E-08	-0.18972023E-12							2
-0.27169579E+05	-0.34201883E+02	0.25431966E+00	0.58351247E-01	-0.40723274E-07							3
-0.34483028E-07	0.16336350E-10	-0.23291682E+05	0.27495401E+02	-0.20683119E+05							4

75-83-2

C6H14 2,2-DIMETHYLBUTANE TRC 1985 DATA EXTRAPOLATED USING WILHOIT'S POLYNOMIALS.  
MAX LST SQ ERROR CP @ 1500 0.36% HF298=-184.68 KJ

C6H14	2,2-DMB	T12/91C	6H	14	0	0G	298.150	5000.000	C	86.17716	1
0.96971555E+01	0.46148235E-01	-0.16623012E-04	0.28333468E-08	-0.18611414E-12							2
-0.28192059E+05	-0.27863620E+02	0.64064618E+00	0.56146894E-01	0.55680943E-05							3
-0.37647313E-07	0.17161290E-10	-0.24881231E+05	0.22759020E+02	-0.22211772E+05							4

79-29-8

C6H14 2,3-DIMETHYLBUTANE TRC 1985 DATA EXTRAPOLATED USING WILHOIT'S POLYNOMIALS.  
MAX LST SQ ERROR CP @ 1300 K 0.64 % HF298=-176.8 KJ

C6H14	2,3-DMB	T12/91C	6H	14	0	0G	298.150	5000.000	C	86.17716	1
0.11052547E+02	0.42967887E-01	-0.15547966E-04	0.26700033E-08	-0.17650517E-12							2
-0.27635374E+05	-0.34063265E+02	-0.24903827E+01	0.76732667E-01	-0.44086761E-04							3
0.11461954E-07	-0.65151136E-12	-0.23564889E+05	0.37180699E+02	-0.21264031E+05							4

3470-17-5

C6N6O6 BENZOTRIFUROXAN (BTF) SIGMA=3 A=B=0.15716 C=0.07858 NU=86(2),104,164,  
183(2),276(2),312,372(2),[420],428(2),509,[570(2)],642(2),649,[651],740(2),  
[736(2),810],785,886,931,[935(2),965(2)],1099,[1082(2)],1290,[1304(2),1415(2)],  
1487,[1570(2)],1602,1659,[1656(2)] REF=Gong, Xiao & Dong Chinese J. Struct.  
Chem. 18,(1999),124-130 NO GASEOUS HEAT OF FORMATION AVAILABLE HF298(Solid)=  
144.9 +/-0.8 kcal REF=Rouse J. Chem. Eng. Data, 21,(1976),16-20. Max Lst Sq  
Error Cp @ 1300 K 0.53 %.

BENZOTRIFUROXAN	T 8/99C	6.N	6.O	6.	0.G	200.000	6000.000	D 252.10284	1
3.25028258E+01	1.96519737E-02	-7.62353333E-06	1.29360949E-09	-8.01216134E-14					2
-1.33442030E+04	-1.47193860E+02	-8.43434844E-01	1.03343605E-01	-6.42039528E-05					3
-7.99732470E-09	1.54458617E-11	-3.76608113E+03	2.69680087E+01	0.00000000E+00					4

Table 4 (continued)

129066-01-9

C7 linear SIGMA=2 STATWT=1 B0=0.030613 Nu=2154,1547,549,2138,1898,1077,  
496(2),190(2),708(2),293(2),80(2) REF=Van-Orden Saykally Chem. Rev. 98,(1998),  
2313 Max Lst Sq Error Cp @ 1300 K 0.47%.

C7 linear	A09/04C	7.	0.	0.	0.G	200.000	6000.000	B	84.07490	1
1.26083266E+01	6.67144456E-03	-2.52621952E-06	4.22093703E-10	-2.58706421E-14						2
1.54955065E+05	-3.71489229E+01	3.38696683E+00	4.56108600E-02	-7.47844134E-05						3
6.56305567E-08	-2.26941954E-11	1.57024331E+05	7.67058229E+00	1.59519683E+05						4

335-57-9

C7F16 PERFLUOROHEPTANE SIGMA=18 CALCULATED and EXTRAPOLATED USING NIST 93 AND  
BOZZELLI & RITTER'S PROGRAM. HF298=-3383.60 KJ REF=DOMALSKI & HEARING JCPRD 22  
(1993) p. 1059 Max Lst Sq Error Cp @ 1400 K 0.2%.

C7F16	T12/94C	7F	16	0	0G	298.150	5000.000	D	388.05145	1
0.49255494E+02	0.15917852E-01	-0.66760164E-05	0.12359725E-08	-0.84204573E-13						2
-0.42550985E+06	-0.20796807E+03	-0.31954899E+01	0.18606616E+00	-0.21215520E-03						3
0.11047553E-06	-0.21600066E-10	-0.41264667E+06	0.55907556E+02	-0.40699560E+06						4

155204-50-5

C7H4 TriEthynylMethane CH(CCH)3 SIGMA=3 STATWT=1 IA=30.2417 IB=30.24999  
IC=56.7183 Nu=3150,3148(2),2880,2232,2223(2),1266(2),995(2),967,960(2),955,  
946(2),921,669,638(2),486,477(2),287,223(2) REF=PM3 HF298=161.6 kcal  
REF=NIST 94 est Max Lst Sq Error Cp @ 200 K & 6000 K 0.50%

C7H4 CH(CCH)3	T08/02C	7.H	4.	0.	0.G	200.000	6000.000	B	88.10666	1
1.29422979E+01	1.62480659E-02	-5.88121491E-06	9.54331104E-10	-5.73366914E-14						2
7.57321451E+04	-4.32325986E+01	-5.84080437E-01	5.22529624E-02	-3.19358974E-05						3
-3.67937454E-09	8.15253334E-12	7.94574218E+04	2.67188586E+01	8.13198132E+04						4

100-47-0

PHENYL-CN (BENZONITRILE) DATA FROM STULL WESTRUM & SINKE EXTRAPOLATED TO 5000K  
USING WILHOIT'S POLYNOMIALS. HF298=52.3 KCAL Max Lst Sq Error Cp @ 1200 K 0.31%

C7H5N	T 3/93C	7H	5N	1	0G	298.150	5000.000	B	103.12344	1
0.13986349E+02	0.21028565E-01	-0.74936815E-05	0.12924836E-08	-0.86479352E-13						2
0.19941209E+05	-0.50121316E+02	-0.30769054E+01	0.68729237E-01	-0.53234449E-04						3
0.16528583E-07	-0.21922909E-12	0.24618574E+05	0.37871666E+02	0.26318232E+05						4

118-96-7

C7H5(NO2)3 TNT Tri-Nitro-Toluene Solid Cp 290-345 REF= Yin,Ziru,Ganghe,  
Chengyun 17th Internat. Pyrotech. Seminar 1991 Vol 1, 515-521 S298=32.93 cal  
Graphic Integ HF298(solid)=-15.1+/-1.2 Kcal REF=Rouse J. Chem. Eng. Data 21  
(1976),16-20 Max Lst Sq Error Cp @ 340 K \*\*1.7 %\*\*

TNT Solid Yin	HF298 C	7.H	5.N	3.O	6.S	290.000	353.800	D	227.13332	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00						2
0.00000000E+00	0.00000000E+00	4.76323267E+03	-6.62925737E+01	3.45483562E-01						3
-7.95964538E-04	6.85394484E-07	-2.83973511E+05	-1.70349206E+04	-7.59857165E+03						4



Table 4 (continued)

118-96-7

C7H5(NO2)3 TNT Tri-Nitro-Toluene SIMNO=2 STATWT=1 IA = 151.9571  
 IB= 161.4057 IC=305.6182 Ir(NO2)para=5.96 ROSYM=2 V(2)=3.11 kcal  
 (Ir(NO2)meta=5.96 ROSYM=2 V(2)=7 kcal)x2 Ir(CH3)=0.51666 ROSYM=3 V(3)=3.5  
 kcal NU=3273(2), 3192, 3160, 3091, 1678(2), 1649, 1635, 1616, 1517, 1501, 1486, 1443, 1434,  
 1407, 1397, 1394, 1362, 1225(2), 1189, 1105, 1064, 1056, 959.5(2), 950, 918, 836, 803, 783,  
 780, 743, 736, 712, 666, 657, 547, 537, 479, 469, 387, 368, 353, 328, 324, 296, 196, 189, 182, 151,  
 122 REF=Burcat B3LYP calc HF298=5.76 kcal REF=Lenchitz et al J. Chem.  
 Thermodyn 3, (1971), 689 Max Lst Sq Error Cp @ 1300 K 0.57%  
 C7H5(NO2)3 (TNT) A 8/05C 7.H 5.N 3.O 6.G 200.000 6000.000 B 227.13122 1  
 3.18243437E+01 2.61420691E-02-1.00880385E-05 1.69978925E-09-1.04624131E-13 2  
 -1.04731295E+04-1.37140750E+02 3.19573446E+00 8.62220253E-02-2.31687328E-05 3  
 -4.31207526E-08 2.63452650E-11-1.60910932E+03 1.54067756E+01 2.89852800E+03 4

479-45-8

C7H5N5O8 Tetryl Solid N Methyl-N,2,4,6-tetranitroaniline Cp 290-345 REF= Yin,  
 Ziru, Ganghe, Chengyun 17th Internat. Pyrotech. Seminar 1991 Vol 1, 515-521  
 S298=34.29 cal Graphic Integ HF298(solid)=9.8+/- 1.1 Kcal REF=NIST 98 (Krien,  
 Licht, Zierath Thermochim Acta 6, (1973), 465-472 Max Lst Sq Error Cp @ 335 K  
 0.70 %  
 Tetryl Solid Yin T 4/99C 7.H 5.N 5.O 8.S 290.000 401.500 D 287.14560 1  
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2  
 0.00000000E+00 0.00000000E+00-2.53679003E+03 2.97271189E+01-1.28541885E-01 3  
 2.45677286E-04-1.74152468E-07 1.72331689E+05 9.49458327E+03 4.93152332E+03 4

100-52-7

BENZALDEHYDE IA=16.033 IB=53.65 IC=69.661 NU=3084, 3063(2), 3036, 3026, 2817, 1728,  
 1614, 1603, 1491, 1460, 1387, 1314, 1276, 1202, 1168, 1160, 1074, 1026, 996, 825, 649, 617,  
 437, 224, 1003, 996, 978, 918, 852, 740, 688, 450, 404, 217 ROSYM=2 IR=1.48 INTERNAL ROT  
 BARRIER V2=1713.8 HF298=-36.8 KJ REF=Ambrose, Connett, Green, Hales, Head, &  
 Martin J. Chem. Thermo. 7 (1975) 1143. Max Lst Sq Error Cp @ 1200 K 0.39%.  
 C7H6O L 3/86C 7H 6O 1 0G 298.150 5000.000 B 106.12404 1  
 0.13650737E+02 0.25680419E-01-0.10466729E-04 0.19413430E-08-0.13483792E-12 2  
 -0.11019744E+05-0.47965796E+02-0.31627334E+01 0.66369245E-01-0.34816353E-04 3  
 -0.62999377E-08 0.85807101E-11-0.61169349E+04 0.40231735E+02-0.44259974E+04 4

3551-27-7

C7H7 2,4,6-Cyclohetatriene-1-yl SIGMA=2 STATWT=2 Ia=22.6219 Ib=22.6281  
 Ic=45.2499 Nu=3198, 3189, 3186, 3171, 3154, 3148(2), 1660, 1636, 1560, 1505, 1494, 1429,  
 1316, 1298, 1256, 1198, 1009, 993, 984, 981, 968, 916, 908, 851, 844, 769, 754, 657, 567, 517,  
 448, 421, 290, 161.6, 70.6 HF298=280.78. kJ HF0=298.3 kJ REF=Burcat G3B3  
 calc. Max Lst Sq Error Cp @ 200 K 0.72%.  
 C7H7 Cyheptatrien A09/05C 7.H 7. 0. 0.G 200.000 6000.000 B 91.13048 1  
 1.37839351E 01 2.32922891E-02-8.36543230E-06 1.35064040E-09-8.08726926E-14 2  
 2.71779724E 04-4.85624908E 01 1.37723080E 00 3.27432725E-02 4.58225372E-05 3  
 -9.07721756E-08 4.08096948E-11 3.16491191E 04 2.10799820E 01 3.37597997E 04 4

2154-56-5

C7H7 BENZYL RAD STATWT=2. SIGMA=2. A0=.1845 B0=.0899 C0=.0605 IR=0.2830  
 ROSYM=2 V(2)=3880 cm-1 NU=3087, 3070, 3056, 3051, 1555, 1465, 1456, 1248, 1151, 1004,  
 958, 801, 513, 923, 803, 343, 378, 947, 862, 744, 675, 657, 463, 195, 3141, 3075, 3058, 1534,  
 1433, 1313, 1295, 1140, 1083, 944, 604, (485 rotor) HF298=208.0+/-1.9 KJ REF=IUPAC  
 DATA SHEET 2003 MAX LST SQ ERROR Cp @ 200 K \*\*1.3%\*\* (0.64% @ 6000 K)  
 C7H7 BENZYL RAD IU3/03C 7.H 7. 0. 0.G 250.000 6000.000 B 91.13048 1  
 0.14723052E+02 0.23034244E-01-0.84847359E-05 0.13916962E-08-0.84247967E-13 2  
 0.17990189E+05-0.55950989E+02-0.12303836E+01 0.48986376E-01 0.13815518E-04 3  
 -0.62587233E-07 0.31595731E-10 0.23192877E+05 0.30555495E+02 0.25016622E+05 4

Table 4 (continued)

68364-31-8

C7H7 Quadricyclane Apex Radical SIGMA=2 STATWT=2 IA=18.1057 IB=18.9705  
 IC=25.2086 Nu=298,530,557,688,727,732,740,770,783,821,859,905,910,914,978,990,  
 1011,1033,1037,1041,1055,1125,1214,1255,1270,1283,1324,1370,1372,3201,3207,3209,  
 3211,3218,3224,3247 HF298=127.753+/-0.5 kcal HF0=132.81 kcal REF=A. Burcat  
 G3B3 calc MAX Lst Sq Error Cp @ 200 K \*\*\*1.8%\*\*\* (0.54% @ 6000 K)  
 C7H7 Quadricyclan T05/04C 7.H 7. 0. 0.G 250.000 6000.000 B 91.13048 1  
 1.45613991E+01 2.25398262E-02-8.08474676E-06 1.30450216E-09-7.80859341E-14 2  
 5.71439268E+04-5.78471674E+01-1.70080734E+00 3.04385802E-02 8.67461662E-05 3  
 -1.54864793E-07 6.96237489E-11 6.29484088E+04 3.38049379E+01 6.42874387E+04 4

177552-63-5

C7H7 Quadricyclane Basis Radical SIGMA=1 STATWT=2 IA=18.3406 IB=18.7504  
 IC=25.3788 Nu=392,530,634,659,735,743,776,820,838,873,906,939,945,962,997,1026,  
 1028,1046,1073,1085,1137,1198,1234,1251,1276,1292,1372,1381,1519,3049,3089,3190,  
 3193,3202,3213,3225 HF298=138.95+/-0.75 kcal HF0=144.32 kcal REF=A. Burcat  
 G3B3 calc Max Lst Sq Error Cp @ 200 K \*\*\*2.0%\*\*\* (0.56% @ 6000 K)  
 C7H7 Quadricyc Bast05/04C 7.H 7. 0. 0.G 250.000 6000.000 B 91.13048 1  
 1.37020207E+01 2.35155030E-02-8.48400888E-06 1.37418106E-09-8.24731805E-14 2  
 6.29321526E+04-5.31007268E+01-8.65667695E-01 2.02947038E-02 1.09980739E-04 3  
 -1.75783782E-07 7.63992292E-11 6.86151415E+04 3.14499535E+01 6.99194396E+04 4

177552-64-6

C7H7 Quadricyclane Shoulder Radical SIGMA=1 STATWT=2 IA=18.1867 IB=19.2528  
 IC=24.8301 Nu=398,523,638,685,725,736,798,807,872,875,904,926,939,950,964,1016,  
 1034,1047,1076,1080,1171,1179,1210,1249,1257,1282,1336,1384,1516,3065,3110,3195,  
 3203,3213,3214,3222 HF298=140.76+/-0.75 kcal HF0=148.13 kcal REF=A. Burcat  
 G3B3 calc Max Lst Sq Error Cp @ 200 K \*\*\*2.03%\*\*\* (0.55% @ 6000 K)  
 C7H7 QuadriShould T05/04C 7.H 7. 0. 0.G 250.000 6000.000 B 91.13048 1  
 1.37942752E+01 2.34051131E-02-8.43790562E-06 1.36605463E-09-8.19586557E-14 2  
 6.38188219E+04-5.36181270E+01-9.44867622E-01 2.05614652E-02 1.10443183E-04 3  
 -1.77155804E-07 7.71416023E-11 6.95385117E+04 3.18007641E+01 7.08327779E+04 4

108-88-3

TOLUENE Liquid REF= TRC 10/86 TABLES. HF298(L)=12.18 kJ. {HF298=12.503+/-0.35 kJ  
 REF=ATcT A} Max Lst Sq Error Cp @ 500 K 0.23%  
 TOLUENE (L) P10/86C 7.H 8. 0. 0.L 178.150 500.000 C 92.14052 1  
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2  
 0.00000000E+00 0.00000000E+00 2.93676022E+01-1.94722686E-01 9.74773096E-04 3  
 -1.91472689E-06 1.48097019E-09-4.16318442E+03-1.12019966E+02 1.46490894E+03 4

108-88-3

C7H8 TOLUENE STATWT=1 SIGMA=1 IA=14.652 IB=33.346 IC=48.000 Ir=0.5214  
 ROSYM=6 V(3)=4.876 cm-1 REF=Rudolph et al Z. Naturforschung 22A, (1967), 940  
 NU=3085,3070,3058,2920,1604,1493,1378,1208,1176,1028,1002,784,524,973,841,406,  
 2979,1455(3),1040,983,893,734,690,467,217,3037,3028,2950,1540,1331,1313,1153,  
 1080,1040,620,347 REF=HITCHCOCK & LAPOSA J. Molec. Spectr.54, (1975), 223  
 HF298=50.17 kJ HF0=73.48 kJ {HF298=50.494+/-0.36 kJ REF=ATcT A; V(3)=3.176  
 cm-1 REF=Melius BAC/MP4 A72L 1987} MAX LST SQ ERROR Cp @ 200 K 0.92 %.  
 C7H8 TOLUENE g 1/93C 7.H 8. 0. 0.G 200.000 6000.000 B 92.13842 1  
 1.29393610E+01 2.66922277E-02-9.68422041E-06 1.57392386E-09-9.46671699E-14 2  
 -6.76971149E+02-4.67249759E+01 1.61200102E+00 2.11179855E-02 8.53239986E-05 3  
 -1.32568501E-07 5.59411406E-11 4.09654820E+03 2.02969771E+01 6.03402967E+03 4

Table 4 (continued)

121-46-0

C7H8 NORBORNADIENE 2,5-BICYCLOHEPTADIENE SIGMA=2 IA=19.32836 IB=28.76499  
 IC=32.96105 REF STRUCT=Boyd et al J. Phys. Chem 75 (1971),1264 NU=3105,3010,  
 2939,1579,1455,1232,1109,938,877,777,729,417,3073,1287,1240,1111,956,904,741,  
 475,3075,3005,1319,1267,1157,944,914,871,801,539,3101,2994,1548,1208,1064,1019,  
 897,656.5,500 REF=Shaw et al J. Chem. Phys 89 (1988),716 HF298=247.6 KJ  
 REF=STEELE J. Chem Thermody. 10, (1978),919 Max Lst Sq Error Cp @ 200 K \*\*1.5%\*\*  
 C7H8 BICY-DIEN T 2/95C 7H 8 0 OG 200.000 6000.000 B 92.14052 1  
 0.13496865E+02 0.25643891E-01-0.92836633E-05 0.15067572E-08-0.90544980E-13 2  
 0.22818374E+05-0.52940311E+02-0.16635648E+01 0.32118722E-01 0.77694587E-04 3  
 -0.13846610E-06 0.61589660E-10 0.28405811E+05 0.33057840E+02 0.29779265E+05 4

278-06-8

C7H8 Quadricyclane (cyclobutane basis, on opposite edges two cyclopropane & their  
 apex connected by CH2) Tetracyclo[3.2.0.0(2,7).0(4,6)]heptane SIGMA=2 STATWT=1  
 IA=19.079 IB=19.2921 IC=25.8763 Nu=396,539,686,719,736,743,783,816,849,878,  
 919,927,943,968,982,1013,1029,1039,1058,1067,1086,1116,1202,1227,1261,1289,1297,  
 1303,1383,1409,1519,3048,3087,3193,3196,3204,3214,3217,3225 HF298=80.6+/- .5  
 kcal HF0=86.86 kcal REF=BURCAT G3B3LYP calc {HF298=336 kJ REF=Roth et al  
 Chem Berich 124, (1991),2499-2521 HF298=339.1+/-2.3 kJ REF=Steele J. Chem.  
 Thermodyn. 10(1978),919-927} HF298(L)=302.1+/-2.2 kJ REF=Steele J. Chem.  
 Thermodyn. 10(1978),919-927 Max Lst Sq Error Cp @ 200 K \*\*\*\* WARNING 2.23% \*\*\*\*  
 C7H8 QuadricycleneT05/04C 7.H 8. 0. 0.G 250.000 6000.000 B 92.13842 1  
 1.35968758E+01 2.61807581E-02-9.41882302E-06 1.52264588E-09-9.12588456E-14 2  
 3.33651653E+04-5.49086727E+01-5.59833875E-01 1.42094434E-02 1.36122373E-04 3  
 -2.06102120E-07 8.81203349E-11 3.92576729E+04 2.92384866E+01 4.05592633E+04 4

544-25-2

C7H8 1,3,5-CYCLOHEPTATRIENE SIGMA=1 IAIBIC=21.43E+114 NU=3050(6),2950,2850,  
 1650(3),1450(3),1400(2),1200(3),1100(2),1000(4),950(2),900(2),800,750,700,650,  
 450(3),350,300,225 REF=DOROFEEVA GURVICH & JORISH HF298=182.8 kJ Max Lst Sq  
 Error Cp @ 200 K 0.86%  
 C7H8 CYTRIENE T 2/95C 7H 8 0 OG 200.000 6000.000 C 92.14052 1  
 0.13258062E+02 0.26861556E-01-0.97467868E-05 0.15841995E-08-0.95289125E-13 2  
 0.15183137E+05-0.49026873E+02 0.85938299E+00 0.28843433E-01 0.66954232E-04 3  
 -0.11395939E-06 0.49164081E-10 0.20057894E+05 0.22487468E+02 0.21985661E+05 4

2396-63-6

C7H8 1,6-HEPTADIYNE SIGMA=2 HF298=395.8 kJ REF=NIST 94 DATA EXTRAPOLATED TO  
 5000 K USING WILHOIT'S POLYNOMIALS Max Lst Sq Error Cp @ 1500 K 0.6%  
 C7H8 1,6-DIYNE T 2/95C 7H 8 0 OG 298.150 5000.000 E 92.14052 1  
 0.13001823E+02 0.25607076E-01-0.83584682E-05 0.13207200E-08-0.81972807E-13 2  
 0.41975255E+05-0.37320914E+02 0.99595662E+00 0.66544712E-01-0.62569423E-04 3  
 0.35335409E-07-0.88673880E-11 0.44836033E+05 0.22638639E+02 0.47603527E+05 4

108-39-4 and 106-44-5 and 95-48-7

C7H7O CRESOL REF=Kudchadker, Kudchadker, Wilhoit & Zwolinski, JPCRD 7 (1978)  
 417. ISOMERS WERE COMBINED BY SETTING T0= DELTA E VALUES. BECAUSE OF SLIGHT  
 DIFFERENCES IN CIS AND TRANS M-CRESOL, THEY WERE COMBINED BY SETTING STATWT=2.  
 OTHER ISOMERS ARE O-CRESOL (CIS AND TRANS) AND P-CRESOL. HF298=-132.298 KJ.  
 Max Lst Sq Error Cp @ 1300 K 0.6%.  
 C7H8O CRESOL L 6/87C 7H 8O 1 OG 200.000 6000.000 B  
 108.13992 1  
 0.15932987E+02 0.27011160E-01-0.99448722E-05 0.16296689E-08-0.98513298E-13 2  
 -0.23592065E+05-0.59732841E+02 0.42258267E+00 0.45551636E-01 0.32012513E-04 3  
 -0.81121959E-07 0.37665658E-10-0.18202621E+05 0.26032903E+02-0.15911701E+05 4

Table 4 (continued)

100-51-6

C7H8O BENZYL ALCOHOL FREQUENCIES AND MOMENTS OF INERTIA EST. FROM BENZALDEHIDE.  
SIGMA=2 IA=15. IB=53. IC=68. IR=0.14 ROSYM=1 POTENTIAL BARRIER V(1)+800.

NU=3084,3063,3036,3026,2817,1035,1614,1603,1500,1491,1460,1314,1276,1202,1168,  
1160,1074,1026,996,825,800,617,437,224,1003,996,978,918,852,740,688,450,404,217,  
2800,1250,1150,1050,3680,1345 REF=KAKAR & REINHART J. CHEM. PHYS 52 (1970), 3803  
HF298=-100.416 KJOULES. REF=Stein et al., NIST Ref Database #25 (1991)

C7H8O	L 7/87C	7H	8O	1	OG	200.000	6000.000	D 108.13992	1
	0.15281154E+02	0.27208501E-01	-0.98584660E-05	0.16012183E-08	-0.96278057E-13				2
	-0.19700471E+05	-0.59418673E+02	0.20642021E+01	0.22775140E-01	0.95972053E-04				3
	-0.15085110E-06	0.64175832E-10	-0.14285021E+05	0.18148312E+02	-0.12077200E+05				4

N/A

C7H10 3,5 DIMETHYL-CYCLO-PENTADIENE ROSYM=2x3 ESTIMATED BY NIST 94 FROM  
2x[C-(H)3]; [CD-(C)2]; [CD-(C)(H)]; [CD-(C)(CD)]; [CD-(CD)(H)]; [C-(CD)2(H)2]  
CYCLO CORRECTION FOR HF 25.1 KJ FOR S 117.2 J HF298=66.7 KJ Max Lst Sq Error  
H-H298 @ 500 K 0.76%

C7H10 CY	T10/94C	7H	10	0	OG	298.150	5000.000	E 94.15640	1
	0.20552365E+02	0.21152399E-01	-0.61510211E-05	0.93381729E-09	-0.57913697E-13				2
	-0.11383855E+04	-0.86816803E+02	-0.31141443E+01	0.88593226E-01	-0.79693884E-04				3
	0.35311116E-07	-0.46666666E-11	0.56494240E+04	0.35689345E+02	0.80221204E+04				4

498-66-8

C7H10 NORBORNENE SIGMA=1 IA=21.42613 IB=24.37202 IC=27.83715 REF= PM3

NU=[3091],3071,[2997],2986,[2981],2972,[2960,2933,2927],2887,1575,1478,1453,  
1452,1340,1300,1286,1284,1271,1254,1206,[1199],1168,1127,1115,1093,1035,1021,  
[967],964,951,939,[928],907,873,833,810,794,769,710,664,[507],472,381,258

IR + [] STO/3-21G calc REF=Shaw et al JPC 89 (1988),716 HF298=90+/-10 kJ

REF=NIST Webbook 2001 estimate MAX Lst Sq Error Cp @ 200 K \*\*1.7%\*\*

C7H10 NORBORNENE	T11/01C	7.H	10.	0.	O.G	200.000	6000.000	D 94.15640	1
	1.37091008E+01	3.18949114E-02	-1.15779814E-05	1.88233002E-09	-1.13241586E-13				2
	3.20331766E+03	-5.53471380E+01	3.10951688E-01	1.46977266E-02	1.40550719E-04				3
	-2.06243618E-07	8.64793395E-11	9.20346303E+03	2.60640025E+01	1.08244503E+04				4

19179-12-5

C7H10N2O2 Cyclo-PRO-GLY Pyperazine ring + Glyoxal fused to Pyrrolidine ring

(-C=O-NH-CH2-C=O-N(-#1)-CH(-#2)-) #1-CH2-CH2-CH2-#2 IA=60.5276 IB=62.9333

IC=118.1002 NU=3597,3149,3137,3127,3105,3085,3064(2),3009,2976,1803,1782,1554,  
1531(2),1521,1489,1460,1412,1389,1367,1363,1342,1321,1304,1266,1257,1241,1219,  
1190,1144,1120,1079,1023,1009,991,938,920,909,867,792,767,665,615,584,580,560,

481,443, 423,345,260,203,163,140,100.8,57.56 REF=Burcat B3LYP/6-31G(d) calc

HF0=-72.0+/-3.0 kcal REF=Ling & C. Lifshitz J. Mass Spect. 33, (1998),25-34.

Max Lst Sq Error Cp @ 1300 K 0.61%.

C7H10N2O2 BiCyclo	A03/05C	7.H	10.N	2.O	2.G	200.000	6000.000	B 154.16658	1
	1.95545314E+01	3.73586527E-02	-1.35449227E-05	2.20085340E-09	-1.32367284E-13				2
	-5.08865962E+04	-7.94221837E+01	4.25843639E+00	2.86043437E-02	1.14423034E-04				3
	-1.73959555E-07	7.21104892E-11	-4.42778012E+04	1.16692503E+01	-4.10355868E+04				4

Table 4 (continued)

279-23-2

C7H12 NORBORNANE (1,4-BICYCLOHEPTANE) SIGMA=2 IA=21.71703 IB=32.0313  
 IC=36.49119 REF=Boyd, Sanwal, Shary-Tehrany & McNally J. PHYS. CHEM. 75, (1971)  
 ,1264 NU=2980,2972,2927,2918,1487,1455(2),1317,1260,1142,993,923,873,818,755,  
 410,2943,2913(2),1306,1298,1220,1115,968,963,542,172,2971,2949,1453,1315,1279,  
 1241,1165,1074,975,800,757,342,2967,2960,2926,1463,1302,1214,1109,1025,954,890,  
 788,451 REF= Shaw, Castro, Dutler, Rauk, Wieser J.Chem Phys 89 (1988),716  
 HF298=-12.84 +/-1.0 KCAL REF= Rogers, Choi, Girellini, Holmes J. PHYS. CHEM. 84  
 , (1980), 1810 Max Lst Sq Error Cp @ 200 K \*\*1.65%\*\*  
 C7H12 NORBORNANE T 2/95C 7H 12 0 OG 200.000 6000.000 B 96.17228 1  
 0.12209671E+02 0.36813654E-01-0.13348120E-04 0.21681847E-08-0.13034960E-12 2  
 -0.13908324E+05-0.48119383E+02 0.29299287E+01-0.51738445E-02 0.19010706E-03 3  
 -0.25143626E-06 0.10128615E-09-0.83354164E+04 0.15423398E+02-0.64613020E+04 4

628-92-2

C7H12 CYCLOHEPTENE SIGMA=2 IAIBIC=32.1E+114 NU=3024,2964,2926,2881,2852(2),  
 2837,1656,1457,1443,1434,1339,1332,1252,1234,1200,1072,1042,983,875,824,746,691,  
 479,417,353,190,3062,2963,2924,2854,2842,1447,1439,1391,1357,1323,1270,1234,  
 1207,1144,1104,1024,985,960,889,832,585,459,312,209 HF298=-9.4 KJ  
 REF=Dorofeeva, Gurvich & Jorish (1986) Max Lst Sq Error Cp @ 200K 0.99% CALCULA-  
 TED DATA DO NOT AGREE WELL WITH THE ORIGINAL DATA  
 C7H12 CY-HEPTENE T 2/95C 7H 12 0 OG 200.000 6000.000 D 96.17228 1  
 0.13885839E+02 0.37228089E-01-0.13526336E-04 0.22001174E-08-0.13239255E-12 2  
 -0.90383223E+04-0.55685410E+02 0.25521022E+01 0.14373533E-01 0.13613489E-03 3  
 -0.19136176E-06 0.77956555E-10-0.33917022E+04 0.15627602E+02-0.11305537E+04 4

N/A

C7H13 1-HEPTENYL-4/5ene SIGMA=2 ROSYM=3 Estimate of NIST-94. EXTRAPOLATED  
 from 1600 K USING WILHOIT'S POLYNOMIALS. HF298=132.2 KJ MAX LST SQ ERROR CP @  
 400 K \*\*1.5%\*\* @ 1500 K 0.56%  
 C7H13 1-Heptenyl T 8/03C 7.H 13. 0. 0.G 298.150 5000.000 E 97.17812 1  
 1.96156993E+01 2.79893895E-02-8.63561102E-06 1.37238476E-09-8.74339134E-14 2  
 6.68057660E+03-7.22430700E+01-7.36601903E+00 1.18305132E-01-1.40059342E-04 3  
 9.69766801E-08-2.75226297E-11 1.38982991E+04 6.44453158E+01 1.59016466E+04 4

592-76-7

C7H14 1-HEPTENE TRC 4/87 DATA EXTRAPOLATED THROUGH WILHOIT'S POLYNOMIALS.  
 HF298=-62.76 kJ HF0=-26.90 kJ MAX LST SQ ERROR Cp @ 200 K 0.71%.  
 C7H14,1-heptene P 4/87C 7.H 14. 0. 0.G 200.000 6000.000 C 98.18606 1  
 2.00329343E+01 3.01875580E-02-9.96912897E-06 1.59376458E-09-9.64314031E-14 2  
 -1.70512608E+04-7.66778730E+01 8.70539860E+00 2.80074488E-03 1.55206000E-04 3  
 -2.09014025E-07 8.40505778E-11-1.12661494E+04-4.46493550E+00-7.54824999E+03 4

291-64-5

C7H14 CYCLOHEPTANE SIGMA=2 IAIBIC=39.1E+114 NU=2925(7),2860(7),1467,1450,  
 1446,1440,1430(3),1360,1350,1310(3),1285(2),1230(3),1210,1200(2),1125,1100,1040,  
 1020,1005(2),950,915,850,830,810,800,735,690,650,513,490,400,335,320,273,186,123  
 HF298=-118.2 KJ REF=Dorofeeva, Gurvich & Jorish (1986) Max Lst Sq Error Cp @  
 200 K \*\*1.1%\*\* CALCULATED DATA DO NOT AGREE WELL WITH THE ORIGINAL DATA.  
 C7H14 CY-HEPTANE T 2/95C 7H 14 0 OG 200.000 6000.000 D 98.18816 1  
 0.14662282E+02 0.41924851E-01-0.15223369E-04 0.24749860E-08-0.14888013E-12 2  
 -0.22745683E+05-0.60364838E+02 0.31165462E+01 0.12618947E-01 0.15692523E-03 3  
 -0.21682238E-06 0.87851529E-10-0.16705601E+05 0.13720905E+02-0.14216111E+05 4

Table 4 (continued)

3356-67-0

N-C7H15 N-HEPTYL RADICAL TRC 10/83 DATA TO 3000 K EXTRAPOLATED USING WILHOIT'S POLYNOMIALS. HF298=4.38 kJ HF0=41.73 kJ MAX LST SQ ERROR CP @ 400 K 0.69%.

C7H15,n-heptyl	P10/83C	7.H 15.	0.	0.G	200.000	6000.000	C	99.19400	1
1.62821576E+01	4.05173319E-02	-1.47864964E-05	2.41765375E-09	-1.45777261E-13					2
-7.70462623E+03	-5.42048086E+01	1.02804605E+01	7.01556769E-04	1.59552077E-04					3
-2.09594137E-07	8.33449128E-11	-3.60308958E+03	-1.03021411E+01	5.27992630E+02					4

59229-47-9 ??

C7H15 3,3-Di-Methyl-1 Pentyl Radical [C2H5C(CH3)2CH2CH2\*] SIGMA=108 Estimated Using the Bozzelli-THERM Prog. Extrapolated Using Wilhoit's Polynomials 1x[C/C4]; 4x[C/C/H3]; 2x[C/C2/H2]; H bond =-101.10 kcal HF298=-1.16 kcal Max Lst Sq Error Cp @ 1500 K 0.37%

C7H15 NEOHEPTYL	T10/99C	7.H 15.	0.	0.G	298.150	5000.000		99.19610	1
1.88589786E+01	3.77585789E-02	-1.41626975E-05	2.49291206E-09	-1.66770014E-13					2
-9.91845317E+03	-7.30310151E+01	1.75482995E+00	5.73984184E-02	3.09997695E-05					3
-8.42656048E-08	3.87583179E-11	-3.78376835E+03	2.20874184E+01	-5.83731332E+02					4

N/A

C7H15 3,3-Di-Methyl-2-Pentyl Radical [C2H5C(CH3)2CH\*CH3] SIGMA=162 Estimated Using the Bozzelli-THERM Prog. Extrapolated Using Wilhoit's Polynomials 1x[C/C4]; 4x[C/C/H3]; 2x[C/C2/H2]; H bond =-98.45 kcal HF298=-3.81 kcal Max Lst Sq Error Cp @ 1500 K 0.41%

C7H15 NEOHEPTYL-2	T10/99C	7.H 15.	0.	0.G	298.150	5000.000	E	99.19610	1
1.81240700E+01	3.84586055E-02	-1.45182003E-05	2.56761683E-09	-1.72327022E-13					2
-1.11163386E+04	-7.02350695E+01	2.09191664E+00	5.73477687E-02	1.54926142E-05					3
-5.34013030E-08	2.27869264E-11	-5.13199239E+03	1.95330456E+01	-1.91725550E+03					4

N/A

C7H15O Neo-HEPTANOL Radical 3,3,-dimethyl-1-pentanoxy radical C2H5C(CH3)2CH2CH2-O\* Estimated Using Bozzelli's THERM program and extrapolated to 5000 K using Wilhoit's polynomials. SIGMA=54 HF298=-34.00 kcal Max Lst Sq Error Cp @ 1000 K 0.54%.

C7H15O 3,3-dimet	T10/99C	7.H 15.O	1.	0.G	298.150	5000.000	E	115.19550	1
2.09858953E+01	3.85709050E-02	-1.46086654E-05	2.59555359E-09	-1.75052645E-13					2
-2.75558714E+04	-9.67484012E+01	1.76386765E-01	7.26245771E-02	2.14651033E-07					3
-5.23551849E-08	2.64458952E-11	-2.03008094E+04	1.71949368E+01	-1.71093666E+04					4

142-82-5

C7H16 liquid n-heptane REF=TRC 10/75 HF298=-224.35 kJ {HF298=-223.845+/-0.7 kJ REF=ATcT A} Max Lst Sq Error Cp @ 200 K 0.04%.

C7H16(L) n-hept	P10/75C	7.H 16.	0.	0.C	182.580	380.000	C	100.20194	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
0.00000000E+00	0.00000000E+00	6.98058594E+01	-6.30275879E-01	3.08862295E-03					3
-6.40121661E-06	5.09570496E-09	-3.68238127E+04	-2.61086466E+02	-2.69829491E+04					4

142-82-5

C7H16 N-HEPTANE TRC 10/85 VALUES EXTRAPOLATED THROUGH WILHOIT'S POLYNOMIALS HF298=-187.78 kJ HF0=-145.88 kJ {HF298=-187.277+/-0.7 kJ REF=ATcT A} MAX LST SQ ERROR Cp @ 200 K 0.75%.

C7H16 n-heptane	P10/85C	7.H 16.	0.	0.G	200.000	6000.000	C	100.20194	1
2.04565203E+01	3.48575357E-02	-1.09226846E-05	1.67201776E-09	-9.81024850E-14					2
-3.25556365E+04	-8.04405017E+01	1.11532994E+01	-9.49419773E-03	1.95572075E-04					3
-2.49753662E-07	9.84877715E-11	-2.67688904E+04	-1.59096837E+01	-2.25846141E+04					4

Table 4 (continued)

C7H16 IsoHeptane 2-methyl-heptane TRC 10/85 DATA to 1500 K extrapolated using Wilhoit's polynomials HF298=-194.6 kJ HF0=-150.40 kJ Max Lst Sq Error Cp @ 200 K 0.44%.

C7H16 ISOHEPTANE	P10/85C	7.H 16.	0.	0.G	200.000	6000.000	C 100.20194	1
1.13546228E+01	5.10820304E-02	-1.80753140E-05	2.28279573E-09	-1.03734486E-13				2
-2.99353806E+04	-3.10112766E+01	4.22047542E+00	3.93948706E-02	7.53934996E-05				3
-1.24221160E-07	5.17527152E-11	-2.68592255E+04	1.24262933E+01	-2.34048669E+04				4

562-49-2

C7H16 NEOHEPTANE 3,3 Di-Methyl-Pentane Estimated Using the Bozzelli-THERM Prog Extrapolated Using Wilhoit's Polynomials 1x[C/C4]; 4x[C/C/H3]; 2x[C/C2/H2]; SIGMA=324 HF298=-50.16 kcal [NIST 94 HF298=-46.89 kcal] Max Lst Sq Error Cp @ 1500 K 0.34%

C7H16 NEOHEPTAN	T10/99C	7.H 16.	0.	0.G	298.150	5000.000	E 100.20404	1
1.89468643E+01	4.04407738E-02	-1.51815251E-05	2.67111667E-09	-1.78560754E-13				2
-3.48922658E+04	-7.70247830E+01	1.55493237E+00	5.93804185E-02	3.04203450E-05				3
-8.22181963E-08	3.74203901E-11	-2.84682415E+04	2.02705469E+01	-2.52414153E+04				4

111-70-6

C7H15OH n-HEPTANOL REF=Stull Westrum & Sinke Extrapolated Using Wilhoit's Polynomials to 5000 K. HF298=-81.2+/-0.39 kcal REF=NIST 1998, (Cox & Pilcher) Max Lst Sq Error Cp @ 1000 K 0.54%.

C7H15OH Normal	T12/98C	7.H 16.O	1.	0.G	298.150	5000.000	E 116.20344	1
1.92489075E+01	4.21234021E-02	-1.57734301E-05	2.77888406E-09	-1.86276082E-13				2
-5.06734146E+04	-6.88916894E+01	3.19682451E+00	6.26125522E-02	7.79555247E-06				3
-4.69733504E-08	2.13096626E-11	-4.45833633E+04	2.09286236E+01	-4.08611933E+04				4

19264-94-9

C7H15OH Neo-Heptanol 3,3,-dimethyl-1-pentanol C2H5C(CH3)2CH2CH2-OH Estimated Using Bozzelli's THERM program and extrapolated to 5000 K using Wilhoit's polynomials. SIGMA=54 HF298=-85.96 kcal Max Lst Sq Error Cp @ 1000 K 0.54%.

C7H15OH 3,3-dime	T10/99C	7.H 16.O	1.	0.G	298.150	5000.000	E 116.20344	1
2.15383565E+01	3.99202307E-02	-1.50184640E-05	2.65913985E-09	-1.78970510E-13				2
-5.39238700E+04	-8.57361104E+01	1.09102491E+00	7.20016043E-02	3.94354014E-06				3
-5.62818094E-08	2.79018977E-11	-4.67188295E+04	2.65734430E+01	-4.32565046E+04				4

88053-51-4

C8H RAD Values calculated using Bozzelli & Ritter's program from C8H2 EXTRAPOLATED USING WILHOIT'S POLYNOMIALS HF298=1162.06 KJ Max Lst Sq Error Cp @ 500 K 0.16%

C8H	T 2/92C	8H	1	0	OG	298.150	5000.000	E 97.09594	1
0.17422244E+02	0.66413688E-02	-0.22557166E-05	0.36657347E-09	-0.23188722E-13				2	
0.13376514E+06	-0.59275082E+02	0.34566807E+01	0.65220393E-01	-0.98141367E-04				3	
0.72046762E-07	-0.20447036E-10	0.13656779E+06	0.77719815E+01	0.13976290E+06				4	

6165-96-4

C8H2 OCTATETRAYNE Calculated using Stein's coefficients J.Phys.Chem 89 (1985) p.3714 BY THE NIST PROGRAM 1991 HF298=223.3 KCAL REF=Kiefer, Sidhu, Kern, Xie, Chen, & Harding 1992. Max Lst Sq Error Cp @ 1200 K 0.25 %

C8H2	T 2/92C	8H	2	0	OG	298.150	5000.000	E 98.10388	1
0.17007524E+02	0.93656848E-02	-0.30485718E-05	0.47653534E-09	-0.29169032E-13				2	
0.10628021E+06	-0.59224564E+02	0.12470437E+01	0.78392526E-01	-0.12416148E-03				3	
0.98381697E-07	-0.30063943E-10	0.10942891E+06	0.16048227E+02	0.11236828E+06				4	

Table 4 (continued)

536-74-3

C8H6 PHENYL-ACETYLENE C6H5CCH SIGMA=2 IA=14.5382 IB=54.405 IC=68.943  
 NU=3271,3032,3028,3019,3009,3000,2150,1614,1586,1488,1437,1312,1190,1166,1159,  
 1087,1056,1008,1007,985,973,938,855,767,736,729,696,687,610,549,525,448,404,370,  
 160.4,142.4 REF=C. MELIUS DATABASE BAC/MP26 #116 P80H HF298=78.43 KCAL Max Lst  
 Sq Error Cp @ 200 K 0.68%

C8H6 C6H5CCH	T 9/96C	8H	6	0	OG	200.000	6000.000	B	102.13564	1
0.15638086E+02	0.22068432E-01	0.80253111E-05	0.13065013E-08	0.78679279E-13						2
0.32272867E+05	0.59610868E+02	0.87234720E+00	0.51839614E-01	0.66079738E-05						3
-0.55950961E-07	0.29284749E-10	0.37461628E+05	0.29096304E+02	0.39467283E+05						4

271-89-6

C8H6O BENZOFURAN SIGMA=1 STATWT=1 IA=21.4215 IB=50.6564 IC=72.07798  
 NU=3291,3263,3219,3205,3195,3183,1670,1642,1592,1518,1493,1403,1372,1297,1287,  
 1203,1180,1161,1129,1067,1037,977,937,912,870,868,864,782(2),763,749,621,598,  
 583,549,432,408,255,221 HF298=17.0 kJ HF0=37.048 kJ REF=Zhu & Bozzelli  
 JPCRD 32, (2003), 1713 {HF298=3.25+/-0.2 kcal REF=NIST 2002, Steele & Chirico  
 1990 Report NIPEP-457} Max Lst Sq Error Cp @ 200 K 0.96%

C8H6O Benzofuran	T03/04C	8.H	6.O	1.	O.G	200.000	6000.000	B	118.13264	1
1.61267559E+01	2.42942790E-02	8.82919089E-06	1.43722155E-09	8.65592465E-14						2
-5.74867958E+03	-6.40564836E+01	-7.85221476E-01	3.96432449E-02	5.69751746E-05						3
-1.14831806E-07	5.19411145E-11	2.15748538E+02	3.02655928E+01	2.04461838E+03						4

255-37-8

C8H6O2 2,3-BENZODIOXIN SIGMA=2 STATWT=1 IA=27.43536 IB=65.59405 IC=93.02894  
 NU=3276,3256,3219,3212,3204,3192,1763,1661,1652,1542,1502,1400,1357,1336,1306,  
 1233,1186,1180,1123,1099,1063,1030,966,931,915,867,857,826,765,755,751,693,585,  
 559,544,498,490,464,387,295,175,78 HF298=-71.2+/-6. kJ HF0=-49.95 kJ  
 REF=Zhu & Bozzelli JPCRD 32, (2003), 1713-1735 Max Lst Sq Error Cp @ 200 K 0.71%  
 Cp @ 1300 K 0.53%.

C8H6O2	T02/04C	8.H	6.O	2.	O.G	200.000	6000.000	B	134.13204	1
1.83621284E+01	2.50459070E-02	9.11651752E-06	1.48553005E-09	8.95329256E-14						2
-1.71240005E+04	-7.46170206E+01	-7.84950560E-01	5.20348763E-02	3.21241586E-05						3
-9.12264124E-08	4.35398430E-11	-1.07661879E+04	3.00336443E+01	-8.56334288E+03						4

95-15-8

C8H6S BENZOTHIOPHENE SIGMA=1 IAIBIC=1.6013E-112 EXPERIMENTAL DATA OF ENTHALPY  
 AND ENTROPY 298-700 K EXTRAPOLATED TO 5000 K USING WILHOITS POLYNOMIALS  
 REF=Chirico, Knipmeyer Nguyen & Steele J. Chem. Thermodynamics 23 (1991), 759  
 HF298=39.74 KCAL REF= Pedley, Naylor & Kirby 1986

C8H6S	T12/93C	8H	6S	1	OG	298.150	5000.000	D	134.20164	1
0.22676902E+02	0.21225910E-01	0.92726789E-05	0.17966329E-08	0.12813338E-12						2
0.89624565E+04	-0.10207224E+03	0.21269350E+02	-0.94299806E-01	0.35966814E-03						3
-0.39367785E-06	0.14307548E-09	0.15380490E+05	-0.65269994E+02	0.19997830E+05						4

N/A

C8H7 STYRENE RADICAL C6H5CH=CH\* REF=Melius Average of data CIS and TRANS equiv  
 of 50-50% mixture SIGMA=2 STATWT=2 IA 16.14 IB=52.3224 IC=68.4804  
 I(red)= 1.6096 V2=4.67 kcal ROSYM=2. NU=3067,3023,3016,3006,2997,2992,  
 2941,1501,1487,1451,1426,1369,1292,1245,1188,1146,1124,1114,1028,971,930,918,  
 899,888,845,797,771,727,701,633,589,578,529,423,418,372,218,205. HF298=93.0 kcal  
 REF=NIST 94 Max Lst Sq Error Cp @ 200 K 0.75%

STYRENE RADICAL	T 2/99C	8.H	7.	0.	O.G	200.000	6000.000	B	103.14358	1
1.80458471E+01	2.21498794E-02	8.05082743E-06	1.30961070E-09	7.88615885E-14						2
3.87090843E+04	-7.17917960E+01	-8.85283632E-01	5.61565120E-02	1.16600084E-05						3
-6.99146159E-08	3.63590274E-11	4.45850990E+04	2.97497087E+01	4.67991499E+04						4



Table 4 (continued)

120-72-9

C8H7N INDOLE (1-BENZAZOLE, 2,3-BENZAPYRROLE) IAIBIC=80998.5 NU=3520,3140,3083(2),3068(2),1617,1578,1510,1489,1458,1410,1348,1300,1275,1245,1205,1150,1122,1082,1068,1015,968,930,900,869,860,800,762,761,738,715,625,608,575,544,428,400(2),240,208 HF298=156.5+/-1.25 KJ REF=Das, Frenkel, Gadalla, Kudchadker, Marsh, Rodgers & Wilhoit JPCRD 22 (1993), 658 Max Lst Sq Error Cp @ 200 K 0.88%

C8H7N INDOLE	T03/95C	8H	7N	1	OG	200.000	6000.000	B	117.15032	1
0.17162122E+02	0.26048457E-01	0.94598392E-05	0.15390002E-08	0.92648224E-13						2
0.10577803E+05	0.69871764E+02	0.14144508E+01	0.48636966E-01	0.43663151E-04						3
-0.10447498E-06	0.48786402E-10	0.16880142E+05	0.32418878E+02	0.18822516E+05						4

277-10-1

C8H8 CUBANE Pentacyclo[4.2.0.0.0.0]Octane SIGMA=24 STATWT=1 IA=IB=IC=24.6449 NU=614.9(2),666.2(3),822.2(3),826.7(3),836.8(3),882.4(2),972,1028,1082.9(3),1111.4(2),1150.2(3),1170.7(2),1235.6(3),1260.7(3),2927.9,2937.5(3),2946(3),2963.5 HF298=155.755 Kcal REF=C. Melius Database of BAC/MP4 data. Private Comm. RK66 {HF298=148.7 kcal Kybett et al JACS 88 (1966), 626.} Max Lst Sq Error Cp @ 200 K \*\*\*2.8 %\*\*\*.

C8H8 CUBANE	T12/94C	8H	8	0	OG	298.150	6000.000	C	104.15152	1
0.16107210E+02	0.27423168E-01	0.10053212E-04	0.16453491E-08	0.99448320E-13						2
0.69973199E+05	0.72553695E+02	0.24663483E+01	0.23435851E-01	0.14037784E-03						3
-0.22354648E-06	0.97222204E-10	0.77230359E+05	0.35253221E+02	0.78381028E+05						4

100-42-5

C8H8 STYRENE C6H5CH=CH2 SIGMA=2 CALCULATED USING TRC 4/89 DATA EXTRAPOLATED WITH WILHOIT'S POLYNOMIALS. HF298=148.3 kJ HF0=169.66 kJ {HF298=147.9+/-1.5 kJ REF=Pedley Naylor & Kirby} Max Lst Sq Error Cp @ 200 K 0.95%

C8H8,styrene	P 4/89C	8.H	8.	0.	OG	200.000	6000.000	C	104.14912	1
1.39192973E+01	2.94553961E-02	1.02697803E-05	1.31095793E-09	6.16742309E-14						2
1.09344570E+04	4.97233295E+01	1.18176309E+00	3.34877555E-02	6.92369418E-05						3
-1.24490988E-07	5.49387246E-11	1.56039775E+04	2.26626016E+01	1.78362886E+04						4

N/A

C8H9 C6H5CH2CH2 RADICAL SIGMA=1 STATWT=2 IA=17.6647 IB=55.7930 IC=69.4678 IR(CH2)=0.29186 ROSYM=2 (V3=1050 cm-1 est.) IR(-C2H4)=3.9049 ROSYM=2 (V(3)=1050. cm-1 est.) Nu= 3276,3208,3196,3188,3178,3174,3167,3016,2953,1665,1644,1546,1502,1488,1482,1376,1364,1347,1226,1214,1198,1192,1110,1103,1060,1020,1018,994,967,921,866,862,783,755,715,636,574,489,468,418,372,277,163 HF298=237.714 kJ REF=BURCAT G3B3 calc {HF298=60.35 kcal REF=C. MELIUS DATABASE BAC/MP26 #175 AA1B} Max Lst Sq Error Cp @ 200 K 0.7 %.

C8H9 C6H5CH2CH2*	A11/04C	8.H	9.	0.	OG	200.000	6000.000	B	105.15706	1
1.61326962E+01	2.82904273E-02	1.01801876E-05	1.64176637E-09	9.81375329E-14						2
2.08791061E+04	6.00115413E+01	7.33299107E-01	4.59053158E-02	3.78257231E-05						3
-9.12367411E-08	4.25589678E-11	2.61572945E+04	2.50411074E+01	2.85902549E+04						4

Table 4 (continued)

100-41-4

C8H10 ETHYL BENZENE C6H5C2H5 SIGMA=1 IA=18.5059 IB=57.7802 IC=69.6147  
 Ir(C2H5)=4.3931 ROSYM=2 (V(3)=3 kcal est.) Ir(CH3)=0.52372 ROSYM=3 V(3)=  
 ibid. NU=3207,3194,3385,3172,3170,3122,3117,3077,3048,3043,1666,1644,1548,1538,  
 1527,1518,1502,1438,1375,1372,1362,1288,1235,1214,1192,1131,1093,1068,1059,1018,  
 993,979,964,920,861,800,787,768,716,637,568,501,418,359,312,225 REF=Burcat G3B3  
 HF298=7.12+/-0.2 kcal REF=Prosen Gillemont Rossini J. Res NBS 34, (1945),65  
 {HF298=7.222 HF0=14.05 kcal REF=Burcat G3B3; HF298=7.0 KCAL REF=NIST 94;  
 HF298=7.15 kcal REF TRC 10/86} Max Lst Sq Error Cp @ 200 K 0.81%.  
 C8H10 C6H5C2H5 A11/04C 8.H 10. 0. 0.G 200.000 6000.000 B 106.16500 1  
 1.56901336E+01 3.23663075E-02-1.16864578E-05 1.88989562E-09-1.13201791E-13 2  
 -4.38669907E+03-6.04442403E+01 1.24076722E+00 3.59132829E-02 7.54222474E-05 3  
 -1.31904301E-07 5.74746803E-11 1.18391719E+03 2.24682133E+01 3.58290266E+03 4

106-42-3

C8H10 1,4-DIMETHYLBENZENE p-Xylene REF=DRAEGER AND SCOTT DATA EXTRAPOLATED  
 THROUGH WILHOIT'S POLYNOMIALS HF298=18.03 KJ MAX LST SQ ERROR CP @ 1300  
 \*\*\* 1.12 % \*\*\*.  
 C8H10 L 2/84C 8H 10 0 0G 300.000 5000.000 B 106.16699 1  
 0.15268401E 02 0.34433573E-01-0.13685810E-04 0.21177802E-08-0.11564062E-12 2  
 -0.61602461E 04-0.59529587E 02-0.16422014E 01 0.58058664E-01 0.55675910E-05 3  
 -0.45693085E-07 0.21727536E-10 0.10412372E 03 0.34509140E 02 0.21641684E+04 4

280-33-1

C8H14 Bicyclo [2,2,2] Octane HC(-CH2CH2-)3CH SIGMA=6 STATWT=1 IA=34.10482  
 IB=35.11210 IC=35.113892 NU=3089.5(2),3082,3064(3),3061,3055,3046(2),3039,  
 3033(2),3031,1553,1531(2),1526,1511.6(2),1404(2),1395,1379,1368(2),1353.5(2),  
 1316.6(2),1275,1272,1271,1175.8(2),1148,1127(2),1073,1040,998,970(2),935,881(2),  
 837,832,803(2),794,639,511,508,376,371,278,271,50 REF=B3LYP/6-31G(d)  
 HF298=-99.04+/-1 kJ HF298(S)=-147.1+/-0.85 kJ REF=Wong & Westrum JACS 93 (1971),  
 5317-5321. Max Lst Sq Error Cp @ 6000 K 0.67%.  
 C8H14 Bicyclo T08/04C 8.H 14. 0. 0.G 200.000 6000.000 C 110.19676 1  
 1.40064576E+01 4.47140230E-02-1.61213297E-05 2.60903788E-09-1.56460968E-13 2  
 -2.05566449E+04-5.89457140E+01 3.73260509E+00-3.32416293E-03 2.11532465E-04 3  
 -2.78026304E-07 1.11137125E-10-1.42481792E+04 1.19565514E+01-1.19111385E+04 4

N/A

C8H15 1-OCTEN-4-YL CH2=CHCH2CH\*C4H9 Estimated using NIST-94. EXTRAPOLATED from  
 1600 K USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1500 K 0.38%  
 HF298=109.1 KJ  
 C8H15 1-octenyl- T 3/00C 8.H 15. 0. 0.G 298.150 5000.000 D 111.20710 1  
 1.86031870E+01 4.07347321E-02-1.52146579E-05 2.66612666E-09-1.77710586E-13 2  
 3.77573497E+03-6.42994408E+01 3.96580128E+00 5.00731521E-02 4.58633610E-05 3  
 -9.55246040E-08 4.20968508E-11 9.47734142E+03 1.90962113E+01 1.31216392E+04 4

111-66-0

C8H16 1-OCTENE TRC 4/87 DATA EXTRAPOLATED THROUGH WILHOIT'S POLYNOMIALS.  
 HF298=-83.59 kJ HF0=-42.77 MAX LST SQ ERROR CP @ 200 K 0.72 %.  
 C8H16,1-octene P 4/87C 8.H 16. 0. 0.G 200.000 6000.000 C 112.21264 1  
 2.43378771E+01 3.22574569E-02-1.03389736E-05 1.65359772E-09-1.00909018E-13 2  
 -2.14383953E+04-9.82405127E+01 1.01483726E+01 1.25438065E-03 1.85245518E-04 3  
 -2.49087148E-07 1.00247926E-10-1.43267638E+04-8.51901783E+00-1.00535089E+04 4

Table 4 (continued)

292-64-8

C8H16 CYCLOOCTANE REF=Dorofeeva Gurvich Jorish JPCRD 15 (1986),437 Original  
Data extrapolated 1600-6000 K using Wilhoit's Polynomials HF298=-124.4+/-1. kJ  
HF0=-72.762 kJ SIGMA=16 Max Lst Sq Error Cp @ 200 K \*\*1.2%\*\* H-Href @ 1300 K  
\*\*1.2%.

C8H16 CYOCTANE	T11/03C	8.H 16.	0.	0.G	200.000	6000.000	D 112.21264	1
1.62542931E+01	4.84250119E-02	-1.75498690E-05	2.85644879E-09	-1.72185344E-13				2
-2.46997499E+04	-6.86502145E+01	6.82277998E+00	-1.12425965E-02	2.39077016E-04				3
-3.05326267E-07	1.20482767E-10	-1.80620391E+04	4.18369785E-01	-1.49617957E+04				4

53358-92-2

N-C8H17 N-OCTYL RADICAL TRC 8/83 DATA TO 3000 K EXTRAPOLATED TO 6000 K USING  
WILHOIT'S POLYNOMIALS. HF298=-16.32 kJ HF0=+25.98 kJ MAX LST SQ ERROR Cp @ 400  
K 0.70%

C8H17,n-octyl	P10/83C	8.H 17.	0.	0.G	200.000	6000.000	C 113.22058	1
1.86450501E+01	4.61979656E-02	-1.68984763E-05	2.76916444E-09	-1.67267916E-13				2
-1.13918705E+04	-6.50893485E+01	1.18083058E+01	-8.50351988E-04	1.87698558E-04				3
-2.45691825E-07	9.75817486E-11	-6.66453488E+03	-1.47299161E+01	-1.96283365E+03				4

111-65-9

n-OCTANE Liquid, DATA TAKEN FROM TRC 10/84 HF298(L)=-250.260 kJ HF0=-227.11 kJ  
{HF298=-249.659+/-0.8 kJ REF=ATcT A} Max Lst Sq Error Cp @ 250 K 0.04%.

C8H18(L),n-octan	P10/84C	8.H 18.	0.	0.C	216.370	400.000	C 114.22852	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2
0.00000000E+00	0.00000000E+00	9.37687938E+01	-8.58272117E-01	3.94831328E-03				3
-7.58573055E-06	5.41151011E-09	-4.23546607E+04	-3.54100158E+02	-3.00991880E+04				4

111-65-9

C8H18 NORMAL OCTANE TRC 4/85 DATA EXTRAPOLATED THROUGH WILHOIT'S POLYNOMIALS  
HF298=-208.75 kJ HF0=-161.89 {-208.153+/-0.8 kJ REF=ATcT A} MAX LST SQ ERROR  
Cp @ 200 K 0.73%.

C8H18,n-octane	P 4/85C	8.H 18.	0.	0.G	200.000	6000.000	C 114.22852	1
2.09430708E+01	4.41691018E-02	-1.53261633E-05	2.30544803E-09	-1.29765727E-13				2
-3.55755088E+04	-8.10637726E+01	1.25245480E+01	-1.01018826E-02	2.21992610E-04				3
-2.84863722E-07	1.12410138E-10	-2.98434398E+04	-1.97109989E+01	-2.51067110E+04				4

540-84-1

C8H18 liquid ISOCTANE DATA TAKEN FROM TRC 10/82 HF298=-61.941 kcal Max Lst  
Sq Error Cp @ 220 K 0.03%.

C8H18(L) isooct	L10/82C	8.H 18.	0.	0.C	165.790	380.000	C 114.22852	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2
0.00000000E+00	0.00000000E+00	1.75199280E+01	1.57483711E-02	7.35946809E-05				3
-6.10398277E-10	4.70619213E-13	-3.77423257E+04	-6.83211023E+01	-3.11696059E+04				4

540-84-1

C8H18 2,2,4 TRIMETHYLPENTANE TRC 4/85 DATA EXTRAPOLATED THROUGH WILHOIT'S  
POLYNOMIALS HF298=-224.01 kJ HF0=-171.54 kJ {HF298=-223.63+/-1.5 kJ  
REF=ATcT A} MAX LST SQ ERROR Cp @ 6000K 0.30% . HF298=-53.54 KCAL

C8H18, isooctane	P 4/85C	8.H 18.	0.	0.G	200.000	6000.000	C 114.22852	1
1.76160941E+01	5.13323108E-02	-1.65307266E-05	2.43232275E-09	-1.35572757E-13				2
-3.63461118E+04	-6.86446285E+01	8.15741071E-01	7.32647307E-02	1.78301503E-05				3
-6.93592790E-08	3.21630852E-11	-3.04774255E+04	2.41511097E+01	-2.69420567E+04				4

Table 4 (continued)

78-00-2

C8H20Pb (C2H5)4Pb TetraEthylLead SIGMA=4 STATWT=1 IA=82.930649 IB=93.663540  
 IC=111.831153 (IR(CH3)=0.52328 ROSYM=3 V(3)=1077 cm-1)x4 NU=88.8,95.1,104,109.5  
 161,219,220,241,269.5,291,303,313,435,470,475,478,495,736,747.5,750,762,930,932,  
 934,940,993,994,997,1005,1125,1126(2),1128,1140,1142,1143.6(2),1194,1204,1208(2)  
 136(2),1370(2),1403,1405(2),1407(2),1410(2),1427,1433(2),1434,1469,3014(2),  
 3016.5(2),3040,3061,3064(2),3066,3068(2),3077,3081(2),3084(2),3155,3166,3168,  
 3175 HF298=109.6+/-5.1 kJ HF0=170.6 kJ HF298(liquid)=53.0+/-5  
 kJ REF=Webbook 2003 Max Lst Sq Error Cp @ 6000 K 0.52%  
 PB(C2H5)4 T 3/04C 8.H 20.PB 1. 0.G 200.000 6000.000 C 323.44440 1  
 2.44253155E+01 5.09078905E-02-1.79998968E-05 2.87408342E-09-1.70711773E-13 2  
 1.56186130E+03-1.01161029E+02 6.60546263E+00 6.31142954E-02 6.45009397E-05 3  
 -1.35534500E-07 6.13504836E-11 8.07613982E+03-7.66773249E-01 1.31817750E+04 4

148549-29-5

C9H4 C(CCH)4 TetraEthynylMetane SIGMA=12 STATWT=1 IA=56.117673 IB=56.133721  
 IC=56.207786 Nu= 3150,3148(3),2245,2230(3),1248(3),961(2),959(3),954(3),715,  
 647(3),627(2),481(3),254(3),188(2) REF=PM3 HF298=218.4 kcal REF=NIST 94 est  
 Max Lst Sq Error Cp @ 6000 K 0.48%  
 C9H4 C(CCH)4 T08/02C 9.H 4. 0. 0.G 200.000 6000.000 B 112.12806 1  
 1.64605249E+01 1.85278175E-02-6.71826859E-06 1.09151934E-09-6.56382337E-14 2  
 1.02991510E+05-6.20998849E+01-1.53821821E+00 7.49142471E-02-7.09672930E-05 3  
 2.98881245E-08-3.00090544E-12 1.07601282E+05 2.91040591E+01 1.09902520E+05 4

71551-80-9

C9H7 INDENYL RADICAL STATWT=2 SIGMA=1 IA=21.31 IB=51.988 IC=73.298 NU=3053,  
 3038,3029,3019,3008,2998,2992,1534,1508,1433,1422,1403,1325,1298,1249,1164,1150,  
 1128,1105,1046,1022,966,937,921,888,852,831,821,804,730,710,691,681,634,562,508,  
 507,490,383,367,222,184.9 HF298=68.26+/-5.22 KCAL REF=C. MELIUS DATABASE  
 BAC/MP26 #205 AAOK Max Lst Sq Error Cp @ 200 K 0.88 %  
 C9H7 INDENYL T 9/96C 9H 7 0 OG 200.000 6000.000 B 115.15458 1  
 0.18554959E+02 0.25035076E-01-0.91457509E-05 0.14934838E-08-0.90133030E-13 2  
 0.25721156E+05-0.76300347E+02-0.26698729E+01 0.62177216E-01 0.15067018E-04 3  
 -0.79645699E-07 0.40918972E-10 0.32386969E+05 0.37861193E+02 0.34349570E+05 4

91-22-5

C9H7N Quinoline BENZO[B]PYRIDINE 1-BEZAZINE SIGMA=1 IAIBIC=159000.4 E-117  
 NU=3074,3062,3048,3035,3017,3006,2980,1619,1595,1568,1500,1469,1431,1391,1370,  
 1312,1253,1216,1189,1140,1117,1093,1032,1012,976,968,952,938,903,864,802,785(2),  
 759,733,627,611,521,505,476,467,389,377,181,168. HF298=200.52+/-1.36 kJ  
 REF= Das et al JPCRD 22 (1993),659 Max Lst Sq Error Cp @ 200 K 0.88%  
 C9H7N QUINOLINE T 5/99C 9.H 7.N 1. 0.G 200.000 6000.000 B 129.16132 1  
 1.85755750E+01 2.79425650E-02-1.02522932E-05 1.67898241E-09-1.01528223E-13 2  
 1.51294620E+04-7.75919222E+01-1.13617529E+00 4.84964316E-02 5.58565955E-05 3  
 -1.20326645E-07 5.49530942E-11 2.20184652E+04 3.18686011E+01 2.41168752E+04 4

119-65-3

C9H7N ISO-QUINOLINE BENZO[C]PYRIDINE 2-BENZAZINE SIGMA=1 IAIBIC=160900.4 E-117  
 NU=3089,3060,3055(2),3025,3008,2990,1627,1587,1552,1497,1460,1432,1381,1377,  
 1315,1273,1255,1179,1140,1118,1095,1034,1013,985,970,959,942,930,831,823,800,  
 778,765,740,637,610,522,504,479,460,375,354,180,169. HF298=204.61+/-1.33 kJ  
 REF= Das et al JPCRD 22 (1993),659 Max Lst Sq Error Cp @ 200 K 0.88%  
 C9H7N ISOQUINOLI T 5/99C 9.H 7.N 1. 0.G 200.000 6000.000 B 129.16132 1  
 1.85146411E+01 2.79810705E-02-1.02625548E-05 1.68026025E-09-1.01589164E-13 2  
 1.56389099E+04-7.71926472E+01-8.22485356E-01 4.62854760E-02 6.07470671E-05 3  
 -1.24938487E-07 5.65402573E-11 2.24802772E+04 3.06200613E+01 2.46087863E+04 4

Table 4 (continued)

95-13-6

C9H8 INDENE SIGMA=1 IA=21.885 IB=52.67 IC=74.043 NU=3044,3022,3019,3007,  
2996,2989,2882,2857,1627,1610,1580,1462,1452,1428,1347,1302,1233,1211,1174,1142,  
1135,1100,1095,1054,999,992,974,954,937,910,874,832,802,776,724,706,697,576,544,  
516,420,385.5,368.6,205.1,189.9 HF298=39.23 KCAL REF=C. MELIUS DATABASE

BAC/MP26 #206 AA0J Max Lst Sq Error Cp @ 200 K 1.01%

C9H8 INDENE	T 9/96C	9H	8	0	OG	200.000	6000.000	B 116.16252	1
0.17318671E+02	0.28982768E-01	0.10605059E-04	0.17334553E-08	0.10467919E-12					2
0.11151429E+05	0.71555323E+02	0.68190289E+00	0.41658733E-01	0.70741234E-04					3
-0.13430875E-06	0.59915845E-10	0.17705036E+05	0.29781396E+02	0.19741190E+05					4

98-83-9

C9H10 ALFA-METHYLSTYRENE (BENZENE, 1-METHYLETHENYL-) DATA TO 1000 K FROM STULL  
WESTRUM & SINKE & NIST 1994 EXTRAPOLATED USING WILHOIT'S POLYNOMIALS. SIGMA=6  
HF298=27.0 KCAL Max Lst Sq Error Cp @ 400 K \*\*1.0%\*\* H @ 800 K 0.9%

C9H10	T 1/96C	9H	10	0	OG	298.150	5000.000	C 118.17840	1
0.18890862E+02	0.31553549E-01	0.12056696E-04	0.21436164E-08	0.14430356E-12					2
0.43332577E+04	0.75568080E+02	0.58431766E+01	0.17489030E-01	0.12112118E-03					3
-0.17951022E-06	0.75443868E-10	0.10316404E+05	0.36919595E+01	0.13586850E+05					4

20685-34-1

C9H12 TETRAVINYL METHANE C(CH=CH2)4 SIGMA=12 IA=44.8365353 IB=57.16084  
IC=66.20476 (IR=3.285879 ROSYM=2 V(2)=700. cm-1)x4 Nu=3146(2),3145(2),3133,  
3120,3128,3127,3038,3037,3034,3032,1863,1858,1854,1844,1357,1353,1345,1324,1298,  
1282,1273,1229,1203,1187,1153,1044,1036,1033,1029,1023,997,977,951,938,931,922,  
920,784,688,662,656,622,538,505,439,408,329,296,270,257,191 REF=PM3

HF298=59.9 kcal REF=NIST 94 est. Max Lst Sq Error Cp @ 6000 K 0.53%

C9H12	C(CH=CH2)4	T08/02C	9.H	12.	0.	0.G	200.000	6000.000	B 120.19158	1
1.88286650E+01	3.55743637E-02	1.27780689E-05	2.04613458E-09	1.21481701E-13						2
2.14164881E+04	7.08074676E+01	3.71153693E+00	5.90790308E-02	1.07786196E-05						3
-5.99861274E-08	2.99665527E-11	2.64195117E+04	1.14903545E+01	3.01426783E+04						4

108-67-8

C9H12 1-3-5-Tri-Methyl-Benzene, also Mesitylene DATA 200-1500 K from Dreager  
J. Chem. Thermo. 17, (1985), 263-275. Extrapolated to 5000 K using Wilhoit's  
polynomials. HF298=-3.84 kcal REF=Stull,Westroom & Sinke 1969. Max Lst sq Error  
Cp @ 1000 K 0.68%

C9H12	1-3-5-TMB	T 8/00C	9.H	12.	0.	0.G	200.000	5000.000	C 120.19428	1
1.67073078E+01	3.98877329E-02	1.54373742E-05	2.77050130E-09	1.87953017E-13						2
-1.09906566E+04	6.54478472E+01	3.70645582E+00	3.04050008E-02	9.36818016E-05						3
-1.42836230E-07	5.85223220E-11	4.96186950E+03	1.31400088E+01	1.93235200E+03						4

95-63-6

C9H12 1-2-4-Tri-Methyl-Benzene, DATA 200-1500 K from Dreager J. Chem. Thermo.  
17, (1985), 263-275. Extrapolated to 5000 K using Wilhoit's polynomials.

HF298=-3.33 kcal REF=NIST Webbook 2000. Max Lst sq Error Cp @ 1000 K 0.66%

C9H12	1-2-4-TMB	T 8/00C	9.H	12.	0.	0.G	200.000	5000.000	C 120.19428	1
1.71329238E+01	3.94083582E-02	1.52208685E-05	2.72757795E-09	1.84838202E-13						2
-1.07469624E+04	6.62588105E+01	5.36104527E+00	2.74614342E-02	9.27107834E-05						3
-1.37606888E-07	5.56796764E-11	5.06812567E+03	5.85157015E+00	1.67571150E+03						4

Table 4 (continued)

N/A

C9H17 1-NONENENYL-4/5 Estimated using NIST-94. EXTRAPOLATED from 1600 K  
 USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1500 K 0.38% HF298=88.4 KJ  
 C9H17 1-nonenyl-4 T 3/00C 9.H 17. 0. 0.G 298.150 5000.000 D 125.23398 1  
 2.10867922E+01 4.61782938E-02-1.72507130E-05 3.02355150E-09-2.01567606E-13 2  
 3.27938951E+01-7.58751351E+01 4.36832491E+00 5.77776115E-02 4.89429265E-05 3  
 -1.04595584E-07 4.61873643E-11 6.51405343E+03 1.91916207E+01 1.06320156E+04 4

124-11-8

C9H18 1-NONENE Estimated using NIST-94. EXTRAPOLATED from 1600 K  
 USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1500 K 0.36% HF298=-103.3 KJ  
 C9H18 1-nonene T 3/00C 9.H 18. 0. 0.G 298.150 5000.000 D 126.24192 1  
 2.18154890E+01 4.80370115E-02-1.79392300E-05 3.14265715E-09-2.09387787E-13 2  
 -6.30911726E+04-8.29167013E+01 2.62429422E+00 7.18302704E-02 1.92494510E-05 3  
 -7.29310566E-08 3.39150762E-11-5.59992986E+04 2.40905648E+01-5.19822816E+04 4

17088-37-8

C9H18O6 TriAcetoneTriPeroxide (TATP) CyclonanoRing; 33,66,99-hexamethyl-1,4,7-cyclonanotriperoxane SIGMA=6 STATWT=1 IA=127.0692 IB=130.3637 IC=200.50556  
 [Ir(CH3)=0.5249 ROSYM=3 V(3)=760. cm-1]x6 REF=MOPAC 2000 PM3 NU=3008(5),  
 3001(7),2947(6),1460(3),1447,1438(8),1377(3),1369(2),1363,1274(2),1234,1204(2),  
 1180(3),1140(3),946(2),938(2),885(2),863,843,784(4),615,574(2),554(2),549(2),  
 467(2),438(3),401(3),369(2),329(2),301(2),243(7) REF=IR from Jubert et al  
 J. Raman Spectro. 30,(1999),45 HF298=-94.52+/-5.3 kcal HF0=-79.23 kcal  
 REF=MOPAC 2000 PM3 {HF298=-115.92 kcal REF=THERGAS no cyclonanoring correcti.}  
 Max Lst Sq Error Cp @ 1300 K 0.55%  
 C9H18O6 TATP A07/05C 9.H 18.O 6. 0.G 200.000 6000.000 D 222.23562 1  
 3.51589772E+01 5.25727977E-02-1.89375944E-05 3.06266814E-09-1.83566557E-13 2  
 -6.29813917E+04-1.61393100E+02-1.19327224E+00 1.68949753E-01-1.71505444E-04 3  
 1.01467377E-07-2.60451321E-11-5.33905344E+04 2.32901330E+01-4.75640393E+04 4

32757-65-6

N-C9H19 N-NONYL RADICAL TRC 10/83 DATA TO 3000 K EXTRAPOLATED TO 6000 K  
 USING WILHOIT'S POLYNOMIALS. HF298=-37.03 kJ HF0=+10.23 kJ MAX LST SQ ERROR Cp  
 @ 400K 0.71 % H  
 C9H19,n-nonyl P10/83C 9.H 19. 0. 0.G 200.000 6000.000 C 127.24716 1  
 2.10145145E+01 5.18616211E-02-1.89952568E-05 3.11574043E-09-1.88328529E-13 2  
 -1.50809093E+04-7.60093216E+01 1.33309614E+01-2.35843645E-03 2.15714140E-04 3  
 -2.81626719E-07 1.11748345E-10-9.72551279E+03-1.91378729E+01-4.45365993E+03 4

111-84-2

C9H20 liq Nonane REF=I.Barin 1987 HF298liq=-275.475 kJ  
 C9H20(L) B01/00C 9.H 20. 0. 0.L 298.150 423.430 C 128.25780 1  
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2  
 0.00000000E+00 0.00000000E+00 3.41721095E+01 2.58204426E-04-6.96987194E-07 3  
 6.20423745E-10 0.00000000E+00-4.33267971E+04-1.47402676E+02-3.31318382E+04 4

111-84-2

N-C9H20 N-NONANE Bureau of Mines Bull 666 1974 DATA TO 1500. K EXTRAPOLATED  
 USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1500 K 0.72 %  
 HF298=-54.71 kcal  
 N-C9H20 NONANE T 5/99C 9.H 20. 0. 0.G 200.000 6000.000 B 128.25780 1  
 2.55877522E+01 4.60770651E-02-1.60860633E-05 2.58274408E-09-1.54734690E-13 2  
 -4.00748448E+04-1.04722466E+02 1.39840225E+01-1.17224978E-02 2.52316467E-04 3  
 -3.25680364E-07 1.29109135E-10-3.28258409E+04-2.38633750E+01-2.75309838E+04 4

Table 4 (continued)

1146-65-2

C10D8 NAPHTHALENE-D8 SIGMA=4 IA=32.0228 IB=76.0297 IC=108.0525 NU=2272,2257,1553,1386,1298,863,835,692,495,785,545,346,875,760,663,410,2302,2275,1604,1330,1030,929,830,490,800,653,507,177,2286,2258,1545,1258,1050,889,715,328,2289,2258,1439,1316,1082,880,825,593,791,628,404,163 REF=CHEN, KUDCHADKER AND WILHOIT  
MAX LST SQ ERROR CP @ 1300 K 0.85 %. HF298=118.05 KJ

C10D8	T 9/82C	10D	8	0	OG	300.000	5000.000	B 136.22281	1
	0.24693802E+02	0.25579888E-01	0.93010221E-05	0.14824513E-08	0.85934623E-13				2
	0.29915154E+04	0.11214200E+03	0.29223614E+01	0.80820084E-01	0.12762395E-04				3
	-0.52788202E-07	0.30022318E-10	0.11687422E+05	0.35703760E+02	0.13205407E+05				4

312310-99-9

C10H6 Naphthyne SYMNO = 1 Ia = 25.100753 Ib = 67.174194 Ic = 92.274938  
Nu = 3134,3133,3123,3110,3099,3095,1994,1610,1533,1410,1442,1401,1363,1326,1286,1212,1203,1154,1127,1089,1082,1020,949,916,890,844,842,780,767,734,701,677,562,544,499,489,407,398,384,359,196,165. REF = Curran Et al JPCRD 29, (2000),463 Hf(298)= 119.7 kcal/mole REF = Wang & Frenklach J. Phys. Chem. 98, (1994),11465. Max Lst Sq Error Cp @ 200 K 0.62%

C10H6 Naphtyne	T 7/98C	10.H	6.	0.	O.G	200.000	6000.000	B 126.15764	1
	1.87728941E+01	2.48768793E-02	9.09940935E-06	1.48730676E-09	8.98228135E-14				2
	5.15727443E+04	7.68608875E+01	1.50617131E+00	6.03325879E-02	1.09063952E-05				3
	-6.91994009E-08	3.54144371E-11	5.80261788E+04	3.24494940E+01	6.02350349E+04				4

10237-50-0

C10H7 Naphtyl radical STATWT = 2 Ia = 25.3426871 Ib = 68.4922226  
Ic = 93.8348672 Nu=3129,3119,3117,3107,3106,3094,3093,2623,1599,1548,1487,1446,1418,1384,1350,1339,1234,1218,1167,1146,1139,1106,1028,1017,949,925,913,898,857,830,775,760,753,742,705,609,588,508,490,489,444,386,347,181,166.  
REF = Curran Et al JPCRD 29, (2000),463 HF298=94.7 kcal REF = Wang & Frenklach J. Phys. Chem. 98, (1994),11465. Max Lst Sq Error Cp @ 200 K 0.81%.

C10H7 Naphtyl rad	T 7/98C	10.H	7.	0.	O.G	200.000	6000.000	B 127.16558	1
	1.83535073E+01	2.77474314E-02	1.00885968E-05	1.64229575E-09	9.89002001E-14				2
	3.89261241E+04	7.48978150E+01	1.89559772E+00	5.83077290E-02	2.79388931E-05				3
	-9.14375172E-08	4.46422302E-11	4.55409775E+04	3.52453263E+01	4.76546183E+04				4

182180-76-3

4-Ethenyl - Phenyl-1-Vinyl Radical C6H4(C2H)C2H2\* STATWT 2. Ia=31.301037  
Ib=54.020658 Ic=69.949573 Ir(-CH=CH())=2.73405 ROSYM=2 V(3)=4.4 kcal/mole  
Nu=3129,3119,3113,3111,3098,3097,3035,1932,1591,1487,1474,1368,1332,1321,1270,1257,1172,1154,1134,1117,1087,1021,1003,951,915,890,882,816,810,781,761,704,675,659,585,548,540,504,443,380,336,322,264,206. REF = Curran et al, JPCRD 29, (2000),463 Hf (298)=147.5 kcal/mole REF = Colomina et al, J. Chem. Thermo. 14, (1982),779. Max Lst Sq Error Cp @ 200 K 0.69%

C6H4(C2H)CH=CH*	T 8/98C	10.H	7.	0.	O.G	200.000	6000.000	B 127.16558	1
	2.00959894E+01	2.63995288E-02	9.54744190E-06	1.54881511E-09	9.30556695E-14				2
	6.51277376E+04	8.23946362E+01	2.07613880E+00	7.07561989E-02	2.27951149E-06				3
	-6.32032786E-08	3.52065658E-11	7.18269865E+04	3.55334903E+01	7.42244582E+04				4

Table 4 (continued)

33490-95-8

C10H7O Naphtoxy radical STATWT = 2 Ia = 42.113955 Ib = 75.532463  
 Ic = 117.64642 NU=3134,3132,3124,3114,3110,3099,3098,1598,1555,1545,1511,1479,  
 1431,1419,1366,1353,1275,1234,1210,1151,1134,1116,1068,1044,1019,964,942,933,  
 866,865,855,787,767,747,706,701,639,563,524,516,458,453,445,401,279,225,167,120.  
 REF = Curran et al, 29, (2000), 463 Hf(298)= 27.6 kcal REF = NIST 1994

Max Lst Sq Error Cp @ 200 K 0.7%

1-C10H7O* Radical T 7/98C 10.H 7.O 1. 0.G 200.000 6000.000 143.16498	1
2.10591364E+01 2.82563070E-02-1.03328686E-05 1.68867034E-09-1.01974767E-13	2
4.09143507E+03-8.84963398E+01-1.15176448E+00 6.11354512E-02 3.20151083E-05	3
-9.94285290E-08 4.79990043E-11 1.14058756E+04 3.25584836E+01 1.38887800E+04	4

275-51-4

C10H8 AZULENE SYGMA=2 IAIBIC=1.88E-112 NU=3070,1690,1634,1621,1577,1535,  
 1482,1442,1389,1367,1295,1290,1265,1201,1150,1114,1055,1045,1036,1007,978,963,  
 945,899,855,820,787,766,940,724,708,694,671,653,610,510,475,350,280,200,3070(7),  
 175 REF=KOVATS, GUNTARD & PLATTNER MAX LST SQ ERROR CP @ 1300 K 0.87 %.  
 HF298=66.9 KCAL REF=STULL WESTRUM & SINKE

H8C10 AZULENE T 9/82H 8C 10 0 0G 300.000 5000. B 128.1732	1
0.19087189E+02 0.28716661E-01-0.98752744E-05 0.14930039E-08-0.81601501E-13	2
0.24276551E+05-0.81975790E+02-0.48537226E+01 0.73454738E-01-0.38748985E-05	3
-0.53900077E-07 0.28514219E-10 0.31977461E+05 0.47005760E+02 0.33667889E+05	4

91-20-3

C10H8 Naphthalene SIGMA = 4 Ia = 26.8532 Ib = 67.4189 Ic = 94.2721  
 Nu= 3092,3090,3065,3060(2),3058,3030,3027,1628,1595,1577,1509,1463,1443,1389,  
 1380,1361,1265,1242,1209,1168,1145,1144,1125,1025,1008,980,970,958,950,936,  
 877,876,841,782,778,761,725,617,581,512,506,472,466,386,359,191,176.  
 REF = CHEN, KUDCHAKER & WILHOIT JPCRD 8, (1979), 527. Hf(298)= 35.99 kcal  
 REF = Colomina et al, J. Chem. Thermo. 14, (1982), 779. Max Lst Sq Error Cp  
 @ 200 K 0.96%

C10H8 Naphthalene T 7/98C 10.H 8. 0. 0.G 200.000 6000.000 B 128.17352	1
1.86129884E+01 3.04494175E-02-1.11224825E-05 1.81615474E-09-1.09601281E-13	2
8.91578988E+03-8.00230396E+01-1.04919475E+00 4.62970781E-02 7.07591636E-05	3
-1.38408111E-07 6.20475407E-11 1.59848987E+04 3.02121626E+01 1.81107678E+04	4

135-19-3

C10H7OH Naphtol Ia = 43.59471 Ib = 75.763548 Ic = 119.35822 Ir = 0.12236  
 ROSYM = 2 V(2) = 3.468 kcal NU = 3652, (3135), 3067, 2967, 2923, 2859, 1946,  
 1905, 1847, 1828, 1820, 1718, 1682, 1634, 1591, 1520, 1462, 1404, 1359, 1277, 1239, 1189, 1152,  
 1089, 1081, 1041, 1014, (943, 925, 894), 874, (848, 819), 790, 766, (742), 715, (704), 583, 570,  
 522, 479, 467, 459, (453, 411, 286, 255, 220, 170). REF = NIST Webbook 1997  
 Hf(298)= -7.36 kcal REF = Da Silva et al. J. Chem Thermo. 20, (1988), 969

Max Lst Sq Error Cp @ 1300 K 0.63%

NAPHTOL C10H8O I T 7/98C 10.H 8.O 1. 0.G 200.000 6000.000 144.17292	1
2.08930252E+01 3.10560066E-02-1.14407562E-05 1.87872866E-09-1.13823881E-13	2
-1.35886443E+04-8.88597101E+01-2.08768263E+00 7.68099506E-02-1.53593023E-05	3
-4.04657632E-08 2.33759779E-11-6.29056385E+03 3.43331051E+01-3.70367466E+03	4



Table 4 (continued)

N/A

C10H9 2-Hydro-Naphthalene Radical STATWT = 2 Ia = 27.990458 Ib = 71.911452  
 Ic = 99.39347 NU= 3126,3110,3106,3095,3093,3090,3082,2851,2843,1636,1575,1528,  
 1473,1430,1416,1397,1375,1353,1319,1260,1218,1185,1150,1137,1135,1112,1029,1016,  
 949,928,900,899,891,886,831,764,761,734(2),678,667,594,525,491,484,445,390,344,  
 256,169,125. REF =Curran et al, JPCRD 29, (2000),463 Hf(298)= 54.86 kcal/mole  
 REF = Marinov et al, Comb. Sci. Technol. 116-117, (1996), 211. Max Lst Sq Error  
 Cp @ 200 K 0.87%

C10H9 2-hydro Rad T 7/98C 10.H 9. 0. 0.G 200.000 6000.000 B 129.18146 1  
 1.96879334E+01 3.20520257E-02-1.16715110E-05 1.90182471E-09-1.14603906E-13 2  
 1.80099777E+04-8.29833882E+01-1.21356342E+00 5.48913745E-02 5.55281159E-05 3  
 -1.24860759E-07 5.75105005E-11 2.52575495E+04 3.28077928E+01 2.76064663E+04 4

N/A

C10H9 1-methyl-1-indenyl Radical SIGMA=1 STATWT=2 IA=32.0588 IB=66.8991  
 Ic=98.4347 Ir=0.549 ROSYM=3 V(3)=~760. cm-1 Nu=3227,3209,3198,3185,3173,  
 3168,3116,3055,3008,1633,1628,1504,1488,1476,1443,1438,1433,1387,1376,1312,1287,  
 1211,1186,1168,1102,1081,1036,1033,1019,987,952.950,895,876,863,794,765,756,733,  
 692,602,560,557,524,459,421,312,228,209,144 HF298=62.7 kcal REF=Lifshitz  
 Dubnikova JPC A 108, (2004),3430 DFT QCISD(T)//B3LYP/(cc-pVDZ) calc Max Lst Sq  
 Error Cp @ 200 K 0.73%.

C10H9 1-methyl A03/05C 10.H 9. 0. 0.G 200.000 6000.000 B 129.17846 1  
 1.90083931E+01 3.18459404E-02-1.15126596E-05 1.86706540E-09-1.12145139E-13 2  
 2.23250010E+04-7.80332683E+01 4.07035729E-01 4.80530672E-02 6.13610491E-05 3  
 -1.25042167E-07 5.63176095E-11 2.89729160E+04 2.60120139E+01 3.15516849E+04 4

536738-49-5

C10H9 1-Methenyl-Indene Radical SIGMA=1 STATWT=2 IA=31.7023 IB=66.6883  
 IC=93.8122 Ir=~0.2919 ROSYM=3 V(3)=~3880. cm-1 Nu=3255,3224,3197,3185,3174,  
 3167,3139,3102,1658,1642,1605,1488,1485,1432,1392,1342,1298,1284,1222,1198,1172,  
 1162,1128,1103,1074,1042,1003,996,964,957,947,889,867,809,778,756,745,727,614,  
 582,553,545,506,432,406,287,264,166,137 HF298=80.7+/-4-5 kcal REF=Lifshitz  
 Dubnikova JPC A 108, (2004),3430 DFT QCISD(T)//B3LYP/(cc-pVDZ) calc. Max Lst Sq  
 Error Cp @ 200 K 0.85%.

C10H9 1-methylen A03/05C 10.H 9. 0. 0.G 200.000 6000.000 B 129.17846 1  
 1.96314392E+01 3.20733859E-02-1.17484015E-05 1.91973968E-09-1.15848061E-13 2  
 3.10756124E+04-8.25158201E+01-1.20688639E+00 5.57000852E-02 5.32772173E-05 3  
 -1.23103519E-07 5.70934182E-11 3.82393435E+04 3.26628275E+01 4.06095849E+04 4

773148-91-7

C10H9 2-Methenyl-Indene SIGMA=1 STATWT=2 IA=22.8241 IB=84.2424 IC=101.8920  
 Ir=~0.2919 ROSYM=3 V(3)=~3880. cm-1 NU=3243,3205,3198,3186,3174,3167,3144,  
 3067,3144,3067,3031,1635,1614,1542,1501,1473,1424,1408,1393,1282,1215,1193,1179,  
 1160,1152,1113,1038,991,981,963,930,886,877,873,821,808,797,759,728,663,597(2),  
 546,488,469,448,427,278,269,199 HF298=63.7+/-4-5 kcal REF=Lifshitz Dubnikova  
 JPC A 108, (2004),3430 DFT QCISD(T)//B3LYP/(cc-pVDZ) calc. Polynomial not calc.

Table 4 (continued)

447-53-0

C10H10 1,2-Dihydro-Naphthalene SIGMA = 1 Ia = 29.06046 Ib = 72.379179  
 Ic = 98.883363 Nu = 3123,3108,3106,3092,3087,3082,3007,3000,2930,2915,1644,  
 1606,1572,1480,1446,1440,1429,1388,1353,1328,1311,1268,1216,1201,1180,1154,1151,  
 1141,1105,1037,1014,998,945,936,919,902,879,851,795,773,738,732,682,672,574,  
 540,490,472,408,376,343,258,148,131. REF = Curran et al JPCRD 29, (2000), 463.  
 Hf(298)= 28. Kcal REF = Pedley & Rylance 1977 Max Lst Sq Error Cp @ 6000 K  
 0.59%

1-2-C10H10	T 7/98C 10.H 10.	0.	0.G	200.000	6000.000	B 130.18940	1
1.92211178E+01	3.51247274E-02	-1.27719042E-05	2.07903232E-09	-1.25191968E-13			2
4.39595221E+03	-8.19390283E+01	-1.92135165E-01	4.50394780E-02	8.64482370E-05			3
-1.56640588E-07	6.88727900E-11	1.16587583E+04	2.82951960E+01	1.40900666E+04			4

N/A

C10H10 1,1'-BiCyclo-2,4-Pentadiene 1,1'-(C5H5)2 SIGMA=2 STATWT=1 IA=26.1914  
 IB=89.7022 IC=89.9448 Ir=12.1181 ROSYM=1 V(3)=524.6 cm-1 (same as biphenyl)  
 Nu=3247(2),3234(2),3219(2),3207(2),2992,2985,1662.5(2),1576(2),1420.5(2),1339,  
 1331,1311,1283,1209,1204,1145,1132,1121.5(2),1076,1045,1032,1015,1007,955(2),  
 952(2),926,880,857,823,813,803,781,727,719,698,656,561,548,398,304,246,129,98.2  
 REF=Burcat B3LYP calc HF298=291.625 kJ HF0=320.336 kJ REF=NIST 94 Max Lst  
 Sq Error Cp @ 200 K \*\*\*1.2%\*\*\*.

C10H10 1,1'-(C5H5)2A05/05C 10.H 10.	0.	0.G	200.000	6000.000	B 130.18640	1
1.96542923E+01	3.33886286E-02	-1.20413130E-05	1.94963753E-09	-1.16973259E-13		2
2.53473433E+04	-8.08051980E+01	1.92659259E+00	2.78897531E-02	1.32941165E-04		3
-2.10257150E-07	9.03339117E-11	3.24585081E+04	2.27839249E+01	3.50742016E+04		4

N/A

C10H10 2,2'-BiCyclo-2,4-Pentadiene 2,2'-(C5H5)2 SIGMA=2 STATWT=1 IA=19.6196  
 IB=104.5829 IC=121.4567 Ir=4.9592 ROSYM=1 V(3)=524.6 cm-1 (same as biphenyl)  
 NU=3049(2),3035,3032,3021(2),2879,2876,2852(2),1632,1621,1566,1553,1415,1412,  
 1357,1344,1312,1297,1244,1232,1185,1124.4(2),1093(2),975,969,960(2),931,923,  
 919(2),896,870,842,787,775(2),692.7(2),514,508,429,414,350,338,260,135,112.4  
 HF298=291.056 kJ HF0=318.773 kJ REF=Melius P81BZ BAC/MP4 calc 1987 Max Lst  
 Sq Error Cp @ 200 K 0.92%

C10H10 2,2'-bicy A05/05C 10.H 10.	0.	0.G	200.000	6000.000	B 130.18640	1
1.99458236E+01	3.42958364E-02	-1.25867035E-05	2.05828616E-09	-1.24255710E-13		2
2.51825371E+04	-8.24439577E+01	1.61705400E+00	3.92928205E-02	9.65351318E-05		3
-1.66381633E-07	7.25256141E-11	3.22188755E+04	2.25929681E+01	3.50057641E+04		4

767-59-9

C10H10 1-MethylIndene SIGMA=1 STATWT=1 IA=32.5366 IB=67.9524 IC=95.7494  
 Ir=0.5249 ROSYM=3 V(3)=760. cm-1 Nu=3217,3196,3193,3183,3171,3165,3113,3103,  
 3031,2991,1660,1645,1612,1488.7(2),1466(2),1398,1389,1348,1303,1293,1241,1221,  
 1180,1166,1127,1098,1076,1068,1043,1009,994,963,950,910,888,866,810,779,753,740,  
 728,617,577,552,526,443,411,289,275,243,166 HF298=44.2 kcal based on the value  
 of 2-Methyl-Indene. REF=Lifshiz Dubnikova QCISD(T)//B3LYP/(cc-pDVZ) calc  
 JPC A 108, (2004), 3430 Max Lst Sq Error Cp @ 200 K 0.82%.

C10H10 1-meIndene A03/05C 10.H 10.	0.	0.G	200.000	6000.000	B 130.18640	1
1.87280048E+01	3.47483381E-02	-1.25510575E-05	2.03419466E-09	-1.22127557E-13		2
1.28512382E+04	-7.85849238E+01	5.74094778E-01	4.29135235E-02	8.39134981E-05		3
-1.50478865E-07	6.59151013E-11	1.96885228E+04	2.47487601E+01	2.22421766E+04		4

Table 4 (continued)

2177-47-1

C10H10 2-MethylIndene SIGMA=1 STATWT=1 IA=22.7818 IB=88.3663 IC=110.1120  
 Ir=0.5249 ROSYM=3 V(3)=760. cm<sup>-1</sup> Nu=3197,3195,3182,3171,3164,3112,3058,3044,  
 3015,3009,1672,1660,1627,1494,1491,1457,1448,1411,1401,1387,1333,1319,1248,1222,  
 1177,1167,1146(2),1113,1042(2),1001,994,955,935,894,878,876,854,803,773,737,651,  
 604,568,477,438,431,421,299,247,213,158 HF298=41.5 kcal based on the value of  
 2-Methyl-Indene. REF=Lifshiz Dubnikova QCISD(T)//B3LYP/(cc-pDVZ) calc JPC A  
 108,(2004),3430 Max Lst Sq Error Cp @ 200 K 0.72%.

C10H10 2-meIndene A03/05C 10.H 10. 0. 0.G 200.000 6000.000 B 130.18640 1  
 1.86540860E+01 3.48863580E-02-1.26166897E-05 2.04645995E-09-1.22929258E-13 2  
 1.15449258E+04-7.76150716E+01 1.18875957E+00 4.18832401E-02 8.16146240E-05 3  
 -1.44935702E-07 6.30963635E-11 1.82030553E+04 2.21078212E+01 2.08834916E+04 4

767-60-2

C10H10 3-MethylIndene SIGMA=1 STATWT=1 IA=33.5942 IB=67.1961 IC=99.74324  
 Ir=0.5249 ROSYM=3 V(3)=760. cm<sup>-1</sup> Nu=3203,3196,3184,3172,3165,3116,3072,3042,  
 3020,3014,1679,1659,1626,1492,1489,1461,1449,1413,1404,1386,1343,1311,1259,1222,  
 1188,1166,1134,1127,1084,1054,1043,1012,995,962,958,936,877,845,793,773,753,738,  
 687,599,557,532,463,454,424,263,229,215,163 HF298=41.4 kcal REF=Lifshiz  
 Dubnikova QCISD(T)//B3LYP/(cc-pDVZ) calc JPC A 108,(2004),3430 Max Lst Sq  
 Error Cp @ 200 K 0.82%.

C10H10 3-meIndene A03/05C 10.H 10. 0. 0.G 200.000 6000.000 B 130.18640 1  
 1.86534258E+01 3.48729778E-02-1.26087006E-05 2.04483255E-09-1.22817979E-13 2  
 1.14946902E+04-7.75807785E+01 1.10113789E+00 4.21733126E-02 8.14199002E-05 3  
 -1.45129384E-07 6.32747506E-11 1.81679841E+04 2.25601758E+01 2.08331700E+04 4

N/A

C10H13 BiCyclo-Pentene-yl Radical C5H7-C5H6\* SIGMA=1 STATWT=2 Rough  
 Approximation Using THERM from C10H14 parent molecule - H. Extrapolated to  
 5000 K using Wilhoit's polynomials. HF298=53.77 kcal {PM3 HF298=42.22 kcal;  
 AM1 HF298=45.11 kcal} Max Lst Sq Error Cp @ 1600 K 0.25%

C10H13 S 8/01C 10.H 13. 0. 0.G 298.150 5000.000 F 133.21322 1  
 1.02070888E+01-2.70757680E-04 2.11426140E-06-3.48818749E-10 1.82240205E-14 2  
 2.25699502E+04-4.95500000E+01-2.49398622E+00 2.70221902E-02-1.26472303E-05 3  
 -4.41162084E-09 4.22721779E-12 2.67189502E+04 1.85757346E+01 2.70579601E+04 4

62862-35-5

C10H14 1,1-BiCycloPentene C5H7-C5H7 SIGMA=2 Rough Approximation Using THERM  
 2x(C/C3/H); 4x(CD/C/H); 4x(C/C/CD/H2) 2x(CY/C5/E) Extrapolated to 5000 K using  
 Wilhoit's polynomials. HF298=21.70 kcal {PM3 HF298=14.03 kcal; AM1 HF298=15.09  
 kcal} Max Lst Sq Error Cp @ 1500 K 0.34%.

C10H14 S 8/01C 10.H 14. 0. 0.G 298.150 5000.000 F 134.22116 1  
 2.15325793E+01 4.14035837E-02-1.45146602E-05 2.45958560E-09-1.61513614E-13 2  
 -4.12936399E+02-9.28924876E+01-9.12022862E+00 1.04360219E-01-2.89513972E-05 3  
 -4.05478829E-08 2.48433320E-11 9.32469775E+03 7.11959534E+01 1.09198016E+04 4

Table 4 (continued)

N/A

C10H15 JP-10 RADICAL IN MIDAPEX POSITION STATWT=2 SIGMA=1 IA=30.37695  
 IB=70.70838 IC=80.0308 NU=164.3,190.2,247.6,309,347,401,502,574,601,837,689,  
 766,797,857,864,918,969,979,1013,1017,1029,1040,1069,1077,1104,1120,1132,1141,  
 1150,1158,1162,1165,1186,1193,1199,1230,1246,1251,1263,1288,1293,1328,1342,1357,  
 1367,1406,1407,1416,1419,1424,1429,1451,1494,1505,2963,2980,3048,3057,3061,3077,  
 3079,3124,3127,3128,3131,3137,3163,3179,3332 REF=AM1 calc HF298=25.251 kcal  
 REF=Dissoc React=98.1 kcal Max Lst Sq Error Cp @ 200 K \*\*\*1.57%\*\*\*  
 C10H15 JP10 RAD. S 4/01C 10.H 15. 0. 0.G 200.000 6000.000 B 135.22910 1  
 1.77659083E+01 4.93981255E-02-1.78151191E-05 2.88413387E-09-1.73012768E-13 2  
 2.12676000E+03-7.93158625E+01 4.06425019E+00-8.85014262E-03 2.70737895E-04 3  
 -3.58057275E-07 1.44165309E-10 1.01359022E+04 1.35328228E+01 1.27067240E+04 4

N/A

C10H15 JP-10 RADICAL ON SIDE TERTIARI CARBON STATWT=2 SIGMA=1 IA=31.92075  
 IB=72.2657 IC=79.747 NU=165.4,192.8,247,319,400,493,554,570,617,668,756,  
 796,841,863,924,957,973,988,996,1005,1017,1045,1052,1077,1106,1121,1140,1149,  
 1150,1152,1159,1172,1187,1202,1227,1247,1264,1265,1283,1291,1318,1337,1350,1358,  
 1406,1411,1419,1423,1429,1437,1458,1471,1496,1533,2951,2968,3048,3061,3064,3077,  
 3081,3103,3124,3130,3131,3132,3140,3162,3169 REF=AM1 calc HF298=23.021 kcal  
 REF=Dissoc React=95.87 kcal Max Lst Sq Error Cp @ 200 K \*\*\*1.68%\*\*\*  
 JP-10 RADICAL ca S 4/01C 10.H 15. 0. 0.G 200.000 6000.000 B 135.22910 1  
 1.71750303E+01 5.00688372E-02-1.80894713E-05 2.93199618E-09-1.76025519E-13 2  
 1.10344712E+03-7.67084714E+01 4.09401552E+00-1.32979467E-02 2.82520168E-04 3  
 -3.69512358E-07 1.48106488E-10 9.11922658E+03 1.37914313E+01 1.15845509E+04 4

N/A

C10H15 Cy-c5h8\*-Cy-C5H7 1-CYCLOPENTENE-2-Cyclopentane-1'-yl STATWT=2 SIGMA=1  
 IA=29.00696 IB=99.0997 IC=100.4662 Ir=26.394 V(2)=1116 cm-1 ROSYM=2  
 Nu=3271,3253,3241,3122,3117,3112,3111(2),3061,3060,3044,3035,3029,3029,3022,  
 3018,1809,1495,1448,1430,1426,1422,1415,1412,1394,1389,1381,1373,1323,1322,1312,  
 1302,1276,1249,1221,1197,1194,1186,1168,1160,1155,1150,1143,1126,1110,1099,1086,  
 1068,1065,1030,988,954,896,850,815,807,778,742,724,681,622,527,389,357,231,214,  
 118.6,79.83,65.57 REF=AM1 Calc. HF298=41.0+/-30 kcal REF=Burcat estimation.  
 Max Lsst Sq Error Cp @ 200 K \*\*\*1.25%\*\*\*,  
 C10H15 Bicyclo RadS 4/01C 10.H 15. 0. 0.G 200.000 6000.000 C 135.22910 1  
 1.84393065E+01 4.76714255E-02-1.71362510E-05 2.76798038E-09-1.65779033E-13 2  
 1.02318584E+04-7.49531448E+01 6.84657726E+00-9.88983515E-03 2.55025973E-04 3  
 -3.35019934E-07 1.34613901E-10 1.73755191E+04 5.50779160E+00 2.06318833E+04 4

Table 4 (continued)

2825-82-3

C10H16 JP-10 TETRAHYDRO-DI-CYCLOPENTADIENE also 4,7-Methano-1H-indene, octahydro SIGMA=1 STATWT=1 IA=31.2575 IB=71.1222 IC=81.9346 NU=131.2, 175.7,267.5,313.3,315.7,393.5,490,529,548,665,732,745,784,819,855,856,880,885, 904,908,917,946,953,982,989,1031,1039,1042,1044,1062,1126,1142,1157,1181,1192, 1197,1215,1239,1249,1276,1288,1293,1299,1304,1314,1317,1330,1336,1354,1358,1477, 1479,1481,1487,1499,1511,2986,2990,2994,3000,3004,3012,3013,3015,3034,3037,3040, 3043,3046,3049,3056,3057 T0=1102.9905 IA=38.1094 IB=61.8407 IC=66.1194 SIGMA=1 NU=157.3,221.1,273.9,283.7,337.1,440.3,451.4,499.2,619,663,696,744,788,813,817, 840,862,876,889,920,930,952,960,971,975,1026,1031,1055,1071,1109,1123,1133,1146, 1170,1187,1189,1226,1243,1262,1268,1291,1295,1307,1313,1317,1324,1329,1348,1351, 1359,1477,1483,1486,1493,1498,1520,2991,2994,3002,3006,3008,3013,3019,3021,3031, 3034,3041,3047,3049,3050,3055,3067 HF298=-20.749 KCAL REF=R.Jaffe NASA Glen, Gaussian CBS-QB3 calc Dec. 2000. Vibrations scaled by 0.99. Eq. mixture of endo 0.00342 and exo 0.99658 isomers. HF298 calc on basis of cyclopentene =33.9+/-1. kJ (TRC). HF0(exo)=-109.853 kJ

C10H16 JP-10	G03/01C	10H	16	0	OG	200.000	6000.000	A	136.23404	1
2.05368497E+01	4.98473675E-02	-1.80332319E-05	2.92541523E-09	-1.75734895E-13						2
-2.21512904E+04	-9.62958904E+01	1.40803444E+00	1.03009739E-02	2.49234729E-04						3
-3.50769059E-07	1.44925987E-10	-1.29353245E+04	2.33764250E+01	-1.04804153E+04						4

N/A

C10H19 1,Decenyl-4/5 CH2=CH-CH2-CH\*-C5H11 Estimated using NIST-94. EXTRAPOLATED from 1600 K USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1500 K 0.37% HF298=67.9 KJ

C10H19 1-deceny	T	3/00C	10.H	19.	0.	0.G	298.150	5000.000	D	139.26086	1
2.37590285E+01	5.13629059E-02	-1.91904058E-05	3.36468639E-09	-2.24370651E-13							2
-3.77181269E+03	-8.85479830E+01	4.94076996E+00	6.39894278E-02	5.64163880E-05							3
-1.18883384E-07	5.24354590E-11	3.56097203E+03	1.85984224E+01	8.16644637E+03							4

N/A

C10H19 1,Decenyl-3 CH2=CH-CH\*-C6H11 Estimated using NIST-94. EXTRAPOLATED from 1600 K USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1500 K 0.76% HF298=2.6 KJ

C10H19 1-deceny	T	3/00C	10.H	19.	0.	0.G	298.150	5000.000	D	139.26086	1
2.47482587E+01	5.14076858E-02	-1.95828774E-05	3.47928330E-09	-2.34079322E-13							2
-1.20167044E+04	-9.35125879E+01	-2.43834540E+01	2.82492767E-01	-4.99496066E-04							3
4.71514086E-07	-1.70502072E-10	-1.41157149E+03	1.41304170E+02	3.12706341E+02							4

872-05-9

C10H20 1-DECENE Estimated using NIST-94. EXTRAPOLATED from 1600 K USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1500 K 0.46% HF298=-123.9 KJ

C10H20 1-Decene	T	3/00C	10.H	20.	0.	0.G	298.150	5000.000	D	140.26880	1
2.43784941E+01	5.33879655E-02	-1.99613482E-05	3.50081948E-09	-2.33453944E-13							2
-2.72997767E+04	-9.49537106E+01	3.47605427E+00	7.65120954E-02	2.93696959E-05							3
-8.88008675E-08	4.03372569E-11	-1.94418036E+04	2.22701279E+01	-1.49016599E+04							4

20063-97-2

C10H20 2-DECENE-trans Estimated using NIST-94. EXTRAPOLATED from 1600 K USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1500 K 0.35% HF298=-136.2 KJ

C10H20 2-decene-	T	3/00C	10.H	20.	0.	0.G	298.150	5000.000	D	140.26880	1
2.38184351E+01	5.39053060E-02	-2.01372708E-05	3.52862934E-09	-2.35146707E-13							2
-2.85920995E+04	-9.22267124E+01	3.74608499E+00	7.49426004E-02	2.93412818E-05							3
-8.58775012E-08	3.85491667E-11	-2.09365775E+04	2.07575646E+01	-1.63810014E+04							4

Table 4 (continued)

19398-37-9

C10H20 3-DECENE-trans Estimated using NIST-94. EXTRAPOLATED from 1600 K  
 USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1500 K 0.34% HF298=-135.5 KJ  
 C10H20 3-decene- T 3/00C 10.H 20. 0. 0.G 298.150 5000.000 D 140.26880 1  
 2.39013980E+01 5.38878964E-02-2.01285612E-05 3.52665091E-09-2.34996859E-13 2  
 -2.85617759E+04-9.25811186E+01 2.73154321E+00 7.88862849E-02 2.51641756E-05 3  
 -8.52509662E-08 3.92427894E-11-2.06898473E+04 2.57333929E+01-1.62968112E+04 4

71941-71-4 ??

N-C10H21 N-DECYL-1 RADICAL TRC 8/83 DATA TO 3000. K EXTRAPOLATED USING  
 WILHOIT'S POLYNOMIALS. HF298=-57.74 kJ HF0=-5.51 kJ MAX LST SQ ERROR Cp @  
 400 K 0.72% {NIST 94 estimate HF298=-43.8 KJ}  
 C10H21,n-decyl P10/83C 10.H 21. 0. 0.G 200.000 6000.000 C 141.27374 1  
 2.33759939E+01 5.75362038E-02-2.10968020E-05 3.46309821E-09-2.09434030E-13 2  
 -1.87658614E+04-8.68825727E+01 1.48510661E+01-3.85330874E-03 2.43710502E-04 3  
 -3.17547576E-07 1.25908377E-10-1.27861722E+04-2.35344919E+01-6.94448621E+03 4

N/A

N-C10H21 N-DECYL-2 RADICAL Estimated using NIST-94. EXTRAPOLATED from 1600 K  
 USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1500 K 0.34 % HF298=-58.1 KJ  
 C10H21 2-decyl T 3/00C 10.H 21. 0. 0.G 298.150 5000.000 D 141.27674 1  
 2.45312418E+01 5.55320406E-02-2.07239376E-05 3.63129156E-09-2.42045771E-13 2  
 -1.95025142E+04-9.36436619E+01 6.86951665E+00 5.57425508E-02 8.72153686E-05 3  
 -1.51902528E-07 6.46180282E-11-1.20143727E+04 9.80863792E+00-6.98778401E+03 4

112320-15-7

N-C10H21 N-DECYL-3 or 4 RADICAL Estimated using NIST 94 EXTRAPOLATED from 1600  
 K USING WILHOIT'S POLYNOMIALS. MAX LST SQ ERROR CP @ 1500 K 0.38% HF298=-58.2 KJ  
 C10H21 3/4-decyl T 3/00C 10.H 21. 0. 0.G 298.150 5000.000 D 141.27674 1  
 2.44433242E+01 5.56583435E-02-2.07686906E-05 3.63847992E-09-2.42490501E-13 2  
 -1.94765658E+04-9.31425601E+01 6.86951665E+00 5.57425508E-02 8.72153686E-05 3  
 -1.51902528E-07 6.46180282E-11-1.20263999E+04 9.80863792E+00-6.99981117E+03 4

124-18-5

C10H22 liq. Decane REF=I.Barin 1987 HF298liq=-301.038 kJ  
 C10H22 (L) B01/00C 10.H 22. 0. 0.L 298.150 446.830 C 142.28468 1  
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2  
 0.00000000E+00 0.00000000E+00 3.77595368E+01 5.43284903E-04-1.44050795E-06 3  
 1.25634293E-09 0.00000000E+00-4.74783720E+04-1.64025285E+02-3.62064632E+04 4

124-18-5

N-C10H22 N-DECANE Bureau of Mines Bull 666 1974 DATA TO 1500. K EXTRAPOLATED  
 USING WILHOIT'S POLYNOMIALS. HF298=-59.64 kcal MAX LST SQ ERROR Cp @ 1300 K 0.7%  
 N-C10H22 DECANE T 5/99C 10.H 22. 0. 0.G 200.000 6000.000 B 142.28468 1  
 2.94782956E+01 4.90518943E-02-1.70317179E-05 2.72919300E-09-1.63370772E-13 2  
 -4.43022624E+04-1.24062121E+02 1.54328173E+01-1.32979232E-02 2.82480581E-04 3  
 -3.65923298E-07 1.45372117E-10-3.58632831E+04-2.79454341E+01-3.00118419E+04 4

Table 4 (continued)

104680-84-4

C10H7C\*O Naphthaldehyde radical STATWT = 2 Ia = 51.315652 Ib = 100.57912  
 Ic = 151.92712 NU=3128,3126,3118,3114,3107,3099,3097,1809,1622,1584,1562,1507,  
 1447,1434,1374,1379,1360,1243,1222,1194,1155,1149,1133,1071,1022,994,962,948,  
 927,905,854,846,791,782,763,727,723,624,612,523,511,494,459,430,392,327,213,178,  
 170,153,78.3 REF = Curran et al. JPCRD 29, (2000), 463 Hf(298)= 41.8  
 kcal REF = Marinov et al, Comb. Sci. Technol, 116-117, (1996), 211.

Max Lst Sq Error Cp @ 1300 K 0.55%

1-C10H7C*O	Radic	T 7/98C	11.H	7.O	1.	0.G	200.000	6000.000	B	155.17598	1	
							2.27592940E+01	2.95236092E-02	-1.08144575E-05	1.76929286E-09	-1.06921871E-13	2
							1.06007552E+04	-9.54682191E+01	2.47024671E-01	6.23078127E-02	3.25268900E-05	3
							-9.98773421E-08	4.79264315E-11	1.80787951E+04	2.74600245E+01	2.10344566E+04	4

66-99-9

C10H7CHO Naphthaldehyde Ia = 50.406846 Ib = 104.13646 Ic = 154.54331  
 Ir = 0.148 ROSYM = 2 V(2) = 4.9 kcal/mole NU=3399,3069,2837,2724,2355,2322,  
 1945,1811,1775,1713,1631,1588,1579,1517,1460,1411,1404,1373,1347,1252,1221,1218,  
 1172,1155,1141,1079,1058,1027,971,955,947,921,888,862,806,789,770,758(2),713,  
 651,616,527,507,492,463,421,389,342,227,206,180,112. REF = NIST Webbook 1997  
 Hf(298)= 7.3 kcal REF = NIST 1994 Max Lst Sq Error Cp @ 1300 K 0.66%

1-C10H7CHO	T 7/98C	11.H	8.O	1.	0.G	200.000	6000.000	B	156.18392	1		
							2.42593357E+01	3.16036997E-02	-1.18467358E-05	1.96728679E-09	-1.20096869E-13	2
							-7.83388781E+03	-1.07718994E+02	-3.75140208E-01	6.11007395E-02	4.92528177E-05	3
							-1.17296000E-07	5.31810720E-11	8.41138142E+02	2.88322573E+01	3.67348166E+03	4

7419-60-5

C11H9 1-C10H7CH2\* 1- Naphtyl Methylene radical STATWT = 2 Ia = 41.8986174  
 Ib = 74.3823227 Ic = 116.2722486 Nu=3193,3128,3121,3118,3106,3105,3099,3096,  
 3094,1610,1559,1537,1500,1486,1439,1433,1395,1362,1347,1282,1230,1214,1168,  
 1151,1135,1090,1075,1032,943,941,927,907,862,850,834,779,775,753,718,710,701,  
 619,566,547,493,492,467,436,433,396,303,232,169,95.8 REF = Curran et al,  
 JPCRD 29, (2000), 463 Hf(298)= 65.2 kcal REF = NIST 94 estimate

Max Lst Sq Error Cp @ 200 K 0.71%

1-C10H7-CH2*	T 7/98C	11.H	9.	0.	0.G	200.000	6000.000		141.19246	1		
							2.18977539E+01	3.26102636E-02	-1.18401218E-05	1.92574628E-09	-1.15903442E-13	2
							2.24571098E+04	-9.41050741E+01	-2.53234304E+00	7.32920338E-02	2.02974707E-05	3
							-9.36547823E-08	4.70753594E-11	3.02906705E+04	3.79638513E+01	3.28097266E+04	4

90-12-0

1-C10H7CH3 1-Methyl-Naphthalene Ia= 43.9442164 Ib= 74.3379622 Ic= 117.7309994  
 Ir = 0.51387 ROSYM = 3 V(3) = 0.01 kcal/mole Nu= 3107,3074,3016,2982,  
 2956,2978,2749,2321,1924,1856,1820,1795,1744,1680,1601,1512,1470,1447,1398,  
 (1360),1261,(1252),1211,1166,1109,1102,1084,1077,1049,(1026,1022),960,(948,934,  
 914,874),858,(846,840),787(2),771,711,699,(616),537,532,490,(462),460,(427,404,  
 269,241,179,161). REF = NIST Webbook 1997 spectrum Hf(298)= 27.75 kcal  
 REF = Speros & Rossini J. Phys. Chem. 64, (1960), 1723. Max Lst Sq Error Cp @  
 200 K 0.68%

1-C10H7-CH3	T 7/98C	11.H	10.	0.	0.G	200.000	6000.000	B	142.20040	1		
							2.17939213E+01	3.60214098E-02	-1.33228698E-05	2.19304403E-09	-1.33071380E-13	2
							3.16261439E+03	-9.48675403E+01	-1.03043715E+00	6.03358177E-02	5.45655719E-05	3
							-1.22769251E-07	5.54507327E-11	1.13241014E+04	3.22970611E+01	1.39642625E+04	4

Table 4 (continued)

1120-21-4

N-C11H24 UNDECANE REF=TRC11/75 TO 1000 K. EXTRAPOLATED USING WILHOIT'S  
POLYNOMIALS. HF298=-64.60 kcal

N-UNDECANE T 5/99C 11.H 24. 0. 0.G 200.000 6000.000 C 156.31156 1  
3.41070654E+01 5.07865991E-02-1.73797396E-05 2.76048145E-09-1.64248726E-13 2  
-4.88486250E+04-1.47546600E+02 1.67589055E+01-1.35771822E-02 3.08216871E-04 3  
-4.00562662E-07 1.59274225E-10-3.89076869E+04-3.15628516E+01-3.25077966E+04 4

N/A

C12D9 O-BIPHENYL RADICAL D9 STATWT=2 SIGMA=1 IA=33.21 IB=170.83 IC=194.34  
IR=8.285 ROSYM=2 V(2)=1500 cal NU=2287,2280,1571,1412,1188,960,869,835,688,300,  
2286,2218,1531,1328,1266,1010,826,790,565,110,832,744,627,540,466,160,790,652,  
346,2288,2284,2281,1568,1346,983,846,816,590,2285,2279,1566,1345,1272,1070,840,  
835,589,355,775,646,539,500,393,232,660,300 HF298=386.5 KJ REF=BURCAT ZELEZNIK  
& MCBRIDE NASA TM-83800 1985

O-C12D9 O-L12/84C 12.D 9. 0. 0.G 300.000 5000.000 B 162.25892 1  
0.30123199E 02 0.28328255E-01-0.10366540E-04 0.16593338E-08-0.96527116E-13 2  
0.33207789E 05-0.13520447E 03-0.73299396E 00 0.89836895E-01-0.13731275E-04 3  
-0.59427020E-07 0.33702430E-10 0.42943094E 05 0.30028793E 02 0.46486410E 05 4

1486-01-7

C12D10 BIPHENYL D10 STATWT=1 SIGMA=4. IA=34.79 IB=171.43 IC=196.03  
IB=8.697 ROSYM=2 V(2)=1500. cal NU=SAME AS FOR C12D9 AND ADDITIONAL 2284,  
952,783 HF298=138.41 KJ REF=BURCAT ZELEZNIK & MCBRIDE NASA-TM-83800 1985.

C12D10 L12/84C 12.D 10. 0. 0.G 300.000 5000.000 B 164.27302 1  
0.30905060E 02 0.30349988E-01-0.11095048E-04 0.17755810E-08-0.10332327E-12 2  
0.28834453E 04-0.14245210E 03-0.15793486E 01 0.95059574E-01-0.14532071E-04 3  
-0.62645597E-07 0.35530079E-10 0.13137422E 05 0.31516678E 02 0.16647502E 05 4

58802-20-3

C12H4OC14 2,3,6,7 Tetra-Chloro-Dibenzo-Furan SIGMA=1 IA=96.411819  
IB= 613.4173648 IC=709.82918 NU=3052(3),3051,1623,1595,1584,1551,1488,1473,  
1412,1379,1330,1311,1262,1244,1232,1215,1125,1099,1036,981,975,948,926,903,836,  
822,796,777,760,732,709,685,676,654,629,577,565,506,473,442,407,392,369,330,282,  
260,234,218,186,173,168,126,118,58,53 REF=Dorofeeva private communication  
HF298=-50. +/- -10. kJ REF=Dorofeeva, Iorish, Moiseeva J. Chem. Eng. Data (1999)  
44,516-523. Max Lst Sq Error Cp @ 1300 K 0.50 %.

C12H4Cl4O 2367 T 7/02C 12.H 4.O 1.CL 4.G 200.000 6000.000 B 305.97036 1  
3.37203056E+01 2.59531836E-02-9.73623386E-06 1.61792141E-09-9.88243946E-14 2  
-1.99774739E+04-1.46328547E+02 8.35008122E-01 1.05239112E-01-5.23532685E-05 3  
-2.50611331E-08 2.27966335E-11-1.04387906E+04 2.60267825E+01-6.01358348E+03 4

64560-17-4

C12H4Cl4O 2,4,6,8 Tetra-Chloro-Dibenzo-Furan SIGMA=2 IA=197.9089427  
IB=445.5922441 IC=653.5011868 NU=3053(2),3051,3050,1624,1588,1582,1542,1489,  
1474,1404,1378,1333,1309,1265,1254,1244,1214,1129,1086,1000,967,952,910,890,884,  
879,851,825,815,769,768,742,701,683,640,574,568,568,547,401(2),392,386,367,363,  
315,231,219,209,194,170,166,145,105,78,39 REF=Dorofeeva private communication  
HF298=-58. +/- -10. kJ REF=Dorofeeva, Iorish, Moiseeva J. Chem. Eng. Data (1999)  
44,516-523. Burcat et al JPCRD 32 (2003),443 Max Lst Sq Error Cp @ 1300 K  
0.50 %.

C12H4Cl4O 2468 T 7/02C 12.H 4.O 1.CL 4.G 200.000 6000.000 B 305.97036 1  
3.37653037E+01 2.59089918E-02-9.71934006E-06 1.61507981E-09-9.86493891E-14 2  
-2.09499311E+04-1.46904227E+02 1.21277591E+00 1.03027906E-01-4.71999359E-05 3  
-3.02796418E-08 2.47102816E-11-1.14514343E+04 2.40113931E+01-6.97575684E+03 4



Table 4 (continued)

1746-01-6

C12H4O2Cl4 2,3,7,8 Tetra-Chloro-Dibenzo-Dioxin SIGMA=4 STATWT=1 IA=96.39084  
 IB=752.11956 IC=847.4184 NU=3235.5(4),1683,1648,1629,1613,1531,1519,1427,1401,  
 1349,1346,1320,1269,1261,1244,1192,1188,1135,1132,992,938,900,884(2),852(2),794,  
 762,693,668,664,652,645,625(2),559,542,499,459,451,448,392.5(2),382,328,286,258,  
 230,222,200,185.3,173,138.3,113.35(2),49.43,20.07 REF=Mhin, Choi & Choi JACS  
 123, (2001),3584-supplement. { HF298=-164.0+/-15. kJ REF=Dorofeeva, Iorish,  
 Moiseeva J. Chem. Eng. Data (1999) 44,516-523.} HF298=136.1+/-10. kJ REF=  
 DOROFEEVA et al JPC 107 (2003),2848 Max Lst Sq Error Cp @ 1300K .49 %.  
 C12H4O2Cl4 2378 T 8/03C 12.H 4.O 2.CL 4.G 200.000 6000.000 C 321.97336 1  
 3.55551539E+01 2.68113836E-02-1.00051732E-05 1.65726833E-09-1.01016088E-13 2  
 -3.09230657E+04-1.55001248E+02 8.42161972E-01 1.18543424E-01-8.34715750E-05 3  
 7.54873814E-09 1.04548677E-11-2.11713374E+04 2.51859725E+01-1.63689742E+04 4

42430-90-0

C12H4O2Cl4 1,3,6,8 Tetra-Chloro-Dibenzo-Dioxin SIGMA=2 IA=177.08439  
 IB=530.21625 IC=707.20877 NU=3246(2),3240(2),1669,1651,1619(2),1513,1509,1457,  
 1441,1355,1338,1326,1267,1245,1235,1218,1193,1111.5(2),989,963,867.5(2),865,  
 858,852(2),827,703(2),682,668,590,576(2),564,537,535,486,463,410,402,372,357,  
 350,298,249,223,203,198,158.5,156.3,154.6,127.9,104.64,48.35,20.12  
 REF=Mhin, Choi & Choi JACS 123, (2001),3584-supplement. {F298=-173.0+/-15. kJ  
 REF=Dorofeeva, Iorish, Moiseeva J. Chem. Eng. Data 44, (1999),516-523.}  
 HF298=128.7+/-17 kJ REF= Dorofeeva et al. JPC 107 (2003) 2848 Max Lst Sq Error  
 Cp @ 1300 K 0.50 %.  
 C12H4O2Cl4 1368 T 8/03C 12.H 4.O 2.CL 4.G 200.000 6000.000 B 321.97336 1  
 3.55414842E+01 2.68126078E-02-1.00031234E-05 1.65667276E-09-1.00969542E-13 2  
 -3.00259258E+04-1.53915980E+02 1.27697078E+00 1.15874285E-01-7.75840253E-05 3  
 1.89840979E-09 1.24410316E-11-2.03341181E+04 2.42875879E+01-1.54789639E+04 4

N/A

C12H4Cl4O3 Dibenzo-p-Dioxine 1,3,6,8-tetrachloro-2-ol SIGMA=1 STATWT=1  
 Ia=183.06492 Ib=587.55552 Ic=770.61573 Ir(OH)==0.13643 V(2)=1116.8 cm-1  
 ROSYM=2 Nu=3855,3062,3058,3057,1800,1795,1766,1761,1637,1611,1598,1555,1512,  
 1426,1404,1337,1330,1326,1289,1241,1174,1114,1105,1033,957,940,932,922,902,839,  
 800,768,729,725,690,661,626,587,565,535,527,514,452,403,401,378,362,343,314,  
 299,289,274,203(2),198,169,158.4,149.2,112.4,106.3,92.9,41.9 REF=PM3  
 HF298=-295.37 kJ REF=DOROFEEVA J.CEData 44, (1999),516 + Bozzelli's increments  
 Burcat et al JPCRD 32 (2003),443 Max Lst Sq Error Cp @ 1300 K 0.51%.  
 C12H4Cl4O3 1368 T 7/02C 12.H 4.O 3.CL 4.G 200.000 6000.000 B 337.97276 1  
 3.65131711E+01 2.81939174E-02-1.05065989E-05 1.73890011E-09-1.05936213E-13 2  
 -5.03536098E+04-1.58210338E+02 1.91091018E+00 1.26862273E-01-1.12283816E-04 3  
 4.42202105E-08-4.87612341E-12-4.08260774E+04 2.00659755E+01-3.55246431E+04 4

574003-31-9

C12H4O2Cl5 2,4-dichloro-phenoxy-1'3'5'-trichloro-phenyl-6-2'-ether Radical  
 Cl2C6H2(O\*) -O-C6H2Cl3 SIGMA=1 STATWT=2 IA=212.47412 IB=647.327722  
 IC=661.92080 Ir(tcb)=84.51393 Ir(dcp)=74.007 (V(2)=1116. cm-1)x2  
 Nu=3059,3056,3048,3042,1878,1766,1754,1673,1626,1571,1517,1448,1414,1385,1315,  
 1308,1263,1191,1162,1156,1090,1079,962,946,937,924,924,897,871,812,789,766,755,  
 716,643,571,553,541,530,518,481,449,423,389,370,365,338,323,310,263,220,194,186,  
 185,169,149,131,129,81.2,57.7,30.5 REF= MOPAC6 PM3 HF298=-30.62+/-6. kcal  
 REF=NIST 94 est+ Dorofeeva 1,3-Cl correction Burcat et al JPCRD 32 (2003),443  
 Max Lst Sq Error Cp@ 1300 K 0.47%.  
 C12H4O2Cl5 T 7/02C 12.H 4.O 2.CL 5.G 200.000 6000.000 B 357.42606 1  
 3.75648982E+01 2.59919632E-02-9.72467483E-06 1.61312689E-09-9.84098487E-14 2  
 -3.03064243E+04-1.54117133E+02 4.22121227E+00 1.20295993E-01-1.01743807E-04 3  
 3.21160499E-08 4.57455537E-13-2.11786130E+04 1.76118180E+01-1.54084943E+04 4

Table 4 (continued)

574003-32-0

C12H4O2Cl6 2,4,6 trichloro-cyclohexa-3,5-diene-1-quinol-2,2-1',3',5' trichloro-phenyl-ether SYMNO=1 STATWT=1 IA=246.48589 IB=629.756 IC=762.77137

Ir(TCP)=72.5050 Ir(TCP-O-)=133.1776 ROSYM=2 (V(2)=1116. cm-1)x2 NU=3059,  
 3055,3044,3040,1973,1842,1828,1767,1749,1574,1512,1417,1383,1333,1308,1300,1205,  
 1177,1158,1139,1085,1077,987,947,941,924,919,903,850,798,790,787,740,716,666,  
 621,570,552,545,531,516,434,424,405(2),372,370,354,338,324,282,220,198,193,  
 186.5,182.6,149,147.1,142.2,130.8,113.8,101.8,50.6,34.15 HF298=~-35.0 kcal  
 REF=PM3 + PM3-UHF HF is very rough estimation. Burcat et al JPCRD 32 (2003),443  
 Max Lst Sq Error Cp @ 1300 K .46%

C12H4O2Cl6 T 7/02C 12.H 4.O 2.CL 6.G 200.000 6000.000 B 392.87876 1  
 4.01072662E+01 2.64099729E-02-9.87725138E-06 1.63801070E-09-9.99097640E-14 2  
 -3.33135529E+04-1.66495471E+02 4.08550482E+00 1.35862415E-01-1.33900143E-04 3  
 6.18063889E-08-9.67607715E-12-2.38039098E+04 1.72309606E+01-1.76125833E+04 4

244037-23-8

C12H4CL6O2 C6HCL3OH-C6HCL3OH 2,4,6,2',4',6'-hexachloro-biphenyl-3,3'-diol.

SIGMA=2 IA=225.75674 IB=649.18009 IC=662.57204 (Ir(OH)=0.14248 ROSYM=2  
 V(2)=1116.8 cm-1)x2 Ir(tcp-tcp)=66,590 ROSYM=2 V(2)=1116 cm-1 NU=3622,3617,  
 3005,3003,1776,1751,1737,1732,1657,1566,1563,1539,1484,1431,1418,1382,1265,1263,  
 1227,1182,1167,1125,1081,955,953,905,818,814,802,773,730,726,700,694,628,612,  
 609,596,561,543,539,455,413,392,378,370,358(2)327,326,303,300,234,198,195,188,  
 168,167,138.7,106.3,105.7,93.3,90.8 HF298=-76.94+/-8.kcal REF=THERM ESTIMATE.  
 Burcat et al JPCRD 32 (2003),443 Max Lst Sq Error Cp @ 1300 K 0.45%

C12H4CL6O2 T 7/02C 12.H 4.CL 6.O 2.G 200.000 6000.000 B 392.87876 1  
 4.05461312E+01 2.56337627E-02-9.51429616E-06 1.57080093E-09-9.55422998E-14 2  
 -5.44633251E+04-1.75242091E+02 1.01096879E+00 1.60030359E-01-1.94327598E-04 3  
 1.24220560E-07-3.27934340E-11-4.46448886E+04 2.31584095E+01-3.87174903E+04 4

591755-81-6

C12H5Cl3O3 DIBENZO-DIOXINE-2,4,7-TRICHLORO-9-OL SIGMA=1 STATWT=1 IA=139.99955

IB=516.76912 IC=656.57445 Ir(OH)=0.1425 V(2)=1116. ROSYM=2 NU=38804,3129,  
 3053,3041,1811,1802,1770,1763,1663,1629,1597,1552,1485,1448,1412,1385,1353,1344,  
 1311,1277,1202,1169,1144,1109,1003,945,933,926,921,908,898,854,763,732,721,713,  
 621,580,569,567,563,533,531,501,463,392,368,356,344,302,271,257,205(2),195,173,  
 172,154.2,119.3,113.1,53.9 REF=PM3 calc HF298=-348.99 kJ REF=Dorofeeva  
 J.CEData,44,(1999),516 + Bozzelli's increments. Burcat et al JPCRD 32 (2003),443  
 Max Lst Sq Error Cp @ 1300 K 0.53%.

C12H5OCl3O3 T 7/02C 12.H 5.O 3.CL 3.G 200.000 6000.000 B 303.52800 1  
 3.39369877E+01 3.03479314E-02-1.12471012E-05 1.85475240E-09-1.12714824E-13 2  
 -5.61302876E+04-1.47572708E+02 1.31429187E+00 1.16707532E-01-8.54167896E-05 3  
 1.75329916E-08 4.64182974E-12-4.68346313E+04 2.20874195E+01-4.19733021E+04 4

591755-82-7

C12H5Cl4O2 Radical 2,4-dichlorophenoxy-1'4'-dichlorophenyl-6-2'-ether STATWT=2

SIGMA=1 IA=187.95423 IB=618.62154 IC=651.94394 Ir(dcp)=79.988 ROSYM=2  
 V(2)=1116 cm-1. Ir(dcb)=48.609 ROSYM=2 V(2)=1116 cm-1 NU=3069,3060,3054,  
 3048,3036,1879,1773,1760,1674,1644,1576,1523,1432,1409,1382,1312,1300,1273,1186,  
 1170,1159,1128,1095,1065,994,974,935,928,913,905,879,857,787,768,745,722,664,  
 617,571,540,534,502,482,444,410,393,391,368,343,320,284,257,214,195,174,161,155,  
 130,111,52.4,33.79 REF=PM3 HF298=-20.44+/-6 kcal REF=NIST 94 estimate +  
 Dorofeeva's 1,3-Cl increments. Burcat et al JPCRD 32 (2003),443 Max Lst Sq  
 Error Cp @ 1300 K 0.49%.

C12H5Cl4O2 RAD T 7/02C 12.H 5.O 2.CL 4.G 200.000 6000.000 B 322.98130 1  
 3.52447272E+01 2.79218605E-02-1.03851978E-05 1.71610191E-09-1.04418334E-13 2  
 -2.45877120E+04-1.44677645E+02 3.38993539E+00 1.11904345E-01-7.74499372E-05 3  
 6.65933244E-09 9.88939812E-12-1.56038201E+04 2.07711496E+01-1.02857486E+04 4

Table 4 (continued)

N/A

C12H5Cl4O3 Benzo-p-Dioxine-hexa-3,5,-diene-2-yl-1-ol-1,3,6,8-tetrachloro Radical  
 STATWT=2 SIGMA=1 IA=190.5625 IB=565.80715 IC=723.24222 IR(OH)=0.1364  
 ROSYM=2 V(2)=1116. cm-1 NU=3887,3068,3061,3057,3056,1788,1784,1775,1672,1608,  
 1565,1497,1440,1412,1379,1361,1327,1317,1274,1247,1194,1173,1125,1103,1101,993,  
 943,930,925,913,885,878,855,765,731,712,685,621,607,566,564,541,536,511,485,460,  
 414,401,373,352,343,303,294,275,247,217,194,177.4,168.6,153.4,131,108.2,98.9,  
 78.9,31.5 REF=PM3-UHF HF=-103.35+/-15. kcal very rough estimation combination  
 Dorofeeva J.CEDData,44,(1999),516 + Bozzelli's increments. Burcat et al JPCRD 32  
 (2003),443 Max Lst Sq Error Cp @ 1300 K 0.49%  
 C12H5Cl4O3 Rad T 7/02C 12.H 5.O 3.CL 4.G 200.000 6000.000 B 338.97710 1  
 3.78627024E+01 2.95127522E-02-1.09455092E-05 1.80598949E-09-1.09795646E-13 2  
 -6.73987047E+04-1.64422619E+02 1.68663349E+00 1.30749832E-01-1.08062036E-04 3  
 3.28510707E-08 9.00638451E-13-5.74323575E+04 2.21930259E+01-5.20074424E+04 4

N/A

C12H5Cl4O3 Benzo-p-Dioxine-hexa-1,4-diene-2-yl-1,3,6,8-tetrachloro Radical  
 STATWT=2 SIGMA=1 IA=187.92913 IB=582.17979 IC=756.07331 IR(OH)=0.1364  
 ROSYM=2 V(2)=1116. cm-1 NU=3888,3062,3059,3051,2852,1791,1785,1745,1653,1616,  
 1565,1514,1415,1370,1359,1348,1335,1325,1308,1301,1204,1174,1111,1090,1044,1014,  
 1011,953,941,922,917,900,839,804,735,727,716,666,623,623,620,576,566,535,512,  
 474,449,401,372,365,349,344,309,274,264,227.9,203.6,198.2,191.8,166.3,155.9,  
 148.6,119.2,92.1,58.29,43.59 REF=PM3 HF298=-76.91+/-15. kcal very rough  
 estimate from Dorofeeva J.CEDData,44,(1999),516 + Bozzelli's increments. Burcat  
 et al JPCRD 32 (2003),443 Max Lst Sq Error Cp @ 1300 K 0.49%  
 C12H5O3Cl4 DOH2 T 7/02C 12.H 5.O 3.CL 4.G 200.000 6000.000 B 338.97710 1  
 3.77083528E+01 2.97513020E-02-1.10549800E-05 1.82623859E-09-1.1115340E-13 2  
 -5.41069240E+04-1.63825524E+02 2.53394872E+00 1.22701309E-01-8.73952730E-05 3  
 1.16842390E-08 8.59557448E-12-4.41665971E+04 1.89081184E+01-3.87023938E+04 4

94888-09-2

C12H5Cl5O2 2,4-dichloro-phenol-trichloro-1',3',5'-phenyl-6-6'ether  
 C12C6H2(OH)-O-C6H2Cl3 SIGMA=1 STATWT=1 IA=236.93934 IB=577.550849  
 IC=706.86084 Ir(tcb)=84.797 Ir(dcp)=73.905 Ir(OH)=0.1364 (V(2)=1116.  
 cm-1)x3 Nu=3855,3062,3058,3053,3045,1781,1773,1767,1752,1623,1581,1565,1515,  
 1451,1429,1384,1347,1330,1292,1200,1174,1159,1107,1081,996,949,939,926,921,908,  
 895,815,789,749,737,729,618,573,565,552,534,530,521,435,424,406,375,371,357,336,  
 316,297,272,217,196.4,191.4,186.2,180,151.5,142.4,139.4,83.3,76.9 REF=MOPAC PM3  
 HF298=-59.79+/-5. kcal REF=NIST 94 est + Dorofeeva 1,3-Cl correction + Bozzelli  
 ortho-Cl-OH correction. Burcat et al JPCRD 32 (2003),443 Max Lst Sq Error Cp @  
 1300 K 0.46%.  
 C12H5O2Cl5 T 7/02C 12.H 5.O 2.CL 5.G 200.000 6000.000 B 358.43400 1  
 3.78525022E+01 2.75151028E-02-1.01717210E-05 1.67476906E-09-1.01670506E-13 2  
 -4.51095646E+04-1.58966651E+02 2.58418823E+00 1.34823485E-01-1.32609390E-04 3  
 6.23672196E-08-1.03965199E-11-3.57970280E+04 2.09115787E+01-3.00873244E+04 4

133617-92-2 ??

C12H6Cl2O 1,6 DiChloroDibenzoFuran SIGMA=1 STATWT=1 IA=93.59345 IB=245.04105  
 IC=338.6345 NU=3237,3230,3224,3220,3202,3200,1677,1645,1632,1620,1524,1511,  
 1462,1454,1394,1370,1307,1282,1264,1226,1199,1172,1166,1093,1084,1050,972,967,  
 941,907,893,865,861,795,785,750,729,710,673,593,589,577(2),540,506,487,411,386,  
 336,330,304,228,180,179,133,99,66 HF298=5.2+/-24.7 kJ HF0=25.245 kJ  
 REF=Zhu & Bozzelli JPCRD 32,(2003), 1713-1735. Max Lst Sq Error Cp @ 1300 K .53%  
 1,6-dichlorodibe T03/04C 12.H 6.CL 2.O 1.G 200.000 6000.000 B 237.08084 1  
 2.81578763E+01 3.03232866E-02-1.11703384E-05 1.83469653E-09-1.11185273E-13 2  
 -1.18306517E+04-1.22613443E+02-2.21247366E-01 8.28615357E-02 5.27378281E-06 3  
 -8.18593533E-08 4.29796179E-11-2.89667449E+03 2.97876049E+01 6.25412682E+02 4

Table 4 (continued)

38178-38-0

C12H6Cl2O2 1,6-DiChloroDibenzoDioxin SIGMA=2 STATWT=1 IA=100.29268  
 IB=291.14376 IC=391.43551 NU=3232(2),3225(2),3208,3207,1673,1660,1630,1625,  
 1529,1516,1506,1488,1366,1340,1336,1277,1252,1250,1215,1196,1175,1165,1096,1090,  
 964,959(2),924,892,891,857,830,775,774,705,693,681,666,617,558,550,546,537,533,  
 517,432,415,367,356,307,280,248,214,174,155,136,57,31 HF298=-89.3+/-26.6 kJ  
 HF0=-67.92+/-26.6 kJ REF=Zhu & Bozzelli JPCRD 32, (2003),1713 {HF298=-86.2+/-  
 30.0 kJ REF=Dorofeeva & Youngman JPC-A,107, (2003),2848} Max Lst Sq Error Cp @  
 1300 K 0.53 %.

C12H6CL2O2 T02/04C 12.H 6.CL 2.O 2.G 200.000 6000.000 B 253.08024 1  
 3.05265612E+01 3.09553854E-02-1.14148452E-05 1.87613213E-09-1.13750031E-13 2  
 -2.40176018E+04-1.33835136E+02-4.61821759E-01 9.62418938E-02-2.03839914E-05 3  
 -5.84410503E-08 3.48744532E-11-1.46011026E+04 3.07817718E+01-1.07402601E+04 4

70870-59-6

C12H6Cl4O2 2,4-Dichlorophenol-6-2'-1',4'-Dichlorophenyl Ether SIGMA=1 STATWT=1  
 IA=182.571414 IB=604.682426 IC=676.9218 Ir(dcp)=48.6075 Ir(dcb)=79.9177  
 Ir(OH)=0.1369 (V(2)=1116 cm-1)x3 NU=3854,3071,3062,3061,3055,3046,1780,1773,  
 1769,1761,1622,1581,1566,1525,1450,1427,1383,1348,1328,1289,1187,1174,1171,1129,  
 1106,1067,1001,987,939,936,923,904,895,860,788,746,736,720,663,615,576,563,548,  
 524,474,442,411,399,392,375,353,321,302,268,258,221,199,189,164,154,142,107,85.8  
 HF298=-49.61 kcal REF=estimated from NIST94 + Dorofeeva & Bozzelli corrections.  
 Burcat et al JPCRD 32 (2003),443Max Lst Sq Error Cp @ 1300 K 0.48%.

C12H6CL4O2 T 7/02C 12.H 6.O 2.CL 4.G 200.000 6000.000 C 323.98564 1  
 3.56559433E+01 2.93270279E-02-1.07879184E-05 1.77037207E-09-1.07228492E-13 2  
 -3.94205538E+04-1.49929054E+02 2.02056763E+00 1.25248291E-01-1.05426156E-04 3  
 3.37523170E-08 2.63176879E-13-3.02692977E+04 2.30604963E+01-2.49645788E+04 4

304905-17-7

C12H7 C10H7CC\* 1-Ethynyl Naphthalene Radical STATWT = 2 Ia = 56.378083  
 Ib = 87.350853 Ic = 143.58234 NU=3143,3132,3123,3122,3113,3103,3102,1805,  
 1604,1558,1541,1503,1438,1429,1393,1374,1324,1255,1221,1198,1163,1151,1132,1076,  
 1030,1015,967,948,934,895,861,848,788,779,755,723,648,628,557,526,523,471,452,  
 437,411,328,306,184,165,118,92.2 REF = Curran et al. 29, (2000),463.  
 Hf(298)= 166.1 kcal REF = NIST 1994 Max Lst Sq Error Cp @ 200 K 0.56  
 1-C10H7-CC\* Radi T 7/98C 12.H 7. 0. 0.G 200.000 6000.000 B 151.18758 1  
 2.28546479E+01 2.94181299E-02-1.07719402E-05 1.76194604E-09-1.06462481E-13 2  
 7.31301345E+04-9.62295750E+01-1.91438001E-01 6.57353329E-02 2.42664513E-05 3  
 -9.15358223E-08 4.48817973E-11 8.06649452E+04 2.89829391E+01 8.35842882E+04 4

208-96-8

C12H8 ACENAPHTHYLENE SIGMA=2 IAIBIC=463 E-114 HF298=259.7 kJ REF=DOROFEEVA  
 & Gurvich IVTAN Preprint # 1-263 1989. {HF298=258+/-5.9 kJ REF=NIST Webbook}  
 Extrapolated to 5000 K using Wilhoit's polynomials. Max Lst Sq Error Cp @ 1300 K  
 0.47 %

C12H8 ACENAPHTH T12/00C 12.H 8. 0. 0.G 200.000 5000.000 152.19552 1  
 1.93183637E+01 3.90205238E-02-1.63352587E-05 3.10041991E-09-2.19199281E-13 2  
 2.15445149E+04-8.32372261E+01-2.81264181E+00 7.04681002E-02 3.15341955E-05 3  
 -1.05176189E-07 5.08713845E-11 2.88462829E+04 3.75755975E+01 3.12345526E+04 4

Table 4 (continued)

15727-65-8

C12H8 C10H7CCH 1-Ethynyl Naphthalene Ia = 57.461762 Ib = 89.485562  
 Ic = 146.94732 Ir = 0. NU=3413,3132,3129,3120,3117,3107,3099,3096,2142,1621,  
 1586,1574,1510,1451,1433,1393,1384,1344,1255,1224,1215,1163,1153,1139,1073,1029,  
 1013,954,938,922,822,850,848,787,781,762,724,686,635,596,571,565,532,507,479,  
 462,441,431,359,337,200,171,132,102. REF = Curran et al. JPCRD 29, (2000),  
 Hf(298)= 90.6 kcal REF = Wang & Frenklach J. Phys. Chem 98, (1994), 11465.  
 Max Lst Sq Error Cp @ 1300 K 0.53%  
 C10H7-CCH T 7/98C 12.H 8. 0. 0.G 200.000 6000.000 B 152.19552 1  
 2.34108373E+01 3.12979308E-02-1.13777419E-05 1.85217551E-09-1.11546889E-13 2  
 3.49196941E+04-1.00594596E+02-2.59169367E+00 8.63306190E-02-1.76590976E-05 3  
 -5.26006488E-08 3.15924760E-11 4.27720678E+04 3.73574503E+01 4.55914299E+04 4

132-64-9

C12H8O DIBENZOFURAN SIGMA = 2 IA=31.1705 IB=139.72989 IC=176.8996  
 NU=3053(4),3050(4),1622,1601,1584,1564,1510,1499,1444,1416,1389,1385,1305,1290,  
 1261,1247,1209,1171(2),1123,1107,1048,1011,1010,1007,986,970,949,888,842,832,  
 823,796,752,738,705,674,623,617,597,579,518,500,458,,430,406,322,289,244,138,118  
 REF=Dorofeeva, Private communication HF298=55.2 kJ REF=Dorofeeva, Iorish,  
 Moiseeva J. Chem. Eng. Data (1999) 44,516-523. {HF298=47.3+/-4.8 kJ REF=NIST  
 WEBBOOK 2000 Sabbah & Antipine 1987} Max Lst Sq Error Cp @ 200 K 0.79%, Cp @  
 1300 K 0.59%  
 C12H8O T 2/02C 12.H 8.0 1. 0.G 200.000 6000.000 C 168.19492 1  
 2.38928699E+01 3.42239370E-02-1.25916314E-05 2.06592304E-09-1.25089220E-13 2  
 -4.81449779E+03-1.07327684E+02-1.94754604E+00 6.63215475E-02 5.55418713E-05 3  
 -1.35401425E-07 6.29515620E-11 4.01745217E+03 3.50605098E+01 6.63742782E+03 4

262-12-4

C12H8O2 Dibenzo-p-Dioxin SIGMA=4 IA=39.2555 IB=176.1272 IC=215.3827  
 NU=3053(4),3051(4),1634,1593,1586,1572,1505,1502,1438,1429,1407,1399,1316,1310,  
 1293,1263,1245,1222,1172,1171,1136,1112,1031,1019,1008(2),954,953,873,859,847,  
 842,829,737,727(2),690,689,653,645,583,547,478,459,457,455,436,373,298,254.5,  
 246.5,219,114.7,50.96 REF=Dorofeeva unpublished results, {HF298=-59.2+/-3.8 kJ.  
 REF=Chirico et.al J.Chem.Thermodynam 22, (1990),1075-1096 HF298(Solid)=-148.7  
 +/-4.4 kJ NIST WEBBOOK 2000, Lukyanova, Kolesov et al Zh. Fiz. Khim,71 (1997),  
 406-408} HF298=50.1+/-2.2 kJ REF=Pimenova et al J.Chem. Thermo 34 (2002),385.  
 Max Lst Sq Error Cp @ 1300 K 0.56%.  
 C12H8O2 T 8/03C 12.H 8.0 2. 0.G 200.000 6000.000 B 184.19432 1  
 2.60370044E+01 3.50780491E-02-1.29210307E-05 2.12161308E-09-1.28529989E-13 2  
 -1.82365905E+04-1.17407370E+02-1.48214627E+00 7.51205359E-02 3.87198163E-05 3  
 -1.19145352E-07 5.69742514E-11-9.05611402E+03 3.29719044E+01-6.02561065E+03 4

444160-65-0

C12H9 1-C10H7CH=CH\* 1-Naphtyl-Vinyl radical STATWT = 2 Ia = 52.035181  
 Ib = 97.671628 Ic = 148.44918 Ir = 2.73405 ROSYM = 2 V(2)= 4.4 kcal  
 NU = 3173,3130,3124,3120,3110,3106,3097,3094,3030,1621,1607,1590,1568,1512,1452,  
 1433,1393,1378,1353,1256,1228,1220,1206,1161,1154,1139,1079,1032,1003,948,934,  
 915,886,876,863,843,832,782,779,762,719,695,661,610,576,528,506,480,462,427,403,  
 321,255,193,172,116. REF = Curran et al. JPCRD 29, (2000), 463  
 Hf(298)= 112.3 kcal REF = Wang & Frenklach J. Phys. Chem 98, (1994), 11465.  
 Max Lst Sq Error Cp @ 200 K 0.72%  
 1-C10H7-CH=CH\* T 7/98C 12.H 9. 0. 0.G 200.000 6000.000 B 153.20346 1  
 2.44441957E+01 3.26961470E-02-1.18995546E-05 1.93488254E-09-1.16386321E-13 2  
 4.52471489E+04-1.05926333E+02-1.42935703E+00 7.39465043E-02 2.97653847E-05 3  
 -1.09318395E-07 5.40951470E-11 5.35782225E+04 3.42505526E+01 5.65112316E+04 4

Table 4 (continued)

304905-16-6

C10H7C\*=CH2 1,-Vinyl Naphthalene STATWT = 2 Ia = 58.410493 Ib = 92.899705  
 Ic = 150.72887 Ir = 3.231365 ROSYM = 2 V(2) = 4.6 kcal NU = 3132,3126,  
 3116,3114,3104,3101,3095,3052,2998,1882,1607,1555,1524,1494,1435,1429,1413,1374,  
 1358,1304,1254,1215,1166,1159,1146,1130,1075,1034,1013,948,947,922,917,852,847,  
 838,818,776,767,749,706,683,611,578,532,524,483,474,431,419,402,339,257,176,163,  
 125. REF = Curran et al. JPCRD 29, (2000), 463 Hf(298)= 98.52 kcal  
 REF = Marinov et al, Comb. Sci. Technol, 116-117, (1996), 211. Max Lst Sq  
 Error Cp @ 200 K 0.65 %.

1-C10H7-C*=CH2	T 7/98C	12.H	9.	0.	0.G	200.000	6000.000	B	153.20346	1
	2.45125261E+01	3.26372895E-02	-1.18731749E-05	1.93107796E-09	-1.16216496E-13					2
	3.83327553E+04	-1.05844161E+02	-1.43370275E+00	7.71544298E-02	1.83225763E-05					3
	-9.54787152E-08	4.85269141E-11	4.65789858E+04	3.40801712E+01	4.95769059E+04					4

3474-38-2

C12H9 O-BIPHENYL RAD SIGMA=1 STATWT=2 IA=27.88 IB=154.77 IC=174.50  
 Ir=6.965 ROSYM=2 V(2)=524.63 cm-1 NU=3080(2),3072,1612,1507,1285,1190,1030,  
 1003,742,315,838,400,609,1595,1452,1376,1316,1156,1090,608,407,970,903,736,698,  
 4847,174,980,897,780,545,441,260,965,838,400,3069(2),3068(2),1570,1432,1383,1283,  
 ,1156,1074,626,116,1597,1482,1176,1008,965 HF298=427.73 kJ HF0=451.89 kJ  
 REF=BURCAT ZELEZNIK AND MCBRIDE NASA TM-83800 1985 MAX LST SQ ERROR Cp @ 200 K  
 0.84 %.

C12H9,o-bipheny	g	8/00C	12.H	9.	0.	0.G	200.000	6000.000	B	153.19986	1
	2.25692222E+01	3.45619984E-02	-1.27020877E-05	2.08111819E-09	-1.25849407E-13						2
	4.05907457E+04	-9.57787051E+01	4.07668089E-01	5.42794698E-02	7.12515775E-05						3
	-1.44404112E-07	6.48497982E-11	4.85351870E+04	2.81980814E+01	5.14438013E+04						4

2051-62-9

C12H9Cl CHLOROBIPHENYL CALCULATED USING BOZZELLI & RITTER'S PROGRAM AND  
 EXTRAPOLATED TO 5000 K SIGMA=2 HF298=148.55 kJ

C12H9CL	T	2/92C	12H	9CL	1	0G	298.150	5000.000	E	188.65616	1
	0.25609923E+02	0.35292178E-01	-0.13556100E-04	0.23746797E-08	-0.15591758E-12						2
	0.58630132E+04	-0.11039461E+03	-0.72831130E+01	0.11977430E+00	-0.82814312E-04						3
	0.15585591E-07	0.42704031E-11	0.15413066E+05	0.61459201E+02	0.17866357E+05						4

86-74-8

C12H9N CARBAZOLE, 9-AZAFLUORENE, DIBENZO-PYRROLE SIGMA=2 IAIBIC=938534.8  
 NU=3421,3094,3084,3077,3055,3050,3039,3030,2940,1625,1594,1576,1490,1481,1452,  
 1449,1380,1334,1320,1288,1233,1205,1204,1158,1152,1136,1118,1107,1022,1012,995,  
 989,939,926,910,893,880,856,835,771,747,741,737,722,691,658,616,566,548,505,467,  
 445,425,410,310,299,222,220,139,104. HF298=200.7+/-4.9 kJ REF= Das et al  
 JPCRD 22 (1993), 659 Max Lst Sq Error Cp @ 200 K 0.79%

C12H9N CARBAZOLE	T	5/99C	12.H	9.N	1.	0.G	200.000	6000.000	B	167.21020	1
	2.55905657E+01	3.50572236E-02	-1.28150596E-05	2.09379140E-09	-1.26416159E-13						2
	1.21368335E+04	-1.15714967E+02	-2.39694034E+00	7.70529957E-02	3.99731799E-05						3
	-1.26020660E-07	6.11915294E-11	2.12953973E+04	3.66013145E+01	2.41385241E+04						4

Table 4 (continued)

826-74-4

C12H10 1-C10H7CH=CH2 Vinyl 1-Naphthalene Ia = 52.618944 Ib = 100.59202  
 Ic = 152.02459 Ir = 3.39278 ROSYM = 2 V(2) = 3.06 kcal Nu = 3168,3130,  
 3124,3120,3110,3105,3096,3093,3083,3074,1644,1620,1591,1576,1513,1455,1435,1416,  
 1393,1379,1348,1295,1250,1226,1217,1164,1154,1139,1089,1035,1021,1000,989,948,  
 935,915,886,883,847,843,788,780,768,722,702,685,587,527,498,482,462,428,397,334,  
 250,199,175,119. REF = Curran et al. JPCRD 29, (2000), 463 Hf(298) = 51.4 kcal  
 REF = NIST 1994 Max Lst Sq Error Cp @ 200 K 0.75%  
 1-C10H7CH=CH2 T11/98C 12.H 10. 0. 0.G 200.000 6000.000 B 154.21140 1  
 2.36421335E+01 3.60544766E-02-1.31138294E-05 2.13119639E-09-1.28115416E-13 2  
 1.46625473E+04-1.02784235E+02-1.19668570E+00 7.06115758E-02 4.27863652E-05 3  
 -1.21989834E-07 5.83744402E-11 2.29191651E+04 3.30370914E+01 2.58653366E+04 4

92-52-4

C12H10 BIPHENYL SIGMA=4 IA=28.67 IB=155.08 IC=175.34 IR=7.166 ROSYM=2  
 V(2)=524.63 NU=3083(2),3052(2),3031,1583(2),1497(2),1275,1151,1025,  
 1019,996,733,969,841,399,1603,1448,1357,1185,1145,1032,606(2),302,904,778,695,  
 543,487,120,955,775,696,531,470,246,3086(2),3067(2),1608,1440,1397,1182,1162(2),  
 1077,140,970,834,397,3038,1046,1012,993,738 REF=KATON AND LIPPINCOTT Spectro-  
 chim. Acta 11, (1959), 627 HF298=182.13 KJ. REF=BURCAT ZELEZNIK & MCBRIDE NASA TM-  
 83800 (1985); Chirico et al J. Chem Thermodyn 21, (1989), 1307 MAX LST SQ ERROR  
 @ 1300 K 0.85 %  
 C12H10,biphenyl g 8/00C 12.H 10. 0. 0.G 200.000 6000.000 B 154.20780 1  
 2.28963620E+01 3.68453189E-02-1.35016357E-05 2.20802787E-09-1.33358137E-13 2  
 1.07395923E+04-1.00509573E+02 1.94600056E-01 5.35259888E-02 8.55000841E-05 3  
 -1.63903525E-07 7.29975666E-11 1.90021492E+04 2.72148992E+01 2.19050792E+04 4

304905-13-3

1-C10H7CH2CH2\* - Ethyl 1-Naphthalene Radical STATWT = 2 Ia = 51.627582  
 Ib = 105.1585 Ic = 155.5285 Ir(-CH2CH2\*) = 3.68853 ROSYM = 2 V(3)=3.0 kcal  
 Ir(-CH2\*)=0.276085 ROSYM = 3 V(3) = 3.0 kcal Nu=3193,3128,3119,3118,3104,  
 3103,3094,3092,3088,2954,2859,1623,1599,1581,1514,1456,1435,1429,1411,1397,1380,  
 1362,1289,1246,1220,1217,1180,1159,1154,1139,1083,1075,1031,1022,975,946,936,  
 913,887,850,836,806,781,778,757,717,692,617,589,527,514,508,472,462,426,400,319,  
 233,202,170,154. REF = Curran et al. JPCRD 29, (2000), 463 Hf(298) = 70. Kcal  
 REF = THERM estimate Max Lst Sq Error Cp @ 200 K 0.64%.  
 C10H7-CH2CH2\* T 7/98C 12.H 11. 0. 0.G 200.000 6000.000 B 155.21934 1  
 2.47911542E+01 3.71007852E-02-1.34341683E-05 2.17751785E-09-1.30703605E-13 2  
 2.36520512E+04-1.07491651E+02-1.76566815E+00 8.31852329E-02 1.56729046E-05 3  
 -9.56306134E-08 4.90427294E-11 3.20816383E+04 3.56277471E+01 3.52251666E+04 4

95591-52-9

1-C10H7CH\*CH3 - Ethyl 1-Naphthalene Radical STATWT = 2 Ia=51.627582  
 Ib=105.1585 Ic=155.5285 Ir(-CH\*CH3)= 4.03467 ROSYM = 2 V(3)=2.9 kcal  
 Ir(-CH3)= 0.417138 ROSYM = 3 V(3)=2.8 kcal Nu = 3193,3128,3119,3118,  
 3104,3103,3094,3092,3088,2954,2859,1623,1599,1581,1514,1456,1435,1429,1411,1397,  
 1380,1362,1289,1246,1220,1217,1180,1159,1154,1139,1083,1075,1031,1022,975,946,  
 936,913,887,850,836,806,781,778,757,717,692,617,589,527,514,508,472,462,426,400,  
 319,233,202,170,154. REF = Curran et al. JPCRD 29, (2000), 463  
 Hf(298) = 52.7 kcal REF = NIST 94 Max Lst Sq Error Cp @200 K 0.63%  
 1-C10H7-CH\*-CH3 T11/98C 12.H 11. 0. 0.G 200.000 6000.000 B 155.21934 1  
 2.45873044E+01 3.73929821E-02-1.36001742E-05 2.21047875E-09-1.32883841E-13 2  
 1.49850894E+04-1.05426141E+02-1.14973681E+00 7.78725206E-02 2.87023997E-05 3  
 -1.08719393E-07 5.37519164E-11 2.33370112E+04 3.42336399E+01 2.65195183E+04 4

Table 4 (continued)

1127-76-0

C12H12 1-C10H7CH2CH3 1- Ethyl Naphthalene Ia = 61.540903 Ib = 92.900467  
 Ic = 147.16558 Ir(C2H5)= 4.472813 ROSYM = 2 V(3) = 2.8 kcal  
 Ir(CH3)= 0.417138 ROSYM = 3 V(3)=2.8 kcal. Nu= 3353,3265,3229,3172,3074,  
 2981,2950,2894,1919,1863,1832,1796,1682,1636,1600,1512,1476,1460,1458,1456,1437,  
 1399,1382,1369,1366,1326,1259,1246,1226,1216,1172,1154,1140,1087,1069,1048,1031,  
 1017,960,938,933,914,893,862,838,786,784,768,734,703,641,630,578,553,572,478,  
 462,429,421,316,289,203,186,171. REF = NIST Webbook 1997 Hf(298)= 23.16 kcal  
 REF=Stull, Westroom & Sinke 1969. Max Lst Sq Error Cp @ 1300 K 0.64%  
 1-C10H7-C2H5 T 7/98C 12.H 12. 0. 0.G 200.000 6000.000 B 156.22728 1  
 2.53697727E+01 4.04594180E-02-1.49784208E-05 2.46402471E-09-1.49382751E-13 2  
 -8.20299732E+02-1.14459910E+02 1.98405802E-02 6.20844325E-02 7.79624479E-05 3  
 -1.55438421E-07 6.85371120E-11 8.47514808E+03 2.80182938E+01 1.16544980E+04 4

773-99-9

C10H7CH2CH2OH 1-Naphtyl-ethanol Ia= 65.973401 Ib=130.12903 Ic=178.19701  
 Ir(-CH2CH2OH)=20.2848 ROSYM = 2 V(3)=2.87 kcal/mole Ir(-CH2OH)=4.75277  
 ROSYM=2 V(3)=2.75 kcal Ir(-OH)=0.139517 ROSYM=1 V(3)=1.03 kcal  
 Nu=3642,3129,3121,3120,3106,3102,3095,3094,3024,3012,2975,2902,1622,1597,1579,  
 1515,1469,1455,1448,1435,1396,1383,1380,1368,1347,1303,1248,1226,1221,1183,  
 1170,1159,1154,1140,1078,1060,1037,1029,984,948,934,916,913,876,858,836,826,  
 782,779,764,720,686,642,577,548,505,482,463,447,426,407,374,318,249,176,170.  
 REF = Curran et al. JPCRD 29, (2000), 463 Hf(298)= -12.6 kcal  
 REF = NIST 1994 Max Lst Sq Error Cp @ 200 K 0.68%  
 1-C10H7CH2CH2OH T11/98C 12.H 12.O 1. 0.G 200.000 6000.000 B 172.22668 1  
 2.58268752E+01 4.06457048E-02-1.47684231E-05 2.39996250E-09-1.44280394E-13 2  
 -1.85903264E+04-1.11344593E+02 1.48378862E-01 7.18508197E-02 5.76461168E-05 3  
 -1.42124444E-07 6.64389673E-11-9.83811550E+03 3.01527814E+01-6.34052999E+03 4

112-40-3

N-C12H26 DODECANE REF=TRC11/75 TO 1000 K. EXTRAPOLATED USING WILHOIT'S  
 POLYNOMIALS. HF298=-69.52 kcal  
 N-DODECANE T 5/99C 12.H 26. 0. 0.G 200.000 6000.000 C 170.33844 1  
 3.70187925E+01 5.54721488E-02-1.92079548E-05 3.08175574E-09-1.84800617E-13 2  
 -5.26984458E+04-1.61453501E+02 2.13264480E+01-3.86394002E-02 3.99476113E-04 3  
 -5.06681097E-07 2.00697878E-10-4.22475053E+04-4.85848300E+01-3.49836226E+04 4

260-94-6

C13H9N ACRIDINE, 10-AZAANTHRACENE, DIBENZO[b,c]PYRIDINE SIGMA=2  
 IAIBIC=1456147.2 E-117 NU=3085(2),3075,3055(2),3037(2),3014(2),1627,1622,1578,  
 1556,1516,1480,1464,1441,1402,1397,1373,1360,1317,1274,1266,1232,1168,1158,1140,  
 1121,1109(3),999,974,965,955,934,939,905,901,861,851,814,785,744,735,712,655,  
 617,600,581,523,477,469,417,401,275,240,217,156,139,106. HF298=273.9+/-4.1 kJ  
 REF= Das et al JPCRD 22 (1993), 659 Max Lst Sq Error Cp @ 200 K 0.89%  
 C13H9N ACRIDINE T 5/99C 13.H 9.N 1. 0.G 200.000 6000.000 B 179.22120 1  
 2.58635113E+01 3.78898227E-02-1.39284598E-05 2.28395317E-09-1.38235768E-13 2  
 2.04600506E+04-1.17880104E+02-8.48162121E-01 6.17087256E-02 8.87124926E-05 3  
 -1.77383638E-07 7.97811734E-11 2.99816376E+04 3.14075642E+01 3.29424103E+04 4



Table 4 (continued)

229-87-8

C13H9N PHENANTHRIDINE, 9-AZAPHENANTHRENE, 3,4-BENZOQUINOLINE SIGMA=2  
 IAIBIC=1612079.0 E-117 NU=3082,3072,3064,3037,3047,3037,3034,3019,3002,1615,  
 1600,1587,1575,1525,1485,1455,1445,1425,1405,1390,1345,1290,1245,1227,1190,1173,  
 1163,1135,1110,1094,1046,1035,1001,970,943,895,876,874,832,819,791,775,750,725,  
 713,712,711,620,576,548,536,505,494,460,435,415,408,395,279,240,234,170,108.  
 HF298=240.5+/-4.2 kJ REF= Das et al JPCRD 22 (1993),659 Max Lst Sq Error Cp  
 @ 1300 K 0.60%  
 C13H9N PHENANTHRI T 5/99C 13.H 9.N 1. 0.G 200.000 6000.000 B 179.22120 1  
 2.65281408E+01 3.72382530E-02-1.36796636E-05 2.24215437E-09-1.35664146E-13 2  
 1.63827924E+04-1.21651719E+02-3.42969371E+00 8.74937697E-02 2.13315768E-05 3  
 -1.06800353E-07 5.35979203E-11 2.60563650E+04 4.04426399E+01 2.89253366E+04 4

20062-22-0

C14H6N6O12 trans HexaNitroStilbene (HNS) C6H2(NO2)3-CH=CH-C6H2(NO2)3 SIGMA=1  
 STATWT=1 IA=315.8696 IB=1077.1432 IC=1347.4667 [Ir(NO2 apex)=6.2354 ROSYM=2  
 V(3)=2448. cm-1]x2 [Ir(NO2 side)=6.3119 ROSYM=2 V(3)=2448. cm-1]x4 [ROSYM=2  
 Ir(C6H2(NO3)2)=85.3947 V(3)=2448 cm-1]x2 Nu=3272(4)3220,3216,1719,1682,  
 1680(2),1678,1657,1655,1635(2),1613(2),1494,1486,1431.3(2),1411,1407,1401,1396,  
 1394,1392,1359,1356,1340,1300,1242,1225,1202(2),1191(2),1099(2),964(2),963(3),  
 949(2),935.5(2),896,836,834,836,821,795,783,776,772,752,749,739,735,725(2),703,  
 687,671,651,572,555,544(2),501,495,469(2),428,405,371,368,363,349,344,326(2),  
 310,294,266,187.5(2),184(2),159,155,152,129,107(2),93.4,88.9,74.8 REF=B3LYP/  
 6-31G(d) HF298=238.4 kJ HF0=285.396 kJ REF=Maranz & Armstrong JCEng Data 13,  
 (1968),455 HF298(s)=58.07 kJ REF=ibid {HF298(s)=68+/-10 kJ REF=Rouse JCEng Data  
 21, (1976),1620} Max Lst Sq Error Cp @ 1300 K 0.59%.  
 C14H6N6O12 HNS A 8/05C 14.H 6.N 6.O 12.G 200.000 6000.000 B 450.23068 1  
 6.55884300E+01 4.18322255E-02-1.67060887E-05 2.87246732E-09-1.79132012E-13 2  
 1.45706534E+03-3.06012560E+02 7.35141779E+00 1.52247536E-01-3.69079521E-06 3  
 -1.32914128E-07 7.04138717E-11 1.99760393E+04 6.96545894E+00 2.86727660E+04 4

120-12-7

C14H10 ANTHRACENE SIGMA=4 IA=39.0139 IB=185.153 IC=224.165 NU=390,624,753,  
 1007,1159,1260,1402,1478,1559,3028,3050,3081,139,488,760,860,980,236,473,739,  
 948,234,652,907,1146,1271,1316,1447,1625,3023,3056,3083,288,526,775,886,915,970,  
 599,809,999,1063,1166,1344,1398,1455,1538,3050,3092,390,523,901,1102,1180,1223,  
 1334,1490,1633,3055,3071,105,166,468,727,876,952 HF298= 230.1 KJ REF=KUDCHADKER  
 KUDCHADKER & ZWOLINSKI J. Chem. Thermodynamics 11, (1979), 1051 MAX LST SQ  
 ERROR @ 200 K 0.87%.  
 C14H10 ANTHRACENE T 1/94C 14H 10 0 OG 200.000 6000.000 B 178.23340 1  
 0.26567127E+02 0.39790904E-01-0.14577610E-04 0.23850396E-08-0.14413090E-12 2  
 0.14850923E+05-0.12283160E+03-0.15665980E+01 0.69536302E-01 0.78609880E-04 3  
 -0.17056214E-06 0.78003880E-10 0.24656643E+05 0.33282196E+02 0.27674511E+05 4

85-01-8

C14H10 PHENANTRENE SIGMA=2 IA=51.7329 IB=147.737 IC=199.470 NU=247,408,548,  
 711,832,1038,1094,1144,1163,1203,1247,1304,1352,1431,1443,1526,1602,1626,3002,  
 3037,3057,3072,3082,123,279,395,513,594,726,763,791,880,946,969,108,234,426,441,  
 494,713,735,819,874,951,441,536,619,712,876,1001,1040,1095,1173,1227,1282,1340,  
 1430,1458,1502,1572,1616,3019,3034,3047,3064,3094 HF298=207.1 KJ REF=KUDCHADKER  
 KUDCHADKER & ZWOLINSKI J. Chem. Thermodynamics 11, (1979), 1051. MAX LST SQ ERROR  
 @ 200 K 0.73%.  
 C14H10 PHENANTHRE T 1/94C 14H 10 0 OG 200.000 6000.000 B 178.23340 1  
 0.26602474E+02 0.39769744E-01-0.14572026E-04 0.23843296E-08-0.14409548E-12 2  
 0.12132838E+05-0.12266672E+03-0.33646717E+01 0.85073271E-01 0.37531110E-04 3  
 -0.12664499E-06 0.61445705E-10 0.22019878E+05 0.40596218E+02 0.24908263E+05 4

Table 4 (continued)

103-30-0

C14H12 t-STILBENE C6H5-CH=CH-C6H5 SIGMA=2 STATWT=1 IA=31.06328 IB=312.8672  
 IC=351.54277 [Ir(C6H5)=10.50126 ROSYM=2 V(3)=1539. cm-1]x2 Nu=3154(2),  
 3091(2),3069(2),3038(2),2959(2),2907(2),1965,1944,1874,1795,1738,1606,1580,  
 1501(2),1453,1392(2),1339(2),1326(2),1212(2),1182(2),1155,1103(2),1072(2),  
 1033(2),985(2),958(2),906(2),845(2),766(2),735(2),691(2),[671,657,650,630,627],  
 547,534,[492,463,378(2),309,276,213,169,115.6,94.8] REF=IR Webbook 2005 [] PM3  
 HF298=223.3+/-4. kJ HF0=255.957 kJ REF=Maranz & Amertrout JCEng Data 13,(1968),  
 455 HF298(s)=136.7 kJ REF=ibid Max Lst Sq Error Cp @ 1300 K 0.58%.  
 C14H12 t-Stilbene A 8/05C 14.H 12. 0. 0.G 200.000 6000.000 B 180.24508 1  
 2.76375532E+01 4.24921182E-02-1.55591594E-05 2.54398669E-09-1.53646182E-13 2  
 1.36607137E+04-1.22903898E+02-3.74515101E-01 7.65060608E-02 6.07336685E-05 3  
 -1.49456020E-07 6.95516583E-11 2.32938089E+04 3.16766006E+01 2.68566638E+04 4

103-29-7

C14H14 BIBENZYL C6H5C2H4C6H5 SIGMA(Exter)=2 STATWT=1 IA=33.8630 IB=314.7877  
 IC=340.5755 (Ir(C6H5)=15.115526 ROSYM=2 V(3)=1035 cm-1)x2 Ir(C6H5CH2)=61.97503  
 ROSYM=2 V(3)=980. cm-1 Nu=3208(2),3195(2),3186(2),3171.5(4),3098,3076,3052,  
 3042,1665(2),1644(2),1546(2),1531,1514,1501(2),1388,1374,1359,1361(2),1312,1311,  
 1234(2),1213(2),1192(2),1177,1121,1098,1058(2),1020,1018(2),1010,993,992,964(2),  
 865,860(2),807,780,775,758,716(2),637,636,625,538,532,483,418(2),374,317,295,  
 237,120.8,61.4 REF=Burcat G3B3 calc. HF298=135+/-1.3 kJ REF=Coleman & Pilcher  
 Trans Faraday Soc. 62,(1966),821-827. {HF298=143.51 KJ REF=Benson.} Max Lst.  
 Sq. Error Cp @ 200 K 0.9%. HF298(Liq)=52.62 kJ HF298(solid)=51.5+/-1.3 kJ  
 C14H14 Bibenzyl T 5/04C 14.H 14. 0. 0.G 200.000 6000.000 B 182.26096 1  
 2.65979897E+01 4.68689340E-02-1.69056103E-05 2.73737090E-09-1.64235887E-13 2  
 3.18810786E+03-1.14827874E+02 1.30521842E+00 5.76220698E-02 1.22418244E-04 3  
 -2.18120750E-07 9.59096665E-11 1.26627763E+04 2.90742354E+01 1.63088384E+04 4

129-00-0

C16H10 PYRENE SIGMA=2 IA=82.22 IB=149.195 IC=231.42 NU=3020,3019,3014,  
 3013,3003,3002,2996,2994,2993,2992,1654,1621,1604,1603,1566,1499,1493,1432,1427,  
 1425,1394,1384,1296,1281,1230,1220,1217,1203,1183,1164,1151,1134,1074,1071,1049,  
 1028,999,992,988,982,975,922,916,911,850,822,807,800,778,777,756,715,704,671(2),  
 569,564,524,523,504,485,483(2),440,392,391,341,255,245,210,149.5,95.1  
 REF=C.MELIUS DATABASE BAC/MP22 #255 AA70 HF298=225.7 KJ REF=Smith et. al,  
 J. Chem. Thermody 12,(1980),919 Max Lst Sq Error Cp @ 200 K 0.8%.  
 C16H10 PYRENE T10/96C 16H 10 0 OG 200.000 6000.000 B 202.25540 1  
 0.29910014E+02 0.42668069E-01-0.15733834E-04 0.25851725E-08-0.15667980E-12 2  
 0.12786491E+05-0.14186953E+03-0.40420321E+01 0.91549657E-01 0.51443344E-04 3  
 -0.15276576E-06 0.73087530E-10 0.24094241E+05 0.43665312E+02 0.27145316E+05 4

54915-71-8

C16H33 n-Hexadecyl Secondary Radical SIGMA=1 STATWT=2 REF=THERM PROGRAM FROM  
 PARENT n-C16H34 - Secondary Proton. HF298=-43.42 kcal Max Lst Sq Error Cp @  
 1500 K 0.46%  
 C16H33 Hexadecyl S05/01C 16.H 33. 0. 0.G 298.150 5000.000 F 225.43802 1  
 3.98439293E+01 8.75342823E-02-3.29289436E-05 5.80687633E-09-3.88795213E-13 2  
 -4.21912004E+04-1.63931267E+02 6.75173475E+00 1.22107685E-01 4.28435207E-05 3  
 -1.27980217E-07 5.58389417E-11-2.94419695E+04 2.27406424E+01-2.18496676E+04 4

Table 4 (continued)

544-76-3

C16H34 n-Hexadecane (Cetane) SIGMA=2 ROSYM=2x13 STATWT=1 HF298=-89.51 kcal  
 REF=NIST 94 + Thergas + THERM Max Lst Sq Error Cp @ 1500 K 0.36

C16H34 Hexadecan	S	5/01C	16.H	34.	0.	0.G	298.150	5000.000	E	226.44596	1	
							3.93197519E+01	9.11470601E-02	-3.39721140E-05	5.94437262E-09	-3.95796331E-13	2
							-6.51665791E+04	-1.66160224E+02	-2.28147400E+00	1.85127971E-01	-9.91782207E-05	3
							1.43398377E-08	3.73230542E-12	-5.17449265E+04	5.60024917E+01	-4.50429238E+04	4

92-24-0

C18H12 Naphthacene (bi-naphthalene) SIGMA=4 IAIBIC=8764. E-114 REF=Dorofeeva & Gurvich Preprint IVTAN 1-238 1988 CALCULATED BY GROUP APPROXIMATIONS. EXTRAPOLATED from 1600 to 5000 K using Wilhoit's POLYNOMIALS. HF298=290. kJ Max Lst Sq Error Cp @ 200 K 0.87%

C18H12	T	2/00C	18.H	12.	0.	0.G	200.000	5000.000	D	228.29328	1	
							2.95586152E+01	5.85686068E-02	-2.41993527E-05	4.54440129E-09	-3.18688238E-13	2
							2.00626643E+04	-1.40019146E+02	-3.28166681E+00	9.79369796E-02	7.11673376E-05	3
							-1.83222246E-07	8.55531781E-11	3.11971518E+04	4.09026837E+01	3.48787842E+04	4

217-59-4

C18H12 TRIPHENYLENE SIGMA=6 IAIBIC=8620. E-114 REF= Dorofeeva & Gurvich 1988 Preprint IVTAN 1-238 1988 CALCULATED BY GROUP APPROXIMATIONS. EXTRAPOLATED from 1600 to 5000 K using Wilhoit's POLYNOMIALS. HF298=274.2 kJ Max Lst Sq Error Cp @ 200 K 0.73%

C18H12	T	2/00C	18.H	12.	0.	0.G	200.000	5000.000	D	228.29328	1	
							2.96559160E+01	5.84891457E-02	-2.41670003E-05	4.53859641E-09	-3.18308300E-13	2
							1.82004887E+04	-1.40400680E+02	-2.34768051E+00	9.51418980E-02	7.53347608E-05	3
							-1.86896616E-07	8.69659877E-11	2.91123994E+04	3.62593629E+01	3.29784918E+04	4

5821-51-2

C20H10 Corannulene (5 benzenes around cyclopentane; not planar) SIGMA=5 STATWT=1  
 IA=164.8814 IB=164.8927 IC=316.5297 Nu=3187(5),3176(5),1870,1805(2),1798(2),  
 1621,1662,1639(2),1614(2),1607(2),1498(2),1479(2),1471(2),1372,1359(2),1279(2),  
 1134,1026(2),992.5(2),980.6(2),976,961,913,890(2),856(2),825(2),806(2),782,  
 700(2),675,665(2),617(2),592(2),576(2),484,460(2),450(2),434(2),316(2),267.5(2),  
 173,135(2) HF298=463.7+/-7.3 kJ REF=Klyobayashi et al JACS 117, (1995), 3270.  
 {HF298=460.7 kJ REF=Slyden & Liebman Chem. Rev 101, (2001), 1563; HF298=459.6 kJ  
 REF=Armitage & Bird Tetrahed. Lett. 34, (1993), 5811.} Max Lst Sq Error Cp @  
 1300 K 0.67%.

C20H10	CORANNUL	A	5/05C	20.H	10.	0.	0.G	200.000	6000.000	B	250.29340	1
							3.06657686E+01	5.29599580E-02	-1.95066691E-05	3.20304721E-09	-1.94054165E-13	2
							4.01719213E+04	-1.49703428E+02	-3.53752796E+00	8.75243280E-02	8.69001904E-05	3
							-1.87189202E-07	8.34302617E-11	5.24972787E+04	4.13547788E+01	5.57699732E+04	4

Table 4 (continued)

198-55-0

C20H12 PERYLENE SIGMA=4 STATWT=1 IA=123.9686 IB=252.2375 IC=384.9360  
 Nu=3059(2), 3034(2), 3018(2), 3015(2), 3000(2), 2997(2), 1642, 1624, 1609, 1598, 1594,  
 1508, 1495, 1472, 1448, 1435, 1427, 1367, 1345, 1318, 1310, 1301, 1291, 1285, 1250, 1197,  
 1185, 1173(3), 1131, 1113, 1099, 1086, 1078, 1063, 1001, 993(2), 986, 983, 970, 949, 927, 922,  
 914, 907, 898, 837, 819, 793, 775, 770, 765, 765, 762(2), 754, 750, 644, 633, 616, 604, 567, 545,  
 523(2), 518(2), 463, 446, 443, 416(2), 345, 338, 292, 243, 236, 204, 173, 118, 93.6, 9.4  
 HF298=196.7+/-20.75 kJ REF=Melius MP2 database AA0P 1996 {HF298=309.6+/-4.2 kJ  
 REF=Pedley & Rylance 1977; HF298=280.3 REF=NIST 94 est.} {HF298(sol)=182.7  
 +/-0.46 kJ REF=Westrum Wong, Mol. Cryst. Liq. Cryst 61, (1980), 207} Max Lst Sq  
 Error Cp @ 200 K 0.78%.

C20H12 Perylene	T03/05C 20.H 12.	0.	0.G	200.000	6000.000	B 252.30928	1
	3.76638387E+01	5.21705496E-02	-1.92428529E-05	3.16234274E-09	-1.91688461E-13		2
	6.71965532E+03	-1.82570533E+02	-4.32109609E+00	1.11780773E-01	6.68921546E-05		3
	-1.92620044E-07	9.18304028E-11	2.07289880E+04	4.70286681E+01	2.46626488E+04		4

135-48-8

C22H14 PENTACENE (5 benzene rings in a row) SIGMA=4 IAIBIC=33150 E-114  
 REF= Dorofeeva & Gurvich 1988 Preprint IVTAN 1-238 1988 CALCULATED BY GROUP  
 APPROXIMATIONS. EXTRAPOLATED from 1600 to 5000 K using Wilhoit's POLYNOMIALS.  
 HF298=355 kJ Max Lst Sq Error Cp @ 200 K 0.73%

C22H14 PENTACENE	T 2/00C 22.H 14.	0.	0.G	200.000	5000.000	D 278.35316	1
	3.58785167E+01	7.04948125E-02	-2.91706302E-05	5.48297466E-09	-3.84747182E-13		2
	2.47407667E+04	-1.74816699E+02	-3.96027507E+00	1.17841522E-01	8.87303666E-05		3
	-2.25804141E-07	1.05493453E-10	3.82520100E+04	4.47088716E+01	4.26964427E+04		4

222-93-5

C22H14 Pentafene SIGMA=2 IAIBIC=39980 E-114 REF= Dorofeeva & Gurvich 1988  
 Preprint IVTAN 1-238 1988 CALCULATED BY GROUP APPROXIMATIONS. EXTRAPOLATED  
 from 1600 to 5000 K using Wilhoit's POLYNOMIALS. HF298=355 kJ Max Lst Sq  
 Error Cp @ 200 K 0.74%

C22H14 Pentafene	T 2/00C 22.H 14.	0.	0.G	200.000	5000.000	D 278.35316	1
	3.61985500E+01	7.00125090E-02	-2.89502373E-05	5.43945174E-09	-3.81596217E-13		2
	2.34318128E+04	-1.75725046E+02	-3.89059592E+00	1.18588915E-01	8.58495971E-05		3
	-2.22381690E-07	1.04152452E-10	3.70146204E+04	4.50315090E+01	4.14937260E+04		4

94227-23-3

C24CL12 PerChloroCoronene STATWT=1 SIGMA=12 IA=1250.17392 IB=1250.63028  
 IC=2463.30815 NU=24.3(2), 41.5, 45.2, 52.07(2), 59.9(2), 64.5, 68.8, 144(2), 166(2),  
 190.3(2), 203.6, 233(2), 240, 248.3(2), 256.3(2), 262, 265, 272.5(3), 283.5, 305, 314,  
 319(2), 323.5(2), 338.5, 372.6, 397(2), 446(2), 455, 497(2), 586(2), 591(2), 625(2), 665,  
 674(2), 689(2), 705, 718.4(2), 756, 767, 784(2), 794, 859, 862(2), 872(2), 918(2), 938, 1008,  
 1061(2), 1237(2), 1256, 1278, 1357, 1406.5(2), 1478(2), 1498, 1551(2), 1559, 1566(2),  
 1627(2), 1647(2), 1684, 1709, 1744.5, 1760, 1778, 1789(2) REF=PM3 HF298=146.6+/-35. kJ  
 REF= ESTIMATE Max Lst Sq Error Cp @ 1300 K 0.53%

C24CL12 ClCoroneneT	8/03C 24.CL12.	0.	0.G	200.000	6000.000	D 713.68920	1
	6.74675357E+01	3.85329684E-02	-1.48783315E-05	2.51718498E-09	-1.55594104E-13		2
	-8.86606352E+03	-3.09600748E+02	5.48199169E+00	2.30027667E-01	-2.53822473E-04		3
	1.50444717E-07	-3.86481388E-11	7.73680444E+03	6.87155182E+00	1.76318268E+04		4

Table 4 (continued)

191-07-1

C24H12 CORONENE (6 benzene ring around a 7TH) SIGMA=12 STATWT=1 IA=250.945567  
 IB=251.1146 IC=501.808336 NU=79.8,83.5,130.8,146,211,278,280,297(2),388(2),  
 417(2),424(2),462,512,542(2),553(2),578,609,631,638,664(2),685,731,739(2),  
 805.5(2),822(2),829,861(2),893,900(2),922,971,973,983(2),995(2),1000(3),1146(2),  
 1153,1203(2),1211,1220.5(2),1253,1267,1280(2),1330,1360(3),1457,1468(2),  
 1529.5(2),1538,1598,1602,1614(2),1631,1672(2),1689,1693,1715,1734,1761,1787,  
 1792,1800,1803.5(2),3178(6),3189(6) REF=MOPAC AM1 { HF298=352.8+/-10. kJ  
 REF=Welsh et al Thermochim Acta 290 (1996), 55. {HF298=322.7 kJ REF=Ferreira  
 Chemosphere 44, (2001),125} HF298=307.5+/-10. kJ Chicos et al J Chem Thermo 34  
 (2002),1195 Max Lst Sq Error Cp @ 1300 K 0.67%.

C24H12 CORONENE	T 8/03C 24.H 12.	0.	0.G	200.000	6000.000	C 300.35208	1
	3.66362791E+01	6.40568636E-02	-2.35898765E-05	3.87302887E-09	-2.34622400E-13		2
	1.83581667E+04	-1.83103895E+02	-3.43656045E+00	1.04563338E-01	9.86369010E-05		3
	-2.14123810E-07	9.51018040E-11	3.28674342E+04	4.09211169E+01	3.69835384E+04		4

N/A

C24H17 TRIPHENYLBENZENE RADICAL (Outer Phenyl Radical in Para Position)  
 CALCULATED FROM PARENT MOLECULE C24H18 - USING THE NIST 1994 APPROXIMATION.  
 PROGRAM EXTRAPOLATED USING WILHOIT'S POLYNOMIALS SIGMA=8 STATWT=2  
 HF298=623.2 KJ

C24H17	T 5/94C 24H 17	0	0G	298.150	5000.000	E 305.39898	1
	0.49910305E+02	0.60606660E-01	-0.21521091E-04	0.37044273E-08	-0.24654232E-12		2
	0.51609915E+05	-0.23666063E+03	-0.16409043E+02	0.22672428E+00	-0.14001458E-03		3
	-0.27875115E-08	0.24713123E-10	0.70999336E+05	0.11051039E+03	0.74953305E+05		4

612-71-5

C24H18 1,3,5-TRIPHENYLBENZENE CALCULATED USING BENSON'S GROUP ADDITIVITY THROUGH  
 BOZZELLI & RITTER'S PROGRAM EXTRAPOLATED USING WILHOIT'S POLYNOMIALS SIGMA=48  
 HF298=373.05 KJ REF=NIST 1994 {HF298(solid)=224.6+/-5.4 kJ REF=Richardson JACS  
 1939}

C24H18	T 2/92C 24H 18	0	0G	298.150	5000.000	E 306.40692	1
	0.51756648E+02	0.59862451E-01	-0.20502137E-04	0.34944485E-08	-0.23287566E-12		2
	0.20652114E+05	-0.25140500E+03	-0.14447245E+02	0.21329283E+00	-0.99995340E-04		3
	-0.44814755E-07	0.40108023E-10	0.40647672E+05	0.98249347E+02	0.44867346E+05		4

99685-96-8

C60 BUCKMINSTERFULLERENE - FOOTBALLNE SYMNO=180. IA=IB=IC=994.2 REF=Froimowitz  
 J. Comp. Chem. 12 (1991),1129 NU=1469,497,1429(3),1183(3),577(3),528(3),273(5),  
 437(5),711(5),773(5),1100(5),1255(5),1427(5),1575(5),943,397(4),461(4),585(4),  
 1021(4),1383(4),1536(4),325(4),611(4),658(4),834(4),1410(4),1535(4),309(5),  
 428(5),503(5),610(5),1122(5),1373(5),1592(5),493(3),705(3),806(5),1274(3),  
 1449(3),457(3),632(3),545(3),315(3),887(3),1139(3),1496(3) REF= Wu et al, Chem.  
 Phys. Let. 137, (1987), 291 HF298=618+/-25 KCAL REF=Beckhaus et al., Angew.  
 Chem Int. Ed. 31 (1992) 63 Max Lst Sq Error Cp @ 1300 K 0.65%

C60	T 6/93C 60	0	0	0G	200.000	6000.000	C 720.66000	1
	0.99843418E+02	0.78857558E-01	-0.30608799E-04	0.51957690E-08	-0.32188408E-12		2	
	0.26670488E+06	-0.54587488E+03	-0.33579084E+02	0.42844440E+00	-0.31712321E-03		3	
	0.47546257E-07	0.27677699E-10	0.30465122E+06	0.14832875E+03	0.31098790E+06		4	

Table 4 (continued)

115383-22-7

C70 (Elipsoid) SYMNO=40. IA=1220.5 IB=IC=1429.5 NU=1568,1465,1383,1232,1185,1062,732,682,571,474,404,260,1532,1452,1298,1146,859,828,653,568,484,1640(2),1568(2),1499(2),1424(2),1383(2),1369(2),1245(2),1200(2),1118(2),961(2),931(2),819(2),748(2),711(2),650(2),585(2),560(2),498(2),412(2),361(2),327(2),1645(2),1583(2),1513(2),1463(2),1433(2),1332(2),1265(2),1212(2),1064(2),966(2),868(2),822(2),781(2),773(2),756(2),722(2),667(2),570(2),501(2),425(2),305(2),216(2),1658,1454,1342,1041,899,774,722,544,335,1565,1389,1270,1217,1168,895,684,592,485,326,1647(2),1592(2),1461(2),1440(2),1360(2),1317(2),1232(2),1186(2),1069(2),909(2),806(2),766(2),753(2),699(2),559(2),538(2),489(2),419(2),243(2),1642(2),1551(2),1531(2),1460(2),1418(2),1358(2),1245(2),1141(2),1107(2),939(2),867(2),819(2),739(2),710(2),682(2),610(2),515(2),405(2),391(2),314(2) REF=BURCAT TAE # 680, 1992 {HF298=692 KCAL} HF298=2652+/-34 kJ REF=Pimenova, Melkhanova & Kolesov J Chem. Thermo. 35 (2003),189 Max Lst Sq Error Cp @ 200 K 0.82%

C70 FOOTBALLENE T 1/03C 70. 0. 0. 0.G 200.000 6000.000 E 840.74900 1  
 1.06784110E+02 1.01992428E-01-3.95570988E-05 6.71117279E-09-4.15612722E-13 2  
 2.68424440E+05-5.99463001E+02-3.13676633E+01 3.34847646E-01 9.85963980E-05 3  
 -4.46661917E-07 2.20100536E-10 3.13337482E+05 1.48919002E+02 3.18960468E+05 4

N/A

JET-A Fuel, Liquid, HF298(L)= -303.5 kJ REF=Gracia-Salcedo,Brabbs & McBride NASA TM 101475 1988. HF298(L)= -265.09 kJ REF=M. Rachner ISRN DLR Mitt-98-01 1998  
 Max Lst Sq Error Cp @ 360 K 0.42%.

Jet-A(L) g 2/96C 12.H 23. 0. 0.C 220.000 550.000 C 167.31102 1  
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2  
 0.00000000E+00 0.00000000E+00 1.90493841E+01-1.69183308E-02 6.30212779E-04 3  
 -1.33364163E-06 9.43345041E-10-4.47959058E+04-6.76893864E+01-3.64907854E+04 4

N/A

JET-A REF=Gracia-Salcedo,Brabbs & McBride NASA TM 101475 1988. and M.Rachner ISRN DLR Mitt-98-01 1998 HF298=-211.47 kJ REF=M. Rachner ISRN DLR Mitt-98-01 1998

JET-A(G) L 6/88C 12H 23 0 0G 273.150 5000.000 C 167.31370 1  
 0.24880201E 02 0.78250048E-01-0.31550973E-04 0.57878900E-08-0.39827968E-12 2  
 -0.38508837E 05-0.95568240E 02 0.20869217E 01 0.13314965E 00-0.81157452E-04 3  
 0.29409286E-07-0.65195213E-11-0.31310966E 05 0.25442305E 02-0.25432647E 05 4

7440-70-2

Ca REFERENCE ELEMENT REF=Alcock et al JPCRD 22 (1993) p.1-85. Generated from original data.

Ca(a) REF ELEMENT L /93CA 1. 0. 0. 0.C 298.150 716.000 B 40.07800 1  
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2  
 0.00000000E+00 0.00000000E+00 3.03325649E+00-1.41800064E-03 7.24487574E-06 3  
 -6.68790594E-09 2.49903889E-12-8.93310508E+02-1.20114288E+01 0.00000000E+00 4  
 Ca(b) L /93CA 1. 0. 0. 0.C 716.000 1115.000 B 40.07800 1  
 5.70111768E+00-5.81056490E-03 4.02212518E-06 0.00000000E+00 0.00000000E+00 2  
 -1.51676361E+03-2.60758134E+01 5.70111768E+00-5.81056490E-03 4.02212518E-06 3  
 0.00000000E+00 0.00000000E+00-1.51676361E+03-2.60758134E+01 0.00000000E+00 4  
 Ca(L) L /93CA 1. 0. 0. 0.L 1115.000 6000.000 B 40.07800 1  
 4.57032345E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2  
 -9.82243308E+02-2.11988643E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 3  
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 4

Table 4 (continued)

7440-70-2

Ca (gas) REF=JANAF 1985 HF298=177.8+/-0.8 kJ

Ca	L 3/93CA 1.	0.	0.	0.G	200.000	6000.000	B	40.07800	1
	1.92707623E+00	1.34909167E-03	-1.07515862E-06		3.25457865E-10	-2.64671538E-14			2
	2.08196210E+04	7.42878398E+00	2.50000000E+00		0.00000000E+00	0.00000000E+00			3
	0.00000000E+00	0.00000000E+00	2.06389279E+04		4.38454833E+00	2.13843029E+04			4

14102-48-8

Ca+ (ion) REF=JANAF 1983 HF298=773.2+/-0.2 kJ

Ca+	J 9/83CA 1.E -1.	0.	0.G	298.150	6000.000	B	40.07745	1
	2.64221438E+00	-1.60517359E-04	-2.70843966E-08		5.13522496E-11	-5.96487048E-15		2
	9.22596379E+04	4.25372628E+00	2.50000000E+00		0.00000000E+00	0.00000000E+00		3
	0.00000000E+00	0.00000000E+00	9.23242106E+04		5.07767503E+00	9.30695856E+04		4

22537-15-1

Cl HF298=121.302+/-0.008 kJ HF0=119.633+/- 0.008 kJ REF=JANAF {HF298=121.302 +/-0.002 kJ REF=ATcT A}

Cl	J 6/82CL 1.	0.	0.	0.G	200.000	6000.000	B	35.45270	1
	2.94658358E+00	-3.85985408E-04	1.36139388E-07		-2.17032923E-11	1.28751025E-15		2	
	1.36970327E+04	3.11330136E+00	2.26062480E+00		1.54154399E-03	-6.80283622E-07		3	
	-1.59972975E-09	1.15416636E-12	1.38552986E+04		6.57020799E+00	1.45891941E+04		4	

7698-05-7

DCl DEUTEROCHLORIC ACID T0=0 STATWT=1 Be=5.444 WE=2144 WEXE=26.9 ALFAE=0.1121

T0=75160 STATWT=2 Be=5.1793 WE=2199 WEXE=26.9 ALFAE=0.1121

T0=76520 STATWT=1 Be=1.555 WE=684.6 WEXE=26.9 ALFAE=0.1121

T0=77525 STATWT=2 Be=4.9605 WE=2114.1 WEXE=26.9 ALFAE=0.1121

HF298=-93.345+/-0.21 kJ REF=JANAF

DCL	J 6/77D 1.CL 1.	0.	0.G	300.000	5000.000	B	37.46680	1
	2.95720340E+00	1.59181600E-03	-6.33202720E-07		1.17556580E-10	-8.15999110E-15		2
	-1.21735150E+04	5.89879666E+00	3.82692130E+00		-2.50133260E-03	6.04661240E-06		3
	-4.48375190E-09	1.13676410E-12	-1.23019210E+04		1.89177776E+00	-1.12270035E+04		4

13770-22-4

DOCl SIGMA=1 STATWT=1 A0=11.052 B0=0.477 C0=0.456 NU=2666,911,723

REF=Jacox NIST Webbook HF298=-79.54+/-2.1 kJ HF0=-76.65 REF=McBride calc.

Max Lst Sq Error Cp @ 400 K &amp; 6000 K 0.28%

DOCL	g 1/01D 1.O 1.CL 1.	0.G	200.000	6000.000	B	53.46620	1
	4.65210175E+00	2.11641809E-03	-7.66161729E-07		1.24270803E-10	-7.46211103E-15	2
	-1.11559090E+04	1.53475660E+00	3.07840297E+00		6.37793362E-03	-3.60099079E-06	3
	-1.14129825E-09	1.40511926E-12	-1.07341490E+04		9.63009270E+00	-9.56625057E+03	4

7790-89-8

ClF T0=0 STATWT=1 Be=0.51409 WE=784.49 WEXE=6.201 ALFAE=0.004329

T0=18721 STATWT=6 Be=0.37026 WE=312.74 WEXE=2.207 ALFAE=0.0139

HF298=-50.292+/-0.42 kJ REF=JANAF

CLF	J 6/77CL 1.F 1.	0.	0.G	300.000	5000.000	B	54.45110	1
	2.84862330E+00	3.17332790E-03	-2.05233870E-06		5.21627330E-10	-3.74722620E-14		2
	-6.92788240E+03	9.31699651E+00	2.64455690E+00		6.24812560E-03	-9.03543510E-06		3
	6.34005750E-09	-1.74353720E-12	-7.04691060E+03		9.63042791E+00	-6.04884780E+03		4

Table 4 (continued)

7790-91-2

CLF3 SIGMA=2 STATWT=1 IA=6.1123 IB=18.1568 IC=24.2691 NU=752,703,528,434,  
326,364 HF298=-158.67+/-2.9 kJ REF=JANAF

CLF3 J 9/65CL 1.F 3. 0. 0.G 300.000 5000.000 B 92.44791 1  
8.95359670E+00 1.17221630E-03-5.08961880E-07 9.75634890E-11-6.88587310E-15 2  
-2.20759680E+04-1.80815549E+01 2.89491190E+00 2.47185500E-02-3.51393230E-05 3  
2.25595910E-08-5.32619780E-12-2.07986400E+04 1.13816921E+01-1.91052460E+04 4

14989-30-1

CLO T0=0 STATWT=4 Be=0.6433 De=2.2 WE=866 WEXE=7.5 ALFAE=0.0069  
HF298=101.22+/-2.1 kJ REF=JANAF {HF298=101.699+/-0.04 REF=ATcT A}

CLO J 6/61CL 1.O 1. 0. 0.G 300.000 5000.000 B 51.45210 1  
4.09126190E+00 5.00031260E-04-1.87782060E-07 3.50976710E-11-2.42050380E-15 2  
1.08532230E+04 3.61889244E+00 2.81793640E+00 4.45313330E-03-4.41248930E-06 3  
1.59209420E-09-1.44862420E-14 1.11713970E+04 1.00579823E+01 1.21736480E+04 4

10049-04-4

CLO2 O-Cl-O SIGMA=2 A000=1.6006 B000=0.33283 C000=0.27553 NU=1109,945,447  
STATWT=2 x11=-4.4 x22=0 x33=-2.0 x12=-3.0 x23=-13 x31=-14.4 g22=0  
HF298=104.6+/-6.3 kJ REF=JANAF

CLO2 (OCLO) J 3/61CL 1.O 2. 0. 0.G 300.000 5000.000 A 67.45150 1  
5.72497580E+00 1.46452300E-03-5.99843510E-07 1.13887500E-10-7.97947760E-15 2  
1.06062640E+04-2.57902748E+00 2.88781660E+00 9.28760080E-03-7.08240400E-06 3  
6.34533760E-10 9.68016050E-13 1.13673770E+04 1.20200293E+01 1.25803228E+04 4

17376-09-9

CLOO RADICAL STATWT=2 IA=1.0968 IB=10.2167 IC=11.3135 NU=1000,300,900  
HF298=23 KCAL MAX LST SQ ERROR CP @ 1300 0.2% REF=Estimated

CLOO L 4/84CL 1.O 2 0 OG 300.000 5000.000 E 67.45180 1  
0.60288639E 01 0.10057015E-02-0.40009184E-06 0.69837636E-10-0.44704535E-14 2  
0.95408711E 04-0.32185535E 01 0.34938974E 01 0.71383193E-02-0.28676532E-05 3  
-0.37120573E-08 0.26473615E-11 0.10247160E 05 0.99912157E 01 0.11574121E 05 4

7616-94-6

CLO3F Perchloryl Fluoride REF=JANAF 3/61 HF298=-5.688 kcal Max Lst Sq Error  
Cp @ 2500 K 0.26%.

CLO3F L 5/95CL 1.O 3.F 1. 0.G 200.000 6000.000 B 102.44930 1  
9.84020286E+00 3.25550966E-03-1.28321227E-06 2.19710639E-10-1.36348643E-14 2  
-6.48553280E+03-2.47267180E+01 6.05661163E-01 3.52831180E-02-4.51135948E-05 3  
2.82788050E-08-7.03541332E-12-4.26508565E+03 2.13532322E+01-2.86229640E+03 4

7782-50-5

CL2 REFERENCE ELEMENT REF=Gurvich 1989 V1 py.1 p.177 HF298=0.00 kcal Max Lst  
Sq Error Cp @ 6000 \*\*1.26%\*\* (Cp @ 700 K 0.08%).

CL2 REF ELEMENT G 8/02CL 2. 0. 0. 0.G 200.000 6000.000 B 70.90600 1  
4.74727507E+00-4.88581697E-04 2.68444865E-07-2.43476072E-11-1.03683156E-15 2  
-1.51101862E+03-3.44538559E-01 2.73638114E+00 7.83525699E-03-1.45104963E-05 3  
1.25730834E-08-4.13247143E-12-1.05880114E+03 9.44557148E+00 0.00000000E+00 4

7791-21-1

CL2O SIGMA=2 STATWT=1 IA=2.0224 IB=23.0829 IC=25.1033 NU=686,640,300  
HF298=87.86+/-6.7 kJ REF=JANAF

CL2O J12/65CL 2.O 1. 0. 0.G 300.000 5000.000 B 86.90480 1  
6.43400620E+00 6.27288090E-04-2.69332520E-07 5.10763940E-11-3.56915450E-15 2  
8.48605300E+03-4.93672407E+00 3.25452380E+00 1.27994490E-02-1.78824600E-05 3  
1.12643830E-08-2.59642520E-12 9.16574230E+03 1.05712106E+01 1.05680184E+04 4



Table 4 (continued)

12292-23-8

CL2O2 (Cl-O-O-Cl) SIGMA=2 IA=5.538 IB=35.2672 IC=38.6944 IR=2.26835 ROSYM=2  
 POTENTIAL BARRIER V(3)=2581. cm-1 REF= BAC/MP4 CALCULATIONS BY MELIUS (private  
 communication). NU=752,650,648,437,328 HF0=34.2 KCAL HF298=33.216 KCAL  
 REF=Lee, Rohlfing & Rice J. Chem Phys.97 (1992), 6593. Max Lst Sq Error Cp @  
 1200 K 0.30%

CL2O2	T 2/94CL	20	2	0	OG	200.000	6000.000	B	102.90420	1
0.97241408E+01	0.29991597E-03	-0.22394766E-06	0.48423798E-10	-0.34559904E-14						2
0.13444436E+05	-0.20745767E+02	0.18634070E+01	0.33285997E-01	-0.57276349E-04						3
0.46928825E-07	-0.14956803E-10	0.15100165E+05	0.17205914E+02	0.16714845E+05						4

7440-47-3

Cr REFERENCE ELEMENT REF=JANAF HF298=0.0 kJ

Cr(cr)REF ELEMENT	J 6/73CR	1.	0.	0.	0.S	200.000	311.500	B	51.99610	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00						2
0.00000000E+00	0.00000000E+00	7.84826024E+00	-1.16276020E-01	8.12369251E-04						3
-2.30807086E-06	2.35328142E-09	-8.98013946E+02	-2.75733139E+01	0.00000000E+00						4
Cr(cr)	J 6/73CR	1.	0.	0.	0.S	311.500	2130.000	B	51.99610	1
4.59782637E+00	-4.81791132E-03	5.84129754E-06	-2.07036847E-09	2.82102268E-13						2
-1.31489668E+03	-2.24454748E+01	1.82863471E+00	4.19562267E-03	-2.82735082E-06						3
-9.15990578E-10	1.55203040E-12	-7.05502663E+02	-8.69806103E+00	0.00000000E+00						4
Cr(L)	J 6/73CR	1.	0.	0.	0.L	2130.000	2952.000	B	51.99610	1
4.73028477E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00						2
5.75359221E+02	-2.45318309E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00						3
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00						4

7440-47-3

Cr Gaseous REF=JANAF HF298=397.48 +/- 4.2 kJ Transition from Liquid to Gas  
 at 2952 K

Cr	J 6/79CR	1.	0.	0.	0.G	200.000	6000.000	B	51.99610	1
3.08497752E+00	-1.44703683E-03	1.08492194E-06	-2.35643635E-10	1.86355816E-14						2
4.68928202E+04	3.65913914E+00	2.50259371E+00	-2.76560170E-05	1.03974095E-07						3
-1.61996406E-10	8.89391985E-14	4.70600237E+04	6.71107210E+00	4.78055833E+04						4

49681-65-4

CrCl ChromiumMonochloride SIGMA=1 From Cp Polynomials HF298=129.9+/-2.7 kJ  
 REF=Ebbinghaus C&F 101, (1995), 311-338 Max Lst Sq Error Cp @ 300 K 0.53%

CrCl	A12/04CR	1.CL	1.	0.	0.G	298.150	3000.000	B	87.44880	1
3.79103889E+00	1.57356548E-03	-1.30343311E-06	4.48647981E-10	-4.78012226E-14						2
1.44632306E+04	8.08526764E+00	2.83722437E+00	8.08793500E-03	-1.59515226E-05						3
1.42928143E-08	-4.80443309E-12	1.45328417E+04	1.20580960E+01	1.56232899E+04						4

14977-61-8

CrCl2O2 SIGMA=2 From Cp Polynomials to 3000 K Extrapolated using Wilhoit.  
 HF298=-519.2+/-4.2 kJ REF=Ebbinghaus C&F 101, (1995), 311-338 Max Lst Sq Error  
 Cp @ 3000 K 0.96%

CrCl2O2	A12/04CR	1.CL	2.O	2.	0.G	298.150	5000.000	B	154.90030	1
1.21316101E+01	3.37565144E-04	1.18813367E-07	-4.97213791E-11	4.50941256E-15						2
-6.64688829E+04	-3.05150563E+01	3.71590088E+00	3.55707786E-02	-6.10226580E-05						3
5.06112478E-08	-1.63324927E-11	-6.46871319E+04	1.01533862E+01	-6.24450509E+04						4

14986-48-2

CrCl6 Chromium Hexachloride From Cp polynomials SIGMA=24 HF298=-345.3+50.?? kJ  
 REF=Ebbinghaus C&F 101, (1995), 311-338 Max Lst Sq Error Cp @ 400 K 0.07%

CrCl6	HF298=-34	A12/04CR	1.CL	6.	0.	0.G	298.150	5000.000	B	264.71230	1
1.83289973E+01	7.77466644E-04	-3.48058994E-07	6.85592495E-11	-4.95622794E-15						2	
-4.72003352E+04	-5.51750147E+01	1.11743747E+01	3.57825048E-02	-6.69030889E-05						3	
5.72907814E-08	-1.85225640E-11	-4.59652557E+04	-2.19248279E+01	-4.15298075E+04						4	

Table 4 (continued)

24094-93-7

CrN(s) Chromium Nitride CONDENSED HF298(S)=-117.15 +/- 8.4 kJ REF=JANAF

CrN(s)	J12/73CR	1.N	1.	0.	0.S	300.000	2500.000	B	66.00284	1
	5.69445390E+00	5.30116900E-04	2.27058290E-07	-8.14832540E-11	1.08037960E-14					2
	-1.58360020E+04	-2.81317040E+01	9.71529040E+00	-2.37753720E-02	5.25610150E-05					3
	-4.83907470E-08	1.62707570E-11	-1.63234220E+04	-4.57300500E+01	-1.41071233E+04					4

24094-93-7

CrN Chromium Nitride T0=0.0 WE=[1000] WEXE=[5.] BE=[0.56115] ALFAE=[0.00375]

RE=[1.65] STATWT=4 T0=[15000] STATWT=8 T0=[20000] STATWT=4 REF=JANAF

HF298=501.01 +/- 20.9 kJ

CrN	J12/73CR	1.N	1.	0.	0.G	300.000	5000.000	C	66.00284	1
	3.86496020E+00	8.51604560E-04	-4.40707580E-07	1.06676010E-10	-8.37314220E-15					2
	5.94774370E+04	5.29506757E+00	2.93046360E+00	3.03770420E-03	-1.27139640E-06					3
	-1.17812490E-09	8.55513490E-13	5.97442030E+04	1.01918812E+01	6.07397802E+04					4

12018-00-7

CrO Chromium Oxide T0=0 WE=898.8 WEXE=6.50 Be=0.5286 ALFAE=0.0050 RE=1.627

STATWT=10 T0=16584.5 STATWT=10 REF=JANAF HF298=188.28 +/- 41.8 kJ

CrO	J12/73CR	1.O	1.	0.	0.G	300.000	5000.000	B	67.99550	1
	4.01398180E+00	6.27002450E-04	-2.79567940E-07	6.00031000E-11	-4.40579160E-15					2
	2.13466930E+04	5.55171510E+00	2.84149960E+00	4.09533580E-03	-3.57764630E-06					3
	8.17104390E-10	2.40720090E-13	2.16460670E+04	1.15179922E+01	2.26454051E+04					4

12018-01-8

CrO2 SIGMA=2 STATWT=3 IAIBIC=332.6337 E-117 NU=998, [300], 1008 REF=JANAF

HF298=-75.312 +/- 41.8 kJ

CrO2	J12/73CR	1.O	2.	0.	0.G	300.000	5000.000	B	83.99490	1
	5.84999980E+00	1.27251010E-03	-5.49205480E-07	1.04974910E-10	-7.39954860E-15					2
	-1.10421830E+04	-1.74497632E+00	3.30126450E+00	8.16258570E-03	-5.89076800E-06					3
	1.61708560E-11	1.08162670E-12	-1.03535690E+04	1.13991138E+01	-9.05799743E+03					4

1333-82-0

CrO3 SIGMA=6 STATWT=1 IA=IB=10.5494 IC=21.0987 REF=Gurvich 1982

HF298=-322.037 kJ Calculated by NASA. Max Lst. Sq. Error Cp @ 1200 K 0.16%

CrO3	T 2/03CR	1.O	3.	0.	0.G	200.000	5000.000	B	99.99430	1
	8.28386164E+00	1.94981497E-03	-8.59416757E-07	1.65569104E-10	-1.14362256E-14					2
	-4.15903861E+04	-1.60755404E+01	2.23347303E+00	2.41293363E-02	-3.23881504E-05					3
	2.06137981E-08	-5.06006431E-12	-4.02225119E+04	1.37499896E+01	-3.87319277E+04					4

12053-27-9

Cr2N Chromium Nitride Crystal HF298(S)=-125.52 +/- 12.6 kJ REF=JANAF

Cr2N(s)	J12/73CR	2.N	1.	0.	0.C	300.000	2500.000	B	117.99894	1
	8.09841850E+00	1.85336110E-03	1.42273060E-06	-5.58963900E-10	6.93071100E-14					2
	-1.76848010E+04	-3.91474720E+01	2.03033880E+00	3.40064410E-02	-6.15249460E-05					3
	5.31425480E-08	-1.67695210E-11	-1.67683130E+04	-1.16006980E+01	-1.50979548E+04					4

1308-38-9

Cr2O3 Chromium Oxide CONDENSED HF298(S)=-1134.70 +/- 8.4 kJ REF=JANAF

Cr2O3(s)	J12/73CR	2.O	3.	0.	0.S	300.000	2603.000	B	151.99040	1
	1.40122350E+01	1.38239780E-03	-2.37792260E-07	1.69950850E-10	-3.77058570E-14					2
	-1.40982170E+05	-7.11015690E+01	2.93327730E+01	-1.02073850E-01	2.36011030E-04					3
	-2.25780190E-07	7.77992890E-11	-1.42404060E+05	-1.35742810E+02	-1.36519668E+05					4
Cr2O3(L)	J12/73CR	2.O	3.	0.	0.L	2603.000	5000.000	B	151.99040	1
	1.88711050E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
	-1.33694980E+05	-9.99614700E+01	1.88711050E+01	0.00000000E+00	0.00000000E+00					3
	0.00000000E+00	0.00000000E+00	-1.33694980E+05	-9.99614700E+01	0.00000000E+00					4

Table 4 (continued)

12068-77-8

Cr<sub>2</sub>FeO<sub>4</sub> Dichromium Ferrum Tetraoxide. Data taken from I. Barin 1989.

HF298(S)=-1458.124 kJ

Cr <sub>2</sub> FeO <sub>4</sub>	B	/89CR	2.FE	1.O	4.	0.S	298.150	2123.000	C	223.83480	1
1.55564505E+01	1.09205438E-02	-6.78459948E-06	2.55612113E-09	-3.64830765E-13							2
-1.80620170E+05	-7.50507389E+01	-1.86852265E+00	1.04789892E-01	-1.95035400E-04							3
1.68861646E-07	-5.48639301E-11	-1.78056165E+05	3.76236322E+00	-1.75371008E+05							4

12012-35-0

Cr<sub>3</sub>C<sub>2</sub> 3-Chromium 2-Carbide Solid. Data taken from I. Barin 1989

HF298(S)=-85.354 kJ

Cr <sub>3</sub> C <sub>2</sub> (S)	B	/89C	2.CR	3.	0.	0.S	298.150	2168.000	C	180.01030	1
1.43803845E+01	2.40334724E-03	9.15436967E-07	-2.48561026E-10	2.79849340E-14							2
-1.50902114E+04	-7.34861883E+01	-1.68140483E+00	7.44936012E-02	-1.22150468E-04							3
9.39505934E-08	-2.71337291E-11	-1.21690265E+04	2.29813080E+00	-1.02656681E+04							4

12075-40-0

Cr<sub>7</sub>C<sub>3</sub> 7-Chromium 3-Carbide Solid. Data taken from I. Barin 1989.

CHF298(S)=-160.666 kJ.

Cr <sub>7</sub> C <sub>3</sub> (S)	B	/89C	3.CR	7.	0.	0.S	298.150	2053.000	C	400.00570	1
2.69325544E+01	8.13786676E-03	1.71106267E-07	2.14298486E-10	-5.73918629E-14							2
-2.81724038E+04	-1.32914128E+02	1.26480339E+00	1.35085980E-01	-2.36886549E-04							3
1.97374948E-07	-6.14407486E-11	-2.39729821E+04	-1.44012483E+01	-1.93235681E+04							4

12105-81-6

Cr<sub>23</sub>C<sub>6</sub> 23-Chromium 6-Carbide Solid. Data taken from I. Barin 1989.

HF298(S)=-328.444 kJ.

C <sub>6</sub> Cr <sub>23</sub>	B	/89C	6.CR	23.	0.	0.S	298.150	1793.000	C	1267.97630	1
9.01158896E+01	-3.96673567E-03	2.71679400E-05	-9.85562288E-09	1.44623799E-12							2
-6.83766452E+04	-4.44799405E+02	1.38920966E+01	3.31573484E-01	-5.26586194E-04							3
3.94794929E-07	-1.08766607E-10	-5.44583198E+04	-8.42575556E+01	-3.95025083E+04							4

16873-17-9

D DEUTERIUM HF298=221.720+/-0.004 kJ REF=JANAF {HF298=221.717+/-2.4E-5

REF=ATcT A}.

D	J	3/82D	1.	0.	0.	0.G	200.000	6000.000	A	2.01410	1
2.50000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00						2
2.59212596E+04	5.91714338E-01	2.50000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00						3
0.00000000E+00	0.00000000E+00	2.59212596E+04	5.91714338E-01	2.66666346E+04							4

14464-47-2

D<sup>+</sup> DEUTERIUM ION HF298=1540.324 kJ HF0=1532.214 kJ REF=Moore 1972 and Gordon 1999. {HF298=1540.321+/-2.7E-5 kJ REF=ATcT A} Max Lst Sq Error N/A

D <sup>+</sup>	g	9/96D	1.E	-1.	0.	0.G	298.150	6000.000	B	2.01355	1
2.50000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00						2
1.84512004E+05	-1.01841452E-01	2.50000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00						3
0.00000000E+00	0.00000000E+00	1.84512004E+05	-1.01841452E-01	1.85257379E+05							4

14452-69-8

D<sup>-</sup> DEUTERIUM ANION REF=Hotop 1985 and Gordon 1999 HF298=142.753 kJ

D <sup>-</sup>	G	9/96D	1.E	1.	0.	0.G	298.150	6000.000	B	2.01465	1
2.50000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00						2
1.64237667E+04	-1.01023912E-01	2.50000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00						3
0.00000000E+00	0.00000000E+00	1.64237667E+04	-1.01023912E-01	1.71691417E+04							4

Table 4 (continued)

14333-26-7

DF DEUTEROFLUORIC ACID T0=0 STATWT=1 Be=11.000 cm-1 WE=2998.19 WEXE=45.76  
 ALPHAE=0.2907 T0=83755 STATWT=1 Be=2.121 cm-1 WE=839.4 WEXE=8.9  
 ALPHAE=0.00712 HF298=-275.51+/- 0.8 kJ REF=JANAF

DF	J 6/77D	1.F	1.	0.	0.G	300.000	5000.000	B	21.01251	1
	2.72646200E+00	1.50912930E-03	-5.17049380E-07	8.54853710E-11	-5.41960240E-15					2
	-3.39369400E+04	5.82982015E+00	3.49813860E+00	2.21767930E-04	-1.33202400E-06					3
	2.56194930E-09	-1.15122410E-12	-3.41832320E+04	1.65507895E+00	-3.31376542E+04					4

13983-20-5

HD PROTODEUTERIUM FROM ORIGINAL TABLES REF=Gurvich 89 HF298=8.5 kJ HF0=8.51 kJ  
 {HF298=0.319 +/-8.3E-5 kJ REF=ATcT A} Max Lst Sq Error Cp @ 1200 K 0.28%

HD	RUS 89H	1.D	1.	0.	0.G	298.150	6000.000	A	3.02204	1
	2.80029834E+00	1.15623360E-03	-3.06064442E-07	4.51518392E-11	-2.62838877E-15					2
	2.38213151E+02	1.23069947E+00	3.43752369E+00	6.17471555E-04	-1.85267846E-06					3
	2.32581486E-09	-8.35140695E-13	-1.77564616E+01	-2.41112115E+00	1.02241948E+03					4

12181-16-7

HD+ PROTODEUTERIUM ION FROM ORIGINAL JANAF TABLES HF298=1496.83 HF0=1490.5 kJ  
 Max Lst Sq Error Cp @ 1300 K 0.79%

HD+	j 9/77H	1.D	1.E	-1.	0.G	298.150	6000.000	B	3.02149	1
	3.63782858E+00	4.58875734E-04	1.13136423E-07	-4.23103495E-11	2.49509008E-15					2
	1.78814567E+05	-2.37056371E+00	3.88006790E+00	-3.06534290E-03	8.17334271E-06					3
	-6.80432062E-09	1.98627839E-12	1.78941448E+05	-2.79172055E+00	1.80021747E+05					4

14940-63-7

DHO STATWT=1 SIGMA=1 A0=23.4105 B0=9.0975 C0=6.4137 NU=2725,1402,3707  
 X11=-41.51 X22=-11.9 X33=-82.34 X12=-16.98 X23=-20.08 X13=-12.91 W0=14.5  
 ALFAA1=0.253 ALFAA2=-1.798 ALFAA3=1.087 ALFAB1=0.199 ALFAB2=-0.147  
 ALFAB3=0.125 ALFAC1=0.1098 ALFAC2=0.071 ALFAC3=0.0881 TAAA=-0.056322  
 TBBB=-0.0024192 TCCC=-0.00047276 TAAB=0.005895 TBBC=-0.00075778  
 TAAC=0.00083015 TABA=-0.0074348 REF=Gurvich 1989 HF298=-245.276 KJ Max Lst  
 Sq Error Cp @ 6000 K 0.22%

HDO	L 5/95H	1D	1O	1	0G	200.000	6000.000	A	19.02144	1
	0.27939505E+01	0.33086588E-02	-0.10334334E-05	0.15472460E-09	-0.87503559E-14					2
	-0.30407527E+05	0.72889151E+01	0.42115416E+01	-0.23855882E-02	0.82921720E-05					3
	-0.71895657E-08	0.22865905E-11	-0.30709525E+05	0.40224847E+00	-0.29499754E+05					4

34322-11-7

DHO2 STATWT=1 SIGMA=1 A0=7.48 B0=.832 C0=.792 BROTI=30.573 BROTI2=.551  
 BROTI3=.0662 V(1)=-2044 cm-1 V(2)=-1292. cm-1 V(3)=-94. cm-1 NU=3620,1332,  
 871,2659,984 X11=-90. X12=-10. X13=-10. X15=-122. X16=-2. X22=-9. X23=-7.  
 X25=-8. X26=-3. X33=-10. X35=-8. X36=-2. X55=-48. X56=-2. X66=-2.  
 ALFAA1=-.23 ALFAA2=.09 ALFAA3=.03 ALFAA5=-.09 ALFAA6=.08 ALFAB1=-.003  
 ALFAB2=-.003 ALFAB3=-.006 ALFAB5=-.001 ALFAB6=-.001 ALFAC1=.001  
 ALFAC2=-.003 ALFAC3=-.012 ALFAC5=.0005 ALFAC6=-.003 DJ=3E-6 DK=.0005  
 DJK=-.000015 REF=Gurvich 1989 HF0=-134.358 KJ Max Lst Sq Error Cp @ 6000 K  
 0.32 %.

HDO2	L 5/95H	1D	1O	2	0G	200.000	6000.000	A	35.02084	1
	0.48569842E+01	0.41449474E-02	-0.14036401E-05	0.22259619E-09	-0.13165755E-13					2
	-0.18651434E+05	0.74277419E-01	0.41089805E+01	0.13881673E-02	0.13185181E-04					3
	-0.18475659E-07	0.76010528E-11	-0.18236260E+05	0.50328708E+01	-0.16865900E+05					4

Table 4 (continued)

13587-54-7

OD DEUTERYL RADICAL FROM ORIGINAL DATA HF0=36.852 KJ REF=GURVICH 89 Max Lst Sq Error Cp @ 6000 K 0.2%

OD	RUS 890	1D	1	0	OG	200.000	6000.000	A	18.01350	1
	0.28342371E+01	0.14734180E-02	-0.50643349E-06	0.84794290E-10	-0.53143844E-14					2
	0.36312839E+04	0.63935773E+01	0.40708924E+01	-0.28210086E-02	0.50328224E-05					3
	-0.30857249E-08	0.68372023E-12	0.33502462E+04	0.26044498E+00	0.44772871E+04					4

17693-79-7

OD- DEUTERYL ION FROM ORIGINAL DATA HF0=-139.198 KJ REF=GURVICH 89  
 {HF298=-138.7+/-0.84 kJ Ref=Schulz, Mead, Jones, Lineberger JCP 77, (1982), 1153}  
 Max Lst Sq Error Cp @ 2500 K 0.11%

OD-	RUS 890	1D	1E	1	OG	298.150	6000.000	A	18.01405	1
	0.27763885E+01	0.15258004E-02	-0.52291732E-06	0.84887426E-10	-0.48226449E-14					2
	-0.18319323E+05	0.53434282E+01	0.35593270E+01	-0.24042233E-03	-0.23249148E-06					3
	0.17198317E-08	-0.94690846E-12	-0.18536277E+05	0.12466308E+01	-0.17484852E+05					4

7789-20-0

DO2 SIGMA=1 STATWT=2 IAIBIC=1.945 E-117 Nu=2530,1020,1123 T0=7030 STATWT=2  
 HF298=6.487 kJ HF0=9.387 kJ REF=Gurvich 89 Max Lst Sq Error Cp @ 400 K 0.36%

DO2	RUS 89D	1.O	2.	0.	O.G	200.000	6000.000	B	34.01290	1
	4.45573114E+00	2.06607643E-03	-5.66117475E-07	7.20169946E-11	-3.62843466E-15					2
	-8.10085761E+02	1.63807075E+00	4.02991705E+00	-2.78860182E-03	1.84192793E-05					3
	-2.24181681E-08	8.78165227E-12	-4.19907996E+02	5.24187832E+00	7.80243694E+02					4

13780-23-9

SD SIGMA=1 T0(STATWT)=0(2) IB=.571167 WE=18865 WEXE=30.95 ALFAE=0.100  
 DE=1.35 E-4 T0(STATWT)=30769(2) IB=.6172119 WE=1417 WEXE=48.85 ALFAE=0.172  
 DE=1.76 E-4 T0(STATWT)=59566(2) IB=.6175838 WE=1859.16 WEXE=29.3 ALFAE=0.105  
 DE=1.35 E-4 T0(STATWT)=63872(4), IB=0.5942658  
 T0(STATWT)=71205(4), IB=0.58986 DE=0.70E-4  
 T0(STATWT)=71328(2) IB=0.58986 DE=1.35E-4  
 T0(STATWT)=76717(4)  
 T0(STATWT)=79320(4), IB=.564292 REF=NIST WEBBOOK HF0=140.14+/-  
 0.52 kJ REF=Csazar Leninger & Burcat JPC 2003 Max Lst Sq Error Cp  
 @ 1300 K 0.32%.

SD	IU2/03S	1.D	1.	0.	O.G	200.000	6000.000	A	34.07910	1
	3.24504866E+00	1.25276603E-03	-4.46274222E-07	7.30968355E-11	-4.33084799E-15					2
	1.57906172E+04	4.90618519E+00	3.69382042E+00	-1.83803156E-03	5.23925510E-06					3
	-3.83522579E-09	8.60488290E-13	1.57961846E+04	3.14078205E+00	1.68548409E+04					4

7782-39-0

D2 REFERENCE ELEMENT HF298=0 HF0=0. FROM ORIGINAL TABLES OF GURVICH 89  
 Max Lst Sq Error Cp @ 6000 K 0.10%

D2	RUS 89D	2.	0.	0.	O.G	200.000	6000.000	B	4.02820	1
	2.73068949E+00	1.48004749E-03	-4.79314695E-07	7.89495975E-11	-4.88380620E-15					2
	-7.95267579E+02	1.64265990E+00	3.49546974E+00	2.58348157E-04	-1.31762502E-06					3
	2.42912017E-09	-1.05982498E-12	-1.04631580E+03	-2.51905534E+00	0.00000000E+00					4

12184-84-8

D2+ From Original JANAF Tables HF298=1498.57 kJ HF0=1492.29 kJ Max Lst Sq Error Cp @ 1300 K 0.76%

D2+	J 9/77D	2.E	-1.	0.	O.G	298.150	6000.000	B	4.02766	1
	3.92368570E+00	2.22864953E-04	1.96265789E-07	-5.64256687E-11	3.39718341E-15					2
	1.78913148E+05	-3.88393204E+00	3.82876883E+00	-3.25946187E-03	1.05345842E-05					3
	-1.02332009E-08	3.41909767E-12	1.79164176E+05	-2.37676862E+00	1.80235315E+05					4

Table 4 (continued)

11081-35-9

D2- SIGMA=2 STATWT=2 We=1202 WeXe=17.5 Be=12.7 ALPHAE=0.141 REF=JANAF 77  
estimated HF298=235.36 kJ HF0=241.42 kJ Max Lst Sq Error Cp @ 1300 K 0.21%

D2-	J 9/77D	2.E	1.	0.	0.G	298.150	6000.000	B	4.02875	1
	3.83396908E+00	8.21355049E-04	-2.61248475E-07	4.43534405E-11	-2.74786624E-15					2
	2.70340679E+04	-3.26230544E+00	3.25565602E+00	5.02863621E-04	4.26580295E-06					3
	-5.93329687E-09	2.34465550E-12	2.72875414E+04	1.93204603E-01	2.83076358E+04					4

7789-20-0

D2O DEUTERATED WATER SIGMA=2 A0=15.4196 B0=7.2704 C0=4.8478 NU=2788.02,  
2671.69,1178.33 X11=-21.94 X22=-9.46 X33=-24.99 X12=-8.77 X13=-85.76

X23=-10.27    ALFAA1=0.246    ALFAA2=-1.188    ALFAA3=0.593    ALFAB1=0.0958

ALFAB2=-0.0728    ALFAB3=0.0418    ALFAC1=0.0768    ALFAC2=0.053    ALFAC3=0.0538

DARD=42.5    TAAA=-0.032153    TBBB=-0.0022233    TCCC=-0.000255518    TAAB=0.0056673

TBBC=-0.00042797    TAAC=0.00015517    TABA=-0.001506    HF298=-249.21+/-0.13 kJ

HF0=-246.261 kJ REF=Gurvich 89 Max Lst Sq Error Cp @ 6000 K 0.36%

D20	α 6/99D	2.0	1.	0.	0.G	200.000	6000.000	A	20.02760	1
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2.94501470E+00 3.54821768E-03-1.20330628E-06 1.90642832E-10-1.12513216E-14 2

-3.09820676E+04 6.12279719E+00 4.09682717E+00-1.67121258E-03 7.73454843E-06 3

-6.88015073E-09 2.18930533E-12-3.11758628E+04 7.23653438E-01-2.99729028E+04 4

6909-54-2

D2O2 DEUTERIUM PEROXIDE SIGMA=2 A0=4.92 B0=0.788 C0=0.733 BROTT1=21.492

BROT2=0.549 BROT3=0.0869 V(1)=-2058 V(2)=-1302 V(3)=-102 1/CM NU=2667,1028,

869,2661,947 X11=-48 X12=-6 X13=-8 X15=-88 X16=-2 X22=-5 X23=-5 X25=-6

X26=-2   X33=-10   X35=-8   X36=-1   X55=-47   X56=-2   X66=-2   ALFA1A=-0.09

ALFA2A=.04    ALFA3A=.03    ALFA5A=-.09    ALFA6A=.07    ALFA1B=-0.001    ALFA2B=-.002

ALFA3B=-.006    ALFA5B=-0.001    ALFA6B=-0.001    ALFA1C=.0005    ALFA2C=-.002

ALFA3C=-.001    ALFA5C=.0005    ALFA6C=-0.003    REF = TSIV 1978    HF298=-144.3 KJ

Max Lst Sq Error Cp @ 6000 K 0.40 %.

D202	α 6/99D	2.0	2.	0.	0.G	200.000	6000.000	B	36.02700	1
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5.14099412E+00 4.24770619E-03-1.51625265E-06 2.48828911E-10-1.50545304E-14 2

-1.92648912E+04 -1.82579388E+00 3.99335958E+00 3.03682596E-03 1.02967795E-05 3

-1.60576667E-08 6.83692371E-12-1.87432656E+04 5.12865282E+00-1.73552019E+04 4

13536-94-2

D2S DEUTERATED SULFIDE SIGMA=2 A0=5.484 B0=4.508 C0=2.444 NU=1999,1896.38,

855.45    X11=-12.91    X22=-2.95    X33=-12.39    X12=-10.14    X13=-48.80    X23=-10.88

$$\text{ALFAA1}=0.0769 \quad \text{ALFAA2}=-0.2164 \quad \text{ALFAA3}=0.1239 \quad \text{ALFAB1}=0.1308 \quad \text{ALFAB2}=-0.1911$$

ALFAB3=0.0984    ALFAC1=0.0501    ALFAC2=0.0445    ALFAC3=0.0389    DARD=26.4

RHO=2.058E-05    HF298=-24.007+/- 0.8 kJ    HF0=-21.114 kJ    REF=Miller et al JCP

46, (1967), 2292-2297 + McBride Max Lst sq Error Cp @ 1300 K 0.49%.

D2S	α 6/01D	2.S	1.	0.	0.G	200.000	6000.000	A	36.09420	1
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3.98099658E+00 2.99684145E-03-1.08624720E-06 1.81265880E-10-1.10816328E-14 2

-4.35437761E+03 2.03253673E+00 3.96539676E+00-9.52689119E-04 9.60156793E-06 3

-9.56853312E-09 3.01603262E-12 -4.09459065E+03 3.23907392E+00 -2.88730785E+03 4

183748-02-9

ELECTRON GAS HF298=0.0 KJ REF=TSIV

ELECTRON GAS	L 6/88E	1	0	0	OG	200.000	6000.000	0.00055	1
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0.25000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2
```

```
-0.74537500E+03-0.11720813E+02 0.25000000E+01 0.00000000E+00 0.00000000E+00 3
```

```
0.00000000E+00 0.00000000E+00-0.74537500E+03-0.11720813E+02 0.00000000E+00 4
```

Table 4 (continued)

14762-94-8

F HF298=79.39+/-0.3 kJ REF=JANAF {HF298=79.223+/-0.16 kJ REF=ATcT A}  
 F J 6/82F 1 0 0 0G 200.000 6000.000 A 18.99840 1  
 0.26716339E+01-0.17461853E-03 0.69066504E-07-0.11953478E-10 0.75236739E-15 2  
 0.87874123E+04 0.39842568E+01 0.24196743E+01 0.29392909E-02-0.89212228E-05 3  
 0.99118537E-08-0.37947152E-11 0.87573220E+04 0.47468987E+01 0.95483679E+04 4

12061-70-0

FO T0=0 STATWT=2 BE=1.05870547 DE=4.28739E-6 WE=1052.99376 WEXE=9.90030  
 WEYE=-0.068456 WEZE=-0.0010881 WX4=-5.945E05 ALPHAE=-0.0138015 T0=193.80  
 STATWT=2 BE=1.05870547 DE=4.28739E-6 WE=1052.99376 WEXE=9.90030  
 WEYE=-0.068456 WEZE=-0.0010881 WX4=-5.945E05 ALPHAE=-0.0138015 REF=Chase  
 HF298=111.267+/-0.69 kJ HF0=110.632 kJ REF=ATcT A {HF298=109. +/-10 KJ  
 REF=M.W.Chase JPCRD 25 (1996),551 also Gurvich 89} Max Lst Sq Error Cp @  
 400 K 0.32%  
 FO ATcT/AF 1.0 1. 0. 0.G 200.000 6000.000 B 34.99780 1  
 4.10435161E+00 3.22444815E-04-6.01630664E-08-1.10998596E-11 1.61567239E-15 2  
 1.20593514E+04 2.35480534E+00 4.34438108E+00-5.37168023E-03 1.77166504E-05 3  
 -2.00073120E-08 7.67510992E-12 1.22051341E+04 2.24948929E+00 1.33822679E+04 4

175861-93-5

FO2 O-F-O SIGMA=2 STATWT=2 IA=2.9573 IB=4.9779 IC=7.9351 [T0=1049.3  
 STATWT=2] NU=1050,600,1200 HF298=378.6+/-20 kJ REF=Chase JPCRD 25 (1996),551  
 Max Lst Sq Error Cp @ 200 K 0.55%.  
 FO2 O-F-O T02/97F 1.0 2. 0. 0.G 200.000 6000.000 C 50.99720 1  
 6.49703714E+00 6.37827524E-04-2.77002473E-07 5.01580874E-11-3.23770263E-15 2  
 4.32340446E+04-7.76454500E+00 3.28036811E+00 2.83373458E-03 1.67141583E-05 3  
 -2.89732189E-08 1.30497405E-11 4.43342884E+04 1.01751445E+01 4.55348541E+04 4

15499-23-7

FO2 F-O-O SIGMA=1 STATWT=2 IA=1.0714 IB=8.3532 IC=9.4246 [T0=8630  
 STATWT=2] NU=1487,376,579.3 HF298=25.4 +/-2. kJ REF=Chase JPCRD 25 (1966),551  
 {HF298=25.497+/-0.47 kJ REF=ATcT A} Max Lst Sq Error Cp @ 1200 K 0.34%.  
 FO2 F-O-O T02/97F 1.0 2. 0. 0.G 200.000 6000.000 B 50.99720 1  
 6.04302238E+00 6.92267660E-04-1.41442202E-07 1.67666488E-11-1.02129739E-15 2  
 1.03557297E+03-3.85061644E+00 3.13625166E+00 1.16477108E-02-1.82583930E-05 3  
 1.50964178E-08-5.01239416E-12 1.73596746E+03 1.05579694E+01 3.05490041E+03 4

7782-41-4

F2 REFERENCE ELEMENT HF298=0. From Original data of Gurvich 89. Max Lst Sq  
 Error Cp @ 6000 K 0.87  
 F2 REF ELEMENT RUS 89F 2. 0. 0. 0.G 200.000 6000.000 A 37.99681 1  
 3.86166219E+00 7.88367679E-04-1.81982940E-07-9.17436560E-12 2.65193472E-15 2  
 -1.23238655E+03 2.04119869E+00 3.20832415E+00 1.25919179E-03 3.89747979E-06 3  
 -7.22184984E-09 3.31837862E-12-1.03425794E+03 5.61903603E+00 0.00000000E+00 4

Table 4 (continued)

7783-41-7

F2O F-O-F SIGMA=2 STATWT=1 IA=1.4392 IB=7.7225 IC=9.1617 NU=925,461,831  
 X11=-4.5 X22=-0.4 X33=-6.3 X12=-6.1 X13=-19.2 X23=-11.0  
 A000=1.960777 B000=.363466 ALFAA1=.001286 ALFAA2=-.023317 ALFAA3=.019514  
 ALFAB1=.002194 ALFAB2=.001413 ALFAB3=.002320 ALFAC1=.000239 ALFAC2=.001777  
 ALFAC3=.003844 TAAAA=-.0002207 TBBBB=-3.167D-06 TCCCC=-1.272D-06 W=-6.9  
 TAABB=1.333D-05 TBBC=-1.928D-06 TAACC=4.090D-06 TABAB=-5.42D-06 C000=.305792  
 RHO 1= 0.12988717E-04 RHO 2= 0. HF298=24.5+/-2. kJ REF+Chase JPCRD 25 (1996)  
 ,551 {HF298=25.439+/-0.85 kJ REF=ATcT A} Max Lst Sq Error Cp @ 200 K 0.24 %.  
 F2O F-O-F g 5/99F 2.0 1. 0. 0.G 200.000 6000.000 A 53.99621 1  
 6.06108975E+00 1.15961203E-03-3.75240266E-07 6.51442886E-11-4.05767505E-15 2  
 8.77698718E+02-5.59764248E+00 2.70030207E+00 1.13302499E-02-1.03150938E-05 3  
 2.39433049E-09 7.96759423E-13 1.72399199E+03 1.14405456E+01 2.94665591E+03 4

7783-44-0

F2O2 F-O-O-F SIGMA=2 STATWT=1 IA=4.1409 IB=16.747 IC=19.247 NU=1210,630.360,  
 202,614,466 HF298=32.87+/-1.3 kJ REF=ATcT A {HF298=19.2+/-2. kJ REF=Chase  
 JPCRD 25 (1996),551} Max Lst Sq Error Cp @ 1200 K 0.24%.  
 F2O2 F-O-O-F ATcT/AF 2.0 2. 0. 0.G 200.000 6000.000 B 69.99561 1  
 8.65306600E+00 1.38757623E-03-5.45322964E-07 9.33107078E-11-5.81240066E-15 2  
 1.04381815E+03-1.69986695E+01 2.14732347E+00 2.93490625E-02-4.95409067E-05 3  
 4.05002590E-08-1.28729207E-11 2.37236337E+03 1.42255077E+01 3.95332978E+03 4

7439-89-6

Fe REFERENCE ELEMENT HF298=0.0 kJ REF=JANAF

Fe(a) J 3/78FE 1. 0. 0. 0.S 200.000 1042.000 B 55.84700 1  
 4.69080173E+03-9.90659991E+00 2.69427446E-03 5.54445321E-06-3.01659823E-09 2  
 -1.41547586E+06-2.49294387E+04 2.41337476E+00-1.57780744E-03 2.14701339E-05 3  
 -3.80171438E-08 2.20426984E-11-7.74380998E+02-1.06560296E+01 0.00000000E+00 4  
 Fe(b) J 3/78FE 1. 0. 0. 0.S 1042.000 1184.000 B 55.84700 1  
 6.59678809E+02-1.14058217E+00 4.96306997E-04 0.00000000E+00 0.00000000E+00 2  
 -2.52106802E+05-3.65665236E+03 0.00000000E+00 0.00000000E+00 0.00000000E+00 3  
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 4  
 Fe(c) J 3/78FE 1. 0. 0. 0.S 1184.000 1665.000 B 55.84700 1  
 6.10109990E+01-1.60945061E-01 1.68369493E-04-7.74563702E-08 1.33091290E-11 2  
 -1.65335454E+04-3.13710668E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 3  
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 4  
 Fe(d) J 3/78FE 1. 0. 0. 0.S 1665.000 1809.000 B 55.84700 1  
 -4.35904698E+02 7.68489448E-01-4.46898892E-04 8.67070913E-08 0.00000000E+00 2  
 1.87925534E+05 2.45057619E+03 0.00000000E+00 0.00000000E+00 0.00000000E+00 3  
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 4  
 Fe(L) J 3/78FE 1. 0. 0. 0.L 1809.000 6000.000 B 55.84700 1  
 5.53538332E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2  
 -1.27428941E+03-2.94772271E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 3  
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 4

7439-89-6

Fe HF298=415.5 +/- 1.3 kJ REF=JANAF

Fe J 3/78FE 1. 0. 0. 0.G 200.000 6000.000 B 55.84700 1  
 3.26197970E+00-1.05582533E-03 5.92906998E-07-1.07189455E-10 7.48064402E-15 2  
 4.90969873E+04 3.52443894E+00 1.70744428E+00 1.06339224E-02-2.76118171E-05 3  
 2.80917854E-08-1.01219824E-11 4.91843725E+04 9.80811099E+00 4.99728787E+04 4



Table 4 (continued)

14067-02-8

Fe+ ion HF298=[1181.144] kJ REF=JANAF

Fe+	J 6/84FE 1.E -1.	0.	0.G	298.150	6000.000	C	55.84645	1
	3.33602399E+00-2.72549262E-04	8.05440344E-09	1.51229089E-11-1.43376595E-15					2
	1.41036455E+05	2.86476968E+00	2.76418106E+00	2.86948238E-03-7.61235651E-06				3
	8.18183334E-09-3.11792199E-12	1.41159039E+05	5.53997981E+00	1.42058161E+05				4

22325-61-7

Fe- ion HF298=[393.338] kJ REF=JANAF

Fe-	J 6/84FE 1.E 1.	0.	0.G	298.150	6000.000	C	55.84755	1
	3.36310586E+00-8.29375042E-04	3.12426241E-07-5.20068355E-11	3.17875241E-15					2
	4.63564307E+04	2.76802421E+00	1.52174510E+00	9.79673193E-03-2.11078670E-05				3
	1.84820903E-08-5.89537134E-12	4.65710215E+04	1.08683385E+01	4.73074180E+04				4

27846-09-9

FeCl Ferrous Chloride T0=0 STATWT=6 WE=404.92 WEXE=1.19 BE=[0.17795]  
 ALFAE=[0.00075] T0=200 STATWT=8 T0=1000 STATWT=8 T0=4000 STATWT=8 REF=JANAF  
 HF298=251.0 +/- 84 kJ

FeCL	J 6/65FE 1.CL 1.	0.	0.G	300.000	5000.000	A	91.29970	1
	4.69406690E+00	1.16040780E-04-2.08401750E-08-1.76265560E-12	5.23138140E-16					2
	2.87903440E+04	4.19355506E+00	3.78858260E+00	4.36780110E-03-6.69223280E-06				3
	4.17074540E-09-8.46867730E-13	2.89200970E+04	8.35336756E+00	3.01925149E+04				4

7758-94-3

FeCl2 Ferric Chloride CONDENSED REF=JANAF HF298(S)=-341.833 +/- 0.42 kJ

FeCL2(s)	J12/70FE 1.CL 2.	0.	0.S	300.000	950.000	C	126.75240	1
	7.11222710E+00	1.10869530E-02-1.70727420E-05	1.35158170E-08-4.13650360E-12					2
	-4.36009850E+04-2.89940550E+01	7.11222710E+00	1.10869530E-02-1.70727420E-05					3
	1.35158170E-08-4.13650360E-12-4.36009850E+04-2.89940550E+01-4.11137739E+04							4
FeCL2(L)	J12/70FE 1.CL 2.	0.	0.L	950.000	5000.000	C	126.75240	1
	1.22888630E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
	-4.11098210E+04-5.31930570E+01	1.22888630E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00			3
	0.00000000E+00	0.00000000E+00-4.11098210E+04-5.31930570E+01	0.00000000E+00					4

7558-94-3

FeCl2 Ferric Chloride T0=0 STATWT=10 B0=0.050489 NU=327,88(2),492 SIGMA=2  
 T0=4800 STATWT=10 T0=7140 STATWT=5 HF298=-141.+/-2.1 kJ REF=JANAF

FeCL2	J12/70FE 1.CL 2.	0.	0.G	300.000	5000.000	B	126.75240	1
	6.94926010E+00	5.33716410E-04	7.02212070E-08-6.14754900E-11	6.79331430E-15				2
	-1.90458320E+04-3.75951441E+00	5.45575050E+00	7.96329270E-03-1.25939640E-05					3
	8.99767340E-09-2.32423630E-12-1.88442970E+04	3.02284219E+00-1.69583047E+04						4

7705-08-0

FeCl3 Ferrun Chloride CONDENSED HF298(S)=-399.405+/-0.84 kJ REF=JANAF

FeCL3(s)	J 6/65FE 1.CL 3.	0.	0.S	200.000	577.000	C	162.20510	1
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			2
	0.00000000E+00	0.00000000E+00-7.39556855E+00	2.02608434E-01-8.44505923E-04					3
	1.59286602E-06-1.07989321E-09-5.00144664E+04	2.44450935E+01-4.80371062E+04						4
FeCL3(L)	J 6/65FE 1.CL 3.	0.	0.L	577.000	6000.000	C	162.20510	1
	1.61031270E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			2
	-4.84135278E+04-6.75758990E+01	1.61031270E+01	0.00000000E+00	0.00000000E+00				3
	0.00000000E+00	0.00000000E+00-4.84135278E+04-6.75758990E+01-4.80371062E+04						4

Table 4 (continued)

7705-08-0

FeCl<sub>3</sub> SIGMA=6 STATWT=6 IA=IB=41.5834 IC=83.1667 nu=130(2),160,310(2),350

HF298=-253.13 +/- 5.0 kJ REF=JANAF

FeCl<sub>3</sub> J 6/65FE 1.CL 3. 0. 0.G 300.000 5000.000 C 162.20510 1  
 9.77711060E+00 2.44213620E-04-1.03139940E-07 1.92074260E-11-1.31792990E-15 2  
 -3.34395700E+04-1.45491463E+01 7.56148730E+00 9.73382490E-03-1.55433050E-05 3  
 1.11863680E-08-3.00229980E-12-3.30136240E+04-3.98583203E+00-3.04431637E+04 4

1345-25-1

FeO Ferric Oxide REF=JANAF HF298(S)=-272.044 kJ

FeO(s) J 6/65FE 1.O 1. 0. 0.S 300.000 1650.000 C 71.84640 1  
 5.83164890E+00 1.42751560E-03-9.32081430E-08-6.59977630E-12-2.25121430E-14 2  
 -3.45669020E+04-2.64469900E+01 5.31954750E+00 2.20965910E-03 1.07217750E-06 3  
 -2.79297290E-09 1.33207330E-12-3.44071650E+04-2.36860340E+01-3.27183475E+04 4  
 FeO(L) J 6/65FE 1.O 1. 0. 0.L 1650.000 5000.000 C 71.84640 1  
 8.20224820E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2  
 -3.38486150E+04-4.00791290E+01 8.20224820E+00 0.00000000E+00 0.00000000E+00 3  
 0.00000000E+00 0.00000000E+00-3.38486150E+04-4.00791290E+01 0.00000000E+00 4

1345-25-1

FeO Ferrum Oxide T0=0 STATWT=10 WE=880.0 WEXE=5.0 BE=[0.4184] ALFAE=0.00293

T0=10000 STATWT=10 T0=16000 STATWT=5 HF298=251.04 +/- 20.9 kJ

FeO J 9/66FE 1.O 1. 0. 0.G 300.000 5000.000 B 71.84640 1  
 4.20498170E+00 2.68384520E-04-8.94267360E-08 3.18559110E-11-3.39225430E-15 2  
 2.88291700E+04 4.83043159E+00 2.82452560E+00 4.30492070E-03-4.10847810E-06 3  
 1.32011890E-09 7.13162170E-14 2.91940350E+04 1.18911760E+01 3.01938519E+04 4

18624-44-7

Fe(OH)<sub>2</sub> Ferric Hydroxide HF298(S)=-574.04 +/- 2.9 kJ REF=JANAF

Fe(OH)<sub>2</sub>(s) J 6/66FE 1.O 2.H 2. 0.C 300.000 1500.000 B 89.86168 1  
 7.40318080E+00 1.19817420E-02-1.49576110E-06-5.05263590E-09 2.00371110E-12 2  
 -7.15922660E+04-3.46732670E+01 1.00912180E+01 4.45231410E-03 4.06668550E-06 3  
 -4.00945250E-09 2.39471640E-13-7.22776880E+04-4.84000340E+01-6.90429813E+04 4

18624-44-7

Fe(OH)<sub>2</sub> Ferrum Hydroxide T0=0 STATWT=5 IA=0.2814 IB=18.6208 IC=18.9022

NU=2300,450,800,750,320,700,400,2600,570 SIGMA=2 HF298=-330.54 +/- 2.1 kJ

Fe(OH)<sub>2</sub> J12/66FE 1.O 2.H 2. 0.G 200.000 6000.000 C 89.86168 1  
 8.96262012E+00 4.20137342E-03-1.61017443E-06 2.68347076E-10-1.63497305E-14 2  
 -4.27994358E+04-1.86912367E+01-1.67667734E+00 6.16931464E-02-1.20738995E-04 3  
 1.09814026E-07-3.72856831E-11-4.11289708E+04 2.96771710E+01-3.97541166E+04 4

1309-33-7

Fe(OH)<sub>3</sub> Ferrum Hydroxide HF298(S)=-832.62 +/-12.6 kJ REF=JANAF

Fe(OH)<sub>3</sub>(s) J 6/66FE 1.O 3.H 3. 0.C 300.000 1500.000 B 106.86902 1  
 8.02239260E+00 1.64201350E-02-1.23693780E-07-6.81928380E-09 2.32769070E-12 2  
 -1.03213360E+05-3.79340200E+01 4.41168360E+00 3.26824620E-02-2.23938150E-05 3  
 2.86467920E-09 2.26223210E-12-1.02718340E+05-2.13310140E+01-1.00141482E+05 4

1317-96-0

FeS Ferrum Monosulfide CONDENSED REF=JANAF HF298(S)=-101.67 +/- 0.8 kJ

FeS(a) J 9/77FE 1.S 1. 0. 0.S 300.000 411.000 B 87.91300 1  
 1.89776270E+01-1.09542820E-01 2.21860160E-04 0.00000000E+00 0.00000000E+00 2  
 -1.49952420E+04-7.81254350E+01 1.89776270E+01-1.09542820E-01 2.21860160E-04 3  
 0.00000000E+00 0.00000000E+00-1.49952420E+04-7.81254350E+01-1.22458515E+04 4

Table 4 (continued)

FeS(b)	J 9/77FE 1.S 1. 0. 0.S	411.000	598.000	B	87.91300	1
8.70285050E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
-1.46897380E+04	-4.20821020E+01	8.70285050E+00	0.00000000E+00	0.00000000E+00		3
0.00000000E+00	0.00000000E+00	-1.46897380E+04	-4.20821020E+01	0.00000000E+00		4
FeS(c)	J 9/77FE 1.S 1. 0. 0.S	598.000	1463.000	B	87.91300	1
-2.68304830E+00	3.67651040E-02	-5.21822740E-05	3.16071700E-08	-6.41260410E-12		2
-1.14986840E+04	1.62391240E+01	9.37241760E+00	9.41620590E-04	-1.58298640E-05		3
1.83808810E-08	-5.77070670E-12	-1.45816850E+04	-4.51415160E+01	0.00000000E+00		4
FeS(L)	J 9/77FE 1.S 1. 0. 0.L	1463.000	5000.000	B	87.91300	1
7.52328060E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
-1.01642370E+04	-3.19709300E+01	7.52328060E+00	0.00000000E+00	0.00000000E+00		3
0.00000000E+00	0.00000000E+00	-1.01642370E+04	-3.19709300E+01	0.00000000E+00		4
1317-96-0						
FeS Ferrum Monosulfide HF298=370.767 kJ Data from I. Barrin Database 1989.						
FeS(G)	B /89FE 1.S 1. 0. 0.G	298.150	3000.000	C	87.91100	1
4.14494627E+00	7.05834738E-04	-5.16986528E-07	1.86466769E-10	-2.22683845E-14		2
4.33002296E+04	6.46991922E+00	2.90286012E+00	6.65546290E-03	-1.14989921E-05		3
9.33240931E-09	-2.89374741E-12	4.35159803E+04	1.22605433E+01	4.45927661E+04		4
7720-78-7						
FeSO4 Ferrous Sulfate REF=JANAF HF298(S)=-928.85 +/-8.4 kJ						
FeSO4(s)	J 6/66FE 1.S 1.0 4. 0.S	300.000	2000.000	C	151.91060	1
1.16089290E+01	1.38046970E-02	-9.81263800E-06	3.60878110E-09	-5.09762790E-13		2
-1.16191860E+05	-5.64778170E+01	3.50576840E+00	3.70297010E-02	-2.90335310E-05		3
4.57785890E-09	2.62020870E-12	-1.14162500E+05	-1.52232410E+01	-1.11717626E+05		4
1309-36-0						
FeS2 Pyrite REF=JANAF HF298(S)=-171.54 +/-2.1 kJ						
FeS2(s)	J 9/77FE 1.S 2. 0. 0.C	300.000	1400.000	C	119.97900	1
-8.85153200E+01	3.27489310E-01	-4.10574390E-04	2.29281460E-07	-4.77644150E-11		2
-4.65124760E+02	4.41730450E+02	4.03456630E-01	4.26746840E-02	-8.40306260E-05		3
7.63014410E-08	-2.54323160E-11	-2.20459270E+04	-5.54563930E+00	-2.06325071E+04		4
23444-30-6						
Fe2Cl4 (FeCl2)2 T0=0 STATWT=10 IA=31.1433 IB=218.7538 IC=IA + IB						
NU=[30,50,80,90,110,125,150,180,200,249,325,438] T0=4600 STATWT=10 T0=7140						
STATWT=5 REF=JANAF HF298=-431.37 +/- 4.2 kJ						
Fe2CL4	J12/70FE 2.CL 4. 0. 0.G	300.000	5000.000	B	253.50480	1
1.53575000E+01	6.42078610E-04	2.08177300E-08	-5.15805590E-11	6.06734950E-15		2
-5.65100370E+04	-3.18965871E+01	1.27382420E+01	1.32355580E-02	-2.16418730E-05		3
1.59936670E-08	-4.35070970E-12	-5.61065790E+04	-1.98247491E+01	-5.18820452E+04		4
16480-60-7						
Fe2Cl6 (FeCl3)2 SIGMA=4 IA=116.3664 IB=194.7424 IC=311.1088 NU=350,310,300,260,250,230,200,120,110(3),100,95,90,85,70,35,18 HF298=-654.38 +/- 8.4 kJ						
REF = JANAF						
Fe2CL6	J 6/65FE 2.CL 6. 0. 0.G	200.000	6000.000	B	324.41020	1
2.15645031E+01	4.62349015E-04	-1.84952078E-07	3.20143043E-11	-2.01002737E-15		2
-8.52432375E+04	-5.86538185E+01	1.42211808E+01	4.35485968E-02	-9.60390188E-05		3
9.37463081E-08	-3.36051626E-11	-8.41996265E+04	-2.59244694E+01	-7.87030865E+04		4

Table 4 (continued)

1317-60-8

Fe<sub>2</sub>O<sub>3</sub> HEMATITE HF298(S)=-824.248 kJ Data from I. Barin Database 1989

Fe <sub>2</sub> O <sub>3</sub> (S) Solid-A	B	/89FE 2.O 3.	0.	0.S	298.150	960.000	C 159.68820	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
0.00000000E+00	0.00000000E+00	1.52218166E-01	6.70757040E-02	-1.12860954E-04				3
9.93356662E-08	-3.27580975E-11	-1.01344092E+05	-6.15024507E+00	-9.91336832E+04				4
Fe <sub>2</sub> O <sub>3</sub> (S) Solid-B	B	/89FE 2.O 3.	0.	0.S	960.000	1700.000	C 159.68820	1
3.53051527E+02	-9.72758065E-01	1.04598367E-03	-4.95511272E-07	8.73647747E-11				2
-1.95976954E+05	-1.81528607E+03	8.01447907E+01	-6.20141606E-02	0.00000000E+00				3
0.00000000E+00	0.00000000E+00	-1.36185811E+05	-4.61194426E+02	-9.91336832E+04				4

12011-67-5

Fe<sub>3</sub>C Triferrumcarbide HF298(S)=25.104 kJ Data from I. Barin database 1989.

Fe <sub>3</sub> C (S) Solid-A	B	/89C 1.FE 3.	0.	0.S	298.150	485.000	C 179.54600	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
0.00000000E+00	0.00000000E+00	9.68770665E+00	1.04155445E-02	-9.03325722E-07				3
7.59127519E-10	0.00000000E+00	-3.25545652E+02	-4.56881802E+01	3.01929999E+03				4
Fe <sub>3</sub> C (S) Solid-B	B	/89C 1.FE 3.	0.	0.S	485.000	1500.000	C 179.54600	1
1.29117933E+01	1.45677470E-03	5.11471347E-08	-2.03130285E-11	2.64589235E-15				2
-1.62949142E+01	-5.96219813E+01	1.28970825E+01	1.48707284E-03	3.83705751E-08				3
-2.70661902E-11	6.58822517E-15	-1.15745541E+01	-5.95430074E+01	3.01929999E+03				4
Fe <sub>3</sub> C (L) Liquid	B	/89C 1.FE 3.	0.	0.L	1500.000	2000.000	C 179.54600	1
1.46661913E+01	-1.66080339E-04	1.41368457E-07	-5.33048944E-11	7.51357777E-15				2
5.30022441E+03	-6.59621815E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00				3
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	3.01929999E+03				4

1309-38-2

Fe<sub>3</sub>O<sub>4</sub> MAGNETITE HF298(s)=-1118.383 kJ Data from I. Barin database 1989

Fe <sub>3</sub> O <sub>4</sub> (S) Solid-A	B	/89FE 3.O 4.	0.	0.S	298.150	850.000	C 231.53260	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
0.00000000E+00	0.00000000E+00	4.84450959E+00	4.39051578E-02	5.24676763E-05				3
-2.20801809E-07	1.74856371E-10	-1.38015344E+05	-2.38418082E+01	-1.34509791E+05				4
Fe <sub>3</sub> O <sub>4</sub> (S) Solid-B	B	/89FE 3.O 4.	0.	0.S	850.000	1870.000	C 231.53260	1
8.84307558E+01	-1.48964861E-01	1.25760044E-04	-4.70060974E-08	6.78732076E-12				2
-1.62143803E+05	-4.63815254E+02	7.97181560E+01	-9.83508037E-02	4.36398095E-05				3
0.00000000E+00	0.00000000E+00	-1.61758880E+05	-4.27156556E+02	-1.34509791E+05				4
Fe <sub>3</sub> O <sub>4</sub> (L) Liquid	B	/89FE 3.O 4.	0.	0.L	1870.000	2000.000	C 231.53260	1
2.45827554E+01	1.11718119E-03	-2.88207928E-07	0.00000000E+00	0.00000000E+00				2
-1.26461365E+05	-1.15899474E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00				3
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	-1.34509791E+05				4

25884-11-1

GeBr Germanium Bromide SIGMA=1 Calculated from Gurvich's original table 1991.

HF298=137.44 kJ HF0=144.47 kJ Max Lst Sq Error Cp @ 700 K 0.14%

GeBr	RUS 91GE 1.BR 1.	0.	0.G	200.000	6000.000	B 152.51400	1
5.37334408E+00	-6.76936973E-04	2.44834869E-07	-3.17858430E-11	1.25231490E-15			2
1.48281157E+04	2.07006807E-01	3.55872665E+00	3.55692441E-03	-5.33454710E-07			3
-4.21585176E-09	2.54436386E-12	1.53226264E+04	9.65613413E+00	1.65299120E+04			4

24415-00-7

GeBr<sub>2</sub> Germanium DiBromide SIGMA=2 STATWT=1 IAIBIC=165000. Nu=288,267,102

HF0=-46.+/ -5kJ HF298=-60.963 REF=Gurvich 1991. Max Lst Sq Error Cp @ 400 K

GeBr <sub>2</sub>	Rus 91GE 1.BR 2.	0.	0.G	200.000	6000.000	B 232.41800	1
6.88516604E+00	1.21917413E-04	-4.87714621E-08	8.44224690E-12	-5.30054609E-16			2
-9.41426303E+03	-9.38759565E-01	4.95506908E+00	1.14288300E-02	-2.51749286E-05			3
2.45541548E-08	-8.79690109E-12	-9.13939058E+03	7.66723245E+00	-7.33210941E+03			4

Table 4 (continued)

57147-09-8

GeBr3 Germanium TriBromo SIGMA=3 STATWT=2 IAIBIC=1700000. Nu=330(2),280,150,110(2) HF298=-119.031 +/-50. kJ HF0=-96.164 kJ REF=Gurvich 1991 Max Lst Sq Error Cp @ 400 K 0.28%.

GeBr3	RUS 91GE 1.BR 3.	0.	0.G	200.000	6000.000	B 312.32200	1
	9.76493341E+00	2.49387982E-04	-9.97238821E-08	1.72573376E-11	-1.08331733E-15		2
	-1.72888982E+04	-1.21585258E+01	5.95663141E+00	2.23501022E-02	-4.89008509E-05		3
	4.74893514E-08	-1.69644626E-11	-1.67392586E+04	4.86495514E+00	-1.43160942E+04		4

13450-92-5

GeBr4 Germanium TetraBromide SIGMA=12 STATWT=1 IAIBIC=6090000. Nu=335.1(3),235.7,111.1(3),74.7(2) HF298=-291+/-6. kJ HF0=-261.287 kJ REF=Gurvich 1991. Max Lst Sq Error Cp @ 400 K 0.27%

GeBr4	RUS 91GE 1.BR 4.	0.	0.G	200.000	6000.000	B 392.22600	1
	1.26993588E+01	3.18891973E-04	-1.27501775E-07	2.20626094E-11	-1.38489060E-15		2
	-3.88643283E+04	-2.49634414E+01	7.87919568E+00	2.82172586E-02	-6.16193016E-05		3
	5.97669067E-08	-2.13326327E-11	-3.81660434E+04	-3.40153686E+00	-3.49990559E+04		4

21110-21-4

GeCl Germanium Chlorid SIGMA=1 STATWT=2 From Gurvich's original table. 1991 HF298=69.03+/-18. kJ HF0=68.66 kJ {HF298=106.9 kJ REF=Wang & Zhang JPC A 108,(2004),10346-353} Max Lst Sq Error Cp @ 400 K & 1300 K 0.17%.

GeCl	A 1/05GE 1.CL 1.	0.	0.G	200.000	6000.000	B 108.06270	1
	5.17762971E+00	-4.66039986E-04	1.42197756E-07	-1.05389955E-11	6.01746946E-17		2
	6.69935596E+03	5.74624469E-03	2.72444852E+00	8.95175345E-03	-1.25463066E-05		3
	6.75349002E-09	-1.04007672E-12	7.19016201E+03	1.18835382E+01	8.30234313E+03		4

10060-11-4

GeCl2 Germanium Dichloride singlet SIGMA=2 STATWT=1 IA=11.8266 IB=32.4945 IC=45.3209 Nu=393,374,152 HF298=-166.9 kJ HF0=-166.39 kJ REF=Wang & Zhang JPC A 108,(2004),10346-353 {HF298=-171. +/-5. kJ REF=Gurvich 1991)} Max Lst Sq Error Cp @ 400 K 0.26%

GeCl2	singlet A 1/05GE 1.CL 2.	0.	0.G	200.000	6000.000	B 143.51540	1
	6.79351478E+00	2.18561190E-04	-8.72823862E-08	1.50910985E-11	-9.46763902E-16		2
	-2.21563223E+04	-3.25039811E+00	3.84255008E+00	1.67529188E-02	-3.57118572E-05		3
	3.40926252E-08	-1.20372990E-11	-2.17097912E+04	1.00619837E+01	-2.00733417E+04		4

158965-68-5 ??

GeCl2 Germanium Dichloride triplet SIGMA=2 STATWT=3 IA=7.1869 IB=41.5489 IC=48.7357 Nu=394,346,108 HF298=102.3 kJ HF0=102.53 kJ REF=Wang & Zhang JPC A 108,(2004),10346-353 Max Lst Sq Error Cp @ 400 K 0.24%

GeCl2	triplet A 1/05GE 1.CL 2.	0.	0.G	200.000	6000.000	B 143.51540	1
	6.81293089E+00	1.98046120E-04	-7.90981674E-08	1.36770236E-11	-8.58091771E-16		2
	1.02206003E+04	-1.95991296E+00	4.11512740E+00	1.53508236E-02	-3.27831640E-05		3
	3.13344673E-08	-1.10725565E-11	1.06275124E+04	1.02027699E+01	1.23037918E+04		4

13569-55-6

GeCl3 Germanium Trichloride SIGMA=3 STATWT=2 IA=IB=40.4236 IC=72.7468 NU=401(2),362,159,126(2) HF298=-234.4 kJ HF0=-233.692 kJ REF=Wang & Zhang JPC A 108,(2004),10346-353 {HF0=-266.102 +/-50. kJ REF=Gurvich 1979 (error in 1991)} Max Lst Sq Error Cp @ 400 K 0.30%

GeCl3	Wang & Z A 1/05GE 1.CL 3.	0.	0.G	200.000	6000.000	B 178.96810	1
	9.66739396E+00	3.52083734E-04	-1.40609944E-07	2.43120518E-11	-1.52528179E-15		2
	-3.11661085E+04	-1.46964485E+01	4.87749855E+00	2.72689732E-02	-5.82615423E-05		3
	5.57079208E-08	-1.96911957E-11	-3.04439818E+04	6.89576825E+00	-2.81916794E+04		4

Table 4 (continued)

10038-98-9

GeCl<sub>4</sub> Germanium Tetrachloride SIGMA=12 STATWT=1 IA=IB=IC=70.6231 Nu=125(3),  
 171.2(3),396.9,459(3) HF298=-500.9 +/-5.0 kJ HF0=-498.55 kJ REF=Wang &  
 Zhang JPC A 108,(2004),10346-353 {HF0=-500. +/-10. kJ REF=Gurvich 1991} Max  
 Lst Sq Error Cp @ 400 K 0.32%

GeCl <sub>4</sub>	Wang &	A 1/05GE 1.CL 4.	0.	0.G	200.000	6000.000	B 214.42080	1
		1.24258326E+01	6.06654290E-04	-2.42012844E-07	4.18147899E-11	-2.62205604E-15		2
		-6.40524947E+04	-2.93922591E+01	4.88842695E+00	4.18964270E-02	-8.77843613E-05		3
		8.28593113E-08	-2.90301372E-11	-6.28780637E+04	4.80674244E+00	-6.01839435E+04		4

13637-65-5

GeH<sub>3</sub>Cl Chlorogermane SIGMA=2 STATWT=1 IA=1.0766 IB=IC=19.8078 Nu=422,602(2),  
 848,874(2),2120,2129(2) HF298=57.7 kJ HF0=67.63 kJ REF=Wang & Zhang JPC A  
 108,(2004),10346-353 Max Lst Sq Error Cp @ 1300 K 0.59%

GeH <sub>3</sub> Cl	A 1/05GE 1.H 3.CL 1.	0.G	200.000	6000.000	B 111.08652	1
	7.05170839E+00	5.69805692E-03	-2.14367790E-06	3.56659527E-10	-2.17964076E-14	2
	4.17257822E+03	-1.06064602E+01	1.12153499E+00	2.60156187E-02	-3.16506126E-05	3
	2.16972347E-08	-6.24282523E-12	5.68867761E+03	1.92353641E+01	6.93967534E+03	4

7782-65-2

GeH<sub>4</sub> Germanium Tetrahydride SIGMA=12 STATWT=1 IA=IB=IC=1.0505 Nu=819(3),  
 931(2),2106,2114(3) HF298=90.3+/-2. kJ REF=Wang & Zhang JPC A 108,(2004),  
 10346-353 {HF298=90.59+/-2 REF=Gunn Green JPC 65,(1961),779} Max Lst Sq Error  
 Cp @ 1300 K 0.65%

GeH <sub>4</sub>	A 1/05GE 1.H 4.	0.	0.G	200.000	6000.000	B 76.64176	1
	5.41474159E+00	7.24155154E-03	-2.71818301E-06	4.51535021E-10	-2.75635275E-14		2
	8.46356611E+03	-7.83419271E+00	2.54992789E+00	7.13885765E-03	1.43758337E-05		3
	-2.33592977E-08	9.65676013E-12	9.69756465E+03	9.02678812E+00	1.08605318E+04		4

12385-13-6

H HF0=211.801 KJ REF=C.E. Moore "Selected Tables of Atomic Spectra" NSRDS-NBS  
 Sec 6 1972 p. A1 I. {HF298=217.998+/-3.4E-5 REF=ATcT A}

H	L 6/94H 1	0	0	OG	200.000	6000.000	A 1.00794	1
	0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			2
	0.25473660E+05	-0.44668285E+00	0.25000000E+01	0.00000000E+00	0.00000000E+00			3
	0.00000000E+00	0.00000000E+00	0.25473660E+05	-0.44668285E+00	0.26219035E+05			4

12408-02-5

H+ HF298=1536.246 kJ HF0=1528.085 kJ REF=Moore NSRDS-NBS 3, SEC6, 1972.  
 {HF298=1536.245+/-3.5E-5 kJ REF=ATcT A} Max Lst Sq Error N/A

H+	g10/00H 1.E -1.	0.	0.G	298.150	6000.000	B 1.00739	1
	2.50000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
	1.84021488E+05	-1.14064664E+00	2.50000000E+00	0.00000000E+00	0.00000000E+00		3
	0.00000000E+00	0.00000000E+00	1.84021488E+05	-1.14064664E+00	1.84766863E+05		4

12184-88-2

H- HF0=132.834 KJ REF=JANAF 1982

H-	L/7/88H 1E 1	0	OG	298.150	6000.000	B 1.00849	1
	0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
	0.15976167E+05	-0.11390139E+01	0.25000000E+01	0.00000000E+00	0.00000000E+00		3
	0.00000000E+00	0.00000000E+00	0.15976167E+05	-0.11390139E+01	0.16721542E+05		4

Table 4 (continued)

10035-10-6

HBr HYDROBROMIC ACID CALCULATED FROM ORIGINAL TABLES REF=Gurvich 1989

HF298=-36.29+/-0.16 kJ {HF298=-36.142+/-0.16 kJ REF=ATcT A} Max Lst Sq Error  
Cp @ 6000 K 0.32%

HBR	RUS 89H	1BR	1	0	OG	200.000	5000.000	B	80.91194	1
	0.28330819E+01	0.14872632E-02	-0.51463345E-06	0.87853840E-10	-0.57591453E-14					2
	-0.52289003E+04	0.74405672E+01	0.34894141E+01	0.27295667E-03	-0.15997163E-05					3
	0.33659948E-08	-0.16408428E-11	-0.54089034E+04	0.39796907E+01	-0.43646589E+04					4

7647-01-0

HCl HYDROCHLORIC ACID CALCULATED FROM ORIGINAL TABLES REF=Gurvich 1989

HF298=-92.31 kJ {HF298=-92.178+/-0.10 kJ REF=ATcT A} Max Lst Sq Error Cp @  
6000 K 0.17%

HCL	RUS 89H	1CL	1	0	OG	200.000	6000.000	B	36.46064	1
	0.27575767E+01	0.14538737E-02	-0.47964697E-06	0.77790943E-10	-0.47957377E-14					2
	-0.11913766E+05	0.65219722E+01	0.34637647E+01	0.47648423E-03	-0.20030122E-05					3
	0.33171437E-08	-0.14495818E-11	-0.12144352E+05	0.26642828E+01	-0.11102278E+05					4

7790-92-3

HOCl SIGMA=1 STATWT=1 IAIBIC=4.357 NU=3609.2,1240,725 HF0=-72.8 kJ

REF=Gurvich 89 Max Lst Sq Error Cp @ 400 K 0.25%

HOCL	RUS 89H	1O	1CL	1	OG	200.000	6000.000	B	52.46004	1
	0.43664934E+01	0.20513656E-02	-0.67087650E-06	0.10131893E-09	-0.57791828E-14					2
	-0.10576070E+05	0.28049555E+01	0.35465037E+01	0.23321738E-02	0.52331522E-05					3
	-0.97366010E-08	0.44672936E-11	-0.10299629E+05	0.73974601E+01	-0.91094784E+04					4

7664-39-3

HF HYDROFLUORIC ACID CALCULATED FROM ORIGINAL TABLES REF=Gurvich 1989

HF298=-273.3+/-0.7 kJ {HF298=-272.864+/-0.16 kJ REF=ATcT A} Max Lst Sq Error  
Cp @ 1200 K 0.35%

HF	RUS 89H	1F	1	0	OG	200.000	6000.000	B	20.00634	1
	0.29204304E+01	0.85796097E-03	-0.16306811E-06	0.13780358E-10	-0.29021238E-15					2
	-0.33685882E+05	0.42144066E+01	0.34811480E+01	0.21334107E-03	-0.68985280E-06					3
	0.85966803E-09	-0.23549086E-12	-0.33913127E+05	0.10259567E+01	-0.32870247E+05					4

14034-79-8

HOF SIGMA=1 STATWT=1 IAIBIC=1.464 NU=3537,1359,886 HF0=-94 kJ

REF=Gurvich 89 Max Lst Sq Error Cp @ 400 K 0.29%

HOF	RUS 89H	1O	1F	1	OG	200.000	6000.000	B	36.00574	1
	0.41252846E+01	0.23151964E-02	-0.77666557E-06	0.11954885E-09	-0.69172673E-14					2
	-0.13072651E+05	0.28986184E+01	0.39203542E+01	-0.13992801E-02	0.13911528E-04					3
	-0.17901805E-07	0.72456494E-11	-0.12851722E+05	0.48785828E+01	-0.11654111E+05					4

10034-85-2

HI HYDROIODIC ACID SIGMA=2 Be=6.512 WE=2309.06 WEXE=39.73 ALFAE=0.1715

HF298=26.359+/-0.21 kJ REF=JANAF {HF298=26.558+/-0.047 kJ REF=ATcT A}

HI	J 9/61H	1.I	1.	0.	O.G	300.000	5000.000	B	127.91241	1
	2.91040080E+00	1.56881880E-03	-5.92276320E-07	1.05370940E-10	-7.03751160E-15					2
	2.25086590E+03	7.86447051E+00	3.69637220E+00	-1.42247550E-03	3.01311880E-06					3
	-1.26664030E-09	-3.50987650E-14	2.10735810E+03	4.08812111E+00	3.17030779E+03					4

Table 4 (continued)

14332-28-6

HNO NITROGEN OXIDE-HYDRIDE Nitrosyl hydride HN=O STATWT=1 SIGMA=1 A0=18.476  
 B0=1.411 C0=1.306 NU=2684,1501,1565 DJ=.4050E-5 DJK=.98E-4 DK=.4485E-2  
 T0=6280 STATWT=3 A0=22.156 B0=1.325 C0=1.242 NU=2850,992,1468  
 T0=13154.4 STATWT=1 A0=22.156 B0=1.325 C0=1.242 NU=2854,981,1421  
 REF=Jacox (1988) HF298=106.842+/-0.125 kJ REF=ATcT A {HF0=105.+/-10.5 kJ  
 REF=Gurvich 1989} Max Lst Sq Error Cp @ 6000 K 0.91%  
 HNO ATcT/AH 1.N 1.O 1. 0.G 200.000 6000.000 A 31.01408 1  
 3.16598124E+00 2.99958892E-03-3.94376786E-07-3.85344089E-11 7.07602668E-15 2  
 1.17726311E+04 7.64511172E+00 4.53525574E+00-5.68543377E-03 1.85198540E-05 3  
 -1.71881225E-08 5.55818157E-12 1.16183003E+04 1.74315886E+00 1.28500657E+04 4

7782-77-6

HNO2 NITROUS ACID STATWT=1 SIGMA=1 A0=3.0783 B0=.41663 C0=.36698 NU=3588,  
 1699,1265,791,593,540 T0=140. STATWT=1 SIGMA=1 A0=2.7899 B0=.43796  
 C0=.37856 NU=3424,1640,1261,853,608,638 REF=Gurvich 1989 HF0=-72.8 KJ Max  
 Lst Sq Error Cp @ 6000 K 0.32 %.  
 HNO2 RUS 89H 1.N 1.O 2 0.G 200.000 6000.000 B 47.01348 1  
 0.57919018E+01 0.36515212E-02-0.12928936E-05 0.20688716E-09-0.12315254E-13 2  
 -0.11565589E+05-0.40558233E+01 0.32141709E+01 0.81276869E-02 0.16602559E-05 3  
 -0.95285182E-08 0.48715058E-11-0.10753237E+05 0.98219504E+01-0.94355439E+04 4

7697-37-2

HNO3 NITRIC ACID STATWT=1 SIGMA=2 A0=.4339999 B0=.403609 C0=.2088327  
 Ir=.1329 v(0)=1134.4 cm-1 ROSYM=2 NU=3550,1710,1326,1303.5,879,647,  
 580,763 REF=Dorofeeva JPCRD 32, (2003), 879 HF0=-124.57 KJ HF298 =134.3+/-0.5 kJ  
 {HF298=-134.112+/-0.18 REF=ATcT A} Max Lst Sq Error Cp @ 1300 K 0.49 %  
 HNO3 T 8/03H 1.N 1.O 3. 0.G 200.000 6000.000 B 63.01288 1  
 8.03098942E+00 4.46958589E-03-1.72459491E-06 2.91556153E-10-1.80102702E-14 2  
 -1.93138183E+04-1.62616537E+01 1.69329154E+00 1.90167702E-02-8.25176697E-06 3  
 -6.06113827E-09 4.65236978E-12-1.74198909E+04 1.71839838E+01-1.61524852E+04 4

3352-57-6

OH HYDROXYL RADICAL T0=0 STATWT=2 WE=3738 WEXE=-84.88 WEYE=0.54 B0=18.550  
 T0=139.7 STATWT=2 T0=32403 STATWT=2 WE=3184.3 WEXE=97.845 BE=17.355 REF=Poly-  
 nomials were calculated directly from Gurvich's Tables wich are direct summation,  
 HF298=37.3+/-0.3 kJ HF0=37.1+/-0.3 kJ REF=Ruscic et al JPC 106, (2002), 2727.  
 Ruscic et al JPCRD 2005 {HF298=37.344+/-0.04 kJ REF=ATcT A} Max Lst Sq Error  
 Cp @ 1200 K 0.28%  
 OH HYDROXYL RADI IU3/03O 1.H 1. 0. 0.G 200.000 6000.000 A 17.00734 1  
 2.83853033E+00 1.10741289E-03-2.94000209E-07 4.20698729E-11-2.42289890E-15 2  
 3.69780808E+03 5.84494652E+00 3.99198424E+00-2.40106655E-03 4.61664033E-06 3  
 -3.87916306E-09 1.36319502E-12 3.36889836E+03-1.03998477E-01 4.48615380E+03 4

12259-29-9

OH+ HYDROXIL POSITIVE ION FROM ORIGINAL DATA HF298=1290.204 KJ REF=TSIV 78  
 OH+ RUS 78O 1.H 1.E -1. 0.G 298.150 6000.000 A 17.00679 1  
 2.68358997E+00 1.57006432E-03-5.39972805E-07 9.37643859E-11-5.70068055E-15 2  
 1.54395744E+05 6.44375888E+00 3.50502572E+00 2.41313749E-04-1.42200949E-06 3  
 2.64780232E-09-1.17038711E-12 1.54127124E+05 1.97907627E+00 1.55174989E+05 4

14280-30-9

OH- HYDROXIL ION FROM ORIGINAL DATA HF0=-150.805 KJ REF=TSIV 78  
 OH- L 3/93O 1.H 1.E 1. 0.G 298.150 6000.000 A 17.00789 1  
 2.83405701E+00 1.07058023E-03-2.62459398E-07 3.08376435E-11-1.31383862E-15 2  
 -1.80186974E+04 4.49464762E+00 3.43279956E+00 6.19656310E-04-1.89930992E-06 3  
 2.37365946E-09-8.55103755E-13-1.82613086E+04 1.06053670E+00-1.72227709E+04 4



Table 4 (continued)

3170-83-0

HO2 RADICAL GROUND STATE STATWT=2 A0=20.356 B0=1.118 C0=1.056 NU=3436.2,  
1391.75,1097.63 EXCITED STATE T0=7029.684 A0=20.486 B0=1.021 C0=0.968  
NU=3268.5,1285,929.068 STATWT=2 REF=JACOX JPCRD 17, (1988) P.269

HF298=12.55 KJ REF=Hills & Howard J. CHEM. PHYS 81 (1984), 4458

{HF298=12.296+/-0.25 REF=ATcT A}

HO2	L 5/89H	10	2	0	OG	200.000	6000.000	B	33.00674	1
	0.41722659E+01	0.18812098E-02	-0.34629297E-06	0.19468516E-10	0.17609153E-15					2
	0.61818851E+02	0.29577974E+01	0.43017880E+01	-0.47490201E-02	0.21157953E-04					3
	-0.24275961E-07	0.92920670E-11	0.29480876E+03	0.37167010E+01	0.15096500E+04					4

13817-06-6

HPO PHOSPHORUS OXYHYDRIDE SIGMA=1 STATWT=1 IAIBIC=5.437 NU=2330,1188,985  
T0=19032.8 STATWT=1 SIGMA=1 HF0=-53. KJ REF=Gurvich 1989 Max Lst Sq Error  
Cp @ 6000 K 0.38%

HPO	RUS 89H	1P	10	1	OG	200.000	6000.000	B	47.98110	1
	0.42999621E+01	0.26002099E-02	-0.99411489E-06	0.16916642E-09	-0.10420412E-13					2
	-0.84075730E+04	0.27172028E+01	0.40742366E+01	-0.31019711E-02	0.18964972E-04					3
	-0.22506453E-07	0.86340185E-11	-0.80437690E+04	0.53965266E+01	-0.68397546E+04					4

13940-21-1

SH T0(STATWT)=0(2), Be=9.461 WE=2711.6 WEXE=59.0 ALFAE=0.27 T0=376.96(2)  
T0=31038(2) Be=8.5214 WE=1979.8 WEXE=97.65 ALFAE=0.464 DE=6.36E-4  
T0=59641(2) Be=8.785 WE=2557. WEXE=56.8 ALFAE=0.259 DE=8.2E-4  
T0=63900(4),71195(4),71318(2),76708(4) Be=9.4611 WE=2711.6 WEXE=59.0  
ALFAE=0.27 DE=4.8E-4 T0=79343(4),80848(4) HF298=141.87+/-0.52 kJ HF0=141.24  
+/-0.52 kJ REF=Csazar Leninger & Burcat J.Chem Phys 2003 Max Lst Sq Error Cp @  
400 K 0.47%.

SH	IU2/03S	1.H	1.	0.	O.G	200.000	6000.000	A	33.07294	1
	3.03153027E+00	1.25805252E-03	-4.05524133E-07	6.19648110E-11	-3.50862111E-15					2
	1.62059674E+04	6.15022140E+00	3.68466877E+00	3.24608824E-03	-1.28635079E-05					3
	1.69512196E-08	-7.07595387E-12	1.59036477E+04	2.01781634E+00	1.70629418E+04					4

62803-12-7

S-OH RADICAL STATWT=2 SIGMA=1 IA=0.1222028 IB=5.0098556 IC=5.132059  
NU=3638,1184,826 HF298=-4.994+/-10. KCAL REF=C. Melius BAC/MP4 DATABASE,  
Private Communication Max Lst Sq Error Cp @ 400 K 0.35%

SOH	T 4/93S	10	1H	1	OG	200.000	6000.000	B	49.07334	1
	0.43544347E+01	0.20549939E-02	-0.67083934E-06	0.10119158E-09	-0.57672355E-14					2
	-0.39895568E+04	0.32303081E+01	0.36922437E+01	0.44545692E-03	0.10785948E-04					3
	-0.15975515E-07	0.68858806E-11	-0.37006791E+04	0.73216957E+01	-0.25130640E+04					4

62470-71-7

HS=O RADICAL STATWT=2 SIGMA=1 IA=0.272571 IB=4.331163 IC=4.603734  
NU=751,1060.5,2543 HF298=-1.143 KCAL estimated. REF=C. MELIUS BAC/MP4 Database  
Private Communication Max Lst Sq Error Cp @ 6000 K 0.32%

HSO	T 4/93H	1S	10	1	OG	200.000	6000.000	B	49.07334	1
	0.45416010E+01	0.22648458E-02	-0.83152058E-06	0.13614796E-09	-0.82290966E-14					2
	-0.21608556E+04	0.23357633E+01	0.34130925E+01	0.32105128E-02	0.38960721E-05					3
	-0.81958128E-08	0.37789804E-11	-0.17554966E+04	0.86522782E+01	-0.57517665E+03					4

Table 4 (continued)

12306-07-9 ~

HSO2 HOSO RADICAL STATWT=2 SIGMA=1 IA=2.397408 IB=8.7861523 IC=11.010938  
 IR=0.11955 NU=403.6,788,1011,1111,3608 ROSYM=2 POT BARRIER V(3)=409.2 cm-1  
 HF298=-61.158 KCAL REF=C. MELIUS BAC/MP4 Database, Private communication

Max Lst Sq Error Cp @ 6000 K 0.19%

HO2S	T11/96H	10	2S	1	OG	200.000	6000.000	B	65.07274	1
6.45143466E+00	2.48602888E-03	-8.43212436E-07	1.30962437E-10	-7.63196759E-15						2
-3.29875786E+04	-4.61876333E+00	3.69601366E+00	9.53437650E-03	-3.92988151E-06						3
-4.41313434E-09	3.33020726E-12	-3.22589853E+04	9.59023664E+00	-3.07751148E+04						4

32750-86-0

HSO3 HOSO2 RADICAL STATWT=2 SIGMA=1 IA=9.4168978 IB=9.7757253 IC=16.401348  
 IR=0.125875 NU=323.6,433,444,675,818,1110,1196,3562 ROSYM=2 POT BARRIER  
 V(3)=954.8 cm-1 REF=C. MELIUS BAC/MP4 Database, Private communication

HF298=-92.1 KCAL REF=Margitan J.J. JPC 88 (1984), 3314 Max Lst Sq Error  
 Cp @ 6000 K 0.18%.

HSO3	T 3/93H	1S	10	3	OG	200.000	6000.000	B	81.07214	1
0.91911575E+01	0.27980912E-02	-0.97493219E-06	0.15441946E-09	-0.91299297E-14						2
-0.49457258E+05	-0.18510636E+02	0.90501684E+00	0.38941616E-01	-0.63379448E-04						3
0.49872276E-07	-0.15179855E-10	-0.47836694E+05	0.21006792E+02	-0.46304593E+05						4

14541-24-3

HS2 HYDROTHIOSULFENO RADICAL SIGMA=1 STATWT=2 A0=9.9261912 B0=0.2643802

C0=0.2571927 Nu=2463,903,595 X11=-57.568 X12=-13.891 X13=1.212

X22=-4.359 X23=-4.537 X33=-2.668 ALFAA1=.2898629 ALFAA2=-.2033949

ALFAA3=.0072196 ALFAB1=-.0006322 ALFAB2=.0003877 ALFAB3=.0016149

ALFAC1=-0.000433 ALFAC2=.0008446 ALFAC3=.0016087 RHO=0.89334E-05

HF0=25.331 kcal REF=JML Martin calc CCSD(T)/cc-pV(Q+d)Z Dec 2001. (HF298=24.71 kcal) {HF298=25+/-2.5 kcal exper. REF=Decker et, al Int. J. Mass. Spec,185-187, (1999),727-747.} Max Lst Sq Error Cp @ 6000 K 0.29%

Hydrothiosulfeno	T 3/03H	1.S	2.	0.	0.G	200.000	6000.000	A	65.13994	1
4.75155728E+00	2.15521745E-03	-7.39343908E-07	1.22229939E-10	-7.35968292E-15						2
1.08214337E+04	2.68990027E+00	2.96279116E+00	8.56185025E-03	-9.91987786E-06						3
6.19874244E-09	-1.52120491E-12	1.12507023E+04	1.15828502E+01	1.24384961E+04						4

14541-24-3

HS2 HYDROTHIOSULFENO RADICAL RRHO SIGMA=1 STATWT=2 A0=9.9261912 B0=0.2643802

C0=0.2571927 Nu=2463,903,595. HF298=25+/-2.5 kcal exper. REF=Decker et, al

Int. J. Mass. Spec,185-187, (1999),727-747. Max Lst Sq Error Cp @ 6000 K 0.29%

HS2 RRHO	T 4/02H	1.S	2.	0.	0.G	200.000	6000.000	B	65.13994	1
5.00284875E+00	1.53333839E-03	-3.71725630E-07	4.12310396E-11	-1.83712860E-15						2
5.09462277E+04	1.36789719E+00	2.96323558E+00	8.55501824E-03	-1.00388287E-05						3
6.25269399E-09	-1.52826367E-12	5.14497883E+04	1.15800366E+01	1.25804170E+04						4

1333-74-0

H2 HF298= 0.0 REF=TSIV

H2 REF ELEMENT	RUS 78H	2	0	0	OG	200.000	6000.000	A	2.01588	1
0.29328305E+01	0.82659802E-03	-0.14640057E-06	0.15409851E-10	-0.68879615E-15						2
-0.81305582E+03	-0.10243164E+01	0.23443029E+01	0.79804248E-02	-0.19477917E-04						3
0.20156967E-07	-0.73760289E-11	-0.91792413E+03	0.68300218E+00	0.00000000E+00						4

Table 4 (continued)

30664-12-1

H2F2 SIGMA=1 IAIBIC=20. NU=4038,4081,171,588,519,226 HF0=-566.5 KJ

REF=Gurvich 89 Max Lst Sq Error Cp @ 1300 K 0.18%

H2F2	RUS 89H	2F	2	0	OG	200.000	6000.000	B	40.01269	1
0.65095969E+01	0.19848359E-02	-0.46422746E-06	0.49022863E-10	-0.18846028E-14						2
-0.70500916E+05	-0.61547561E+01	0.33553129E+01	0.22103635E-01	-0.43986009E-04						3
0.40099889E-07	-0.13495484E-10	-0.70212768E+05	0.72994688E+01	-0.68545684E+05						4

7732-18-5

H2O Water CONDENSED REF=NASA Unpublished HF298=-285.83 kJ {HF298=-285.819+/-0.03 kJ REF=ATcT A}.

H2O(s)	L 8/89H	2.O	1.	0.	0.S	200.000	273.150		18.01528	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
0.00000000E+00	0.00000000E+00	5.29677970E+00	-6.75749247E-02	5.16942109E-04						3
-1.43853360E-06	1.52564794E-09	-3.62266557E+04	-1.79220428E+01	-3.59742186E+04						4
H2O(L)	L 8/89H	2.O	1.	0.	0.L	273.150	600.000	C	18.01528	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
0.00000000E+00	0.00000000E+00	7.25575005E+01	-6.62445402E-01	2.56198746E-03						3
-4.36591923E-06	2.78178981E-09	-4.18865499E+04	-2.88280137E+02	-3.43772513E+04						4

7732-18-5

H2O REF=Wooley J. RES. NBS 92 (1987), 35. HF298=-241.826+/-0.04 KJ based on HF298(L) from Cox, Wagman & Medvedev CODATA KEY VAL. for THERMO, Hemisphere 1989 p.21 and heat of vap. from Haar, Gallagher & Kell NBS/NRC Tables, Hemisphere 1984. {HF298=-241.815+/-0.03 kJ REF=ATcT A}.

H2O	L 5/89H	2O	1	0	OG	200.000	6000.000	A	18.01528	1
0.26770389E+01	0.29731816E-02	-0.77376889E-06	0.94433514E-10	-0.42689991E-14						2
-0.29885894E+05	0.68825500E+01	0.41986352E+01	-0.20364017E-02	0.65203416E-05						3
-0.54879269E-08	0.17719680E-11	-0.30293726E+05	-0.84900901E+00	-0.29084817E+05						4

7722-84-1

H2O2 liquid Hydrogen Peroxide REF=Gurvich 1989 HF298=-44.880 kcal

{HF298=-187.676+/-0.06 REF=ATcT A} Max Lst Sq Error Cp @ 2000 K 0.0017%

H2O2(L)	RUS/89H	2.O	2.	0.	0.L	272.740	6000.000	B	34.01468	1
1.07426738E+01	1.64789013E-06	-7.92451706E-10	1.53610575E-13	-1.04359108E-17						2
-2.57871325E+04	-4.80251356E+01	1.07394015E+01	2.99630938E-05	-7.13210384E-08						3
7.09751854E-11	-2.53463009E-14	-2.57871465E+04	-4.80128553E+01	-2.25843640E+04						4

7722-84-1

H2O2 Hydrogen Peroxide SIGMA=2 IAIBIC=2.976026 E-117 Ir=0.071093 NU=3599, 1388,875,3611,1266 X11=90.9 x12=11 x13=11 x15=167.6 x16=3 x22=10 x23=7

x25=11.5 x26=4 x33=10 x35=11.1 x36=2 x55=90.2 x56=3 x66=3 ALFAA1=0.234

ALFAA2=-0.104 ALFAA3=-0.034 ALFAA5=0.234 ALFAA6=-0.174 ALFAB1=0.003

ALFAB2=0.004 ALFAB3=.007 ALFAB5=.003 ALFAB6=.003 ALFAC1=-.001 ALFAC2=.004

ALFAC3=.013 ALFAC5=-.001 ALFAC6=.007 HF298= -135.88+/-0.2 KJ HF0=-129.9

REF=Dorofeeva et al JPCRD 32 (2003),879 {HF298=-135.77+/-0.07 REF=ATcT A}

Max Lst Sq Error CP @ 6000 K 0.29% Calculated directly from Original tables

H2O2 DOROFEEVA e	T 8/03H	2.O	2.	0.	0.G	200.000	6000.000	A	34.01468	1
4.57977305E+00	4.05326003E-03	-1.29844730E-06	1.98211400E-10	-1.13968792E-14						2
-1.80071775E+04	6.64970694E-01	4.31515149E+00	-8.47390622E-04	1.76404323E-05						3
-2.26762944E-08	9.08950158E-12	-1.77067437E+04	3.27373319E+00	-1.63425145E+04						4

Table 4 (continued)

7783-06-4

H2S CALCULATED FROM ORIGINAL VALUES REF=Gurvich 1989 HF298=-20.60 KJ

Max Lst Sq Error Cp @ 6000 K 0.38%

H2S	RUS 89H	2S	1	0	OG	200.000	6000.000	B	34.08188	1
0.29770813E+01	0.36005325E-02	-0.12328487E-05	0.19692654E-09	-0.11677327E-13						2
-0.35155970E+04	0.67868340E+01	0.41194112E+01	-0.18771599E-02	0.82066045E-05						3
-0.70594243E-08	0.21405829E-11	-0.36819294E+04	0.15345832E+01	-0.24775964E+04						4

7664-93-9

H2SO4 Liquid Sulfuric Acid HF298=-813.989+/-0.67 kJ REF= JANAF 1977.

H2SO4 (L)	J 9/77H	2.S	1.O	4.	0.L	300.000	1000.000	C	98.07948	1
9.94215250E+00	2.17863690E-02	3.49744580E-06	-3.35488570E-09	1.16995860E-12						2
-1.01859790E+05	-4.43986950E+01	9.94215250E+00	2.17863690E-02	3.49744580E-06						3
-3.35488570E-09	1.16995860E-12	-1.01859790E+05	-4.43986950E+01	-9.79023828E+04						4

7664-93-9

H2SO4 SULFURIC ACID SIGMA=2 STATWT=1 IAIBIC=4669.95E-117 NU=3563,1216,1136,831,548,420,355,3567,1452,1157,882,558,475, Ir=0.8097 HF0=-720.8+/-2 KJ

HF298=-732.7 kJ REF=Dorofeeva et al JPCRD 32 (2003),879 Max Lst Sq Error Cp @ 6000 K 0.25%. Calculated from original tables.

H2SO4	T 8/03H	2.S	1.O	4.	0.G	200.000	6000.000	B	98.07948	1
1.13355392E+01	5.60829109E-03	-1.94574192E-06	3.07136054E-10	-1.81109544E-14						2
-9.21087435E+04	-2.96094003E+01	4.53388173E+00	3.10347679E-02	-4.10421795E-05						3
2.95752341E-08	-8.81459071E-12	-9.05459072E+04	3.93961412E+00	-8.81230524E+04						4

63344-86-5

H2S2 HS-SH DISULFANE SIGMA=2 STATWT=1 Ia=0.5381381 Ib=10.4557619 Ic=10.9939

REF=MOPAC AM1-UHF NU=2557,2556,883,882,516,416 REF= Jacox+Shimanouchi NIST

Webbook 2000 HF298=15.5 kcal REF=Kerr CRC Handbook of Chem and Phys 2002.

Max Lst Sq Error Cp @ 6000 K 0.37%

Disulfane H-S-S-	T 3/03H	2.S	2.	0.	0.G	200.000	6000.000	B	66.14788	1
5.69402902E+00	3.90495326E-03	-1.41886468E-06	2.30688658E-10	-1.38745854E-14						2
-1.65807167E+02	-3.74138641E+00	2.09117166E+00	1.94220358E-02	-2.89395611E-05						3
2.30251562E-08	-7.20187083E-12	5.91056782E+02	1.35883795E+01	1.86421088E+03						4

16904-65-7

H3F3 SIGMA=3 IAIBIC=2000. NU=3200(3),275(3),1000(3),550.(3) HF0=-873. KJ

Max Lst Sq Error Cp @ 6000 K 0.27%

H3F3	RUS 89H	3F	3	0	OG	200.000	6000.000	C	60.01903	1
0.87390503E+01	0.59975373E-02	-0.20456662E-05	0.31840506E-09	-0.18565610E-13						2
-0.10935328E+06	-0.18233375E+02	0.15442408E+01	0.38576820E-01	-0.59195549E-04						3
0.45635939E-07	-0.13570689E-10	-0.10801711E+06	0.15744454E+02	-0.10628128E+06						4

13968-08-6

H3O+ HYDRONIUM ION SIGMA=3 STATWT=1 IAIBIC=.0287 NU=3490,960,3610(2),1590(2)

HF298=598. KJ REF=Gurvich 1989 Max Lst Sq Error Cp @ 6000 K 0.29%

H3O+	RUS 89H	3O	1E	-1	OG	298.150	6000.000	B	19.02267	1
0.24964777E+01	0.57284481E-02	-0.18395322E-05	0.27357729E-09	-0.15409386E-13						2
0.70972911E+05	0.74585048E+01	0.37929561E+01	-0.91087830E-03	0.11636414E-04						3
-0.12136548E-07	0.42616180E-11	0.70751240E+05	0.14715543E+01	0.71922458E+05						4

Table 4 (continued)

51912-69-7

H4F4 SIGMA=4 IAIBIC=17000. NU=3200(4),275(4),1000(4),550(4),40,20

HF0=-1174. KJ REF=Gurvich 89 Max Lst Sq Error Cp @ 6000 K 0.26%

H4F4	RUS 89H	4F	4	0	OG	200.000	6000.000	C	80.02537	1
0.12317199E+02	0.79983433E-02	-0.27282048E-05	0.42465241E-09	-0.24761183E-13						2
-0.14704897E+06	-0.31058240E+02	0.26932762E+01	0.51626337E-01	-0.79360527E-04						3
0.61278889E-07	-0.18250746E-10	-0.14526330E+06	0.14381384E+02	-0.14275433E+06						4

74835-81-7

H5F5 SIGMA=5 IAIBIC=100000. NU=3200(5),275(5),1000(5),550(5),40(2),20(2)

HF0=-1475. REF=Gurvich 89 KJ Max Lst Sq Error Cp @ 6000 K 0.26%

H5F5	RUS 89H	5F	5	0	OG	200.000	6000.000	C	100.03172	1
0.15895341E+02	0.99991630E-02	-0.34107496E-05	0.53090070E-09	-0.30956799E-13						2
-0.18474466E+06	-0.44099390E+02	0.38423046E+01	0.64675877E-01	-0.99525494E-04						3
0.76921762E-07	-0.22930752E-10	-0.18250949E+06	0.12802019E+02	-0.17922738E+06						4

24993-08-6

H6F6 SIGMA=6 STATWT=1 IAIBIC=495000. NU=3065,1029,203,537,26,551(2),3322(2),991(2),327(2),33(2),550,3403,979,356,53,3153(2),1017(2),252(2),545(2),15(2)

HF0=-1788. KJ Max Lst Sq Error Cp @ 6000 K 0.25%.

H6F6	RUS 89H	6F	6	0	OG	200.000	6000.000	B	120.03806	1
0.19464060E+02	0.11926891E-01	-0.40493043E-05	0.62823170E-09	-0.36546130E-13						2
-0.22389232E+06	-0.56827093E+02	0.47664477E+01	0.78603132E-01	-0.12115664E-03						3
0.93614852E-07	-0.27894457E-10	-0.22117213E+06	0.12546784E+02	-0.21715593E+06						4

74835-82-8

H7F7 SIGMA=7 IAIBIC=1800000. NU=3200(7),275(7),1000(7),550(7),40(4),20(4)

REF=Gurvich 89 HF0=-2080. KJ Max Lst Sq Error Cp @ 6000 K 0.25%

H7F7	RUS 89H	7F	7	0	OG	200.000	6000.000	C	140.04440	1
0.23051635E+02	0.14000785E-01	-0.47758323E-05	0.74339634E-09	-0.43347992E-13						2
-0.26049687E+06	-0.70563434E+02	0.61403336E+01	0.90775247E-01	-0.13985636E-03						3
0.10820867E-06	-0.32291248E-10	-0.25736269E+06	0.92617199E+01	-0.25253430E+06						4

7440-59-7

He HF298=0.0 KJ REF=McBride, Heilmel, Ehlers &amp; Gordon "Thermodynamic Properties to 6000K ..." NASA SP-3001 1963.

He REF ELEMENT	L10/90HE	1.	0.	0.	0.G	200.000	6000.000	B	4.00260	1
2.50000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			2
-7.45375000E+02	9.28723974E-01	2.50000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			3
0.00000000E+00	0.00000000E+00	-7.45375000E+02	9.28723974E-01	0.00000000E+00						4

14234-48-1

He+ HF298=2378.521 kJ HF0=2372.324 kJ REF=C.E. Moore U.S. Nat. Bur. Stand.

NSRDS-NBS 34 1970. {HF298=2378.520+/-2.2E-5 kJ REF=ATcT A} Max Lst Sq Error N/A

He+	g 3/97HE	1.E	-1.	0.	0.G	298.150	6000.000	B	4.00205	1
2.50000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			2
2.85323374E+05	1.62166556E+00	2.50000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			3
0.00000000E+00	0.00000000E+00	2.85323374E+05	1.62166556E+00	2.86068749E+05						4

7349-97-6

Hg REFERENCE ELEMENT REF=JANAF 1961 For the liquid phase above 630 K HF(T) is no longer 0.

Hg(cr)	J12/61HG	1.	0.	0.	0.S	200.000	234.290	B	200.59000	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			2
0.00000000E+00	0.00000000E+00	2.43103385E+00	4.24646658E-03	0.00000000E+00						3
0.00000000E+00	0.00000000E+00	-1.17886806E+03	-7.11248114E+00	0.00000000E+00						4

Table 4 (continued)

Hg (L) J12/61HG 1. 0. 0. 0.L 234.290 2000.000 B 200.59000 1  
 3.03653487E+00 3.16006666E-04 6.43901172E-08-2.92306991E-11 4.86860918E-15 2  
 -8.88170502E+02-8.17243018E+00 3.79685248E+00-2.09026109E-03 2.22267107E-06 3  
 -1.08605655E-10-4.28087248E-13-1.05834631E+03-1.19626936E+01 0.00000000E+00 4

7349-97-6

Hg (G) HF298=61.38+/-0.04 kJ HF0=-64.53 kJ REF=JANAF 1984 For the gas phase above 630 K the HF(T)=0 as for the reference element. See CODATA J. Chem. Therm 10, (1978), 903.

Hg J 9/84HG 1. 0. 0. 0.G 200.000 6000.000 B 200.59000 1  
 2.50953611E+00-1.98827279E-05 1.38910849E-08-3.93542920E-12 3.90959219E-16 2  
 6.63358064E+03 6.74847966E+00 2.50000000E+00 0.00000000E+00 0.00000000E+00 3  
 0.00000000E+00 0.00000000E+00 6.63690008E+03 6.80020154E+00 7.38227508E+03 4

7789-47-1

HgBr2 HF298=-40.5 kcal REF=NASA OLD Polynomial Database quoting JANAF 1962 tables which were not included in following editions.

HgBr2(s) J 3/62HG 1.BR 2. 0. 0.S 300.000 514.000 E 360.39800 1  
 8.28297140E+00 1.63023640E-03 3.42298790E-06 7.09619920E-10-4.33538620E-12 2  
 -2.29524380E+04-2.73452760E+01 8.28297140E+00 1.63023640E-03 3.42298790E-06 3  
 7.09619920E-10-4.33538620E-12-2.29524380E+04-2.73452760E+01-2.03808119E+04 4  
 HgBr2(L) J 3/62HG 1.BR 2. 0. 0.C 514.000 5000.000 E 360.39800 1  
 1.22787990E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2  
 -2.25008980E+04-4.68512120E+01 1.22787990E+01 0.00000000E+00 0.00000000E+00 3  
 0.00000000E+00 0.00000000E+00-2.25008980E+04-4.68512120E+01 0.00000000E+00 4

7789-47-1

HgBr2 (Gas) HF298=-20.424 kcal REF=NASA OLD polynomial database quoting JANAF 1962 tables not included in following editions.

HgBr2 J 3/62HG 1.BR 2. 0. 0.G 300.000 5000.000 E 360.39800 1  
 7.42269900E+00 7.86876630E-05-2.99103070E-08 4.84982280E-12-2.79309330E-16 2  
 -1.25220200E+04-3.86733971E+00 6.71889210E+00 2.57827430E-03-2.91802370E-06 3  
 9.58184420E-10 1.38723070E-13-1.23714340E+04-4.13670823E-01-1.02774216E+04 4

7546-30-7

HgCl Calomel (Gas) HF298=78.45 kJ REF= HF298 and Data taken from Webbook 2003 quoting JANAF 1961 loose leaf. Data do not match. Max Lst Sq Error Cp @ 298 K 0.1 % and @ 1300 K 0.02%

HgCl gas Calomel T12/03HG 1.CL 1. 0. 0.G 298.150 5000.000 F 236.04270 1  
 4.45021150E+00 1.51707424E-04-2.26822222E-08 4.20577307E-12-2.88049761E-16 2  
 8.08558085E+03 5.83071658E+00 3.74145448E+00 3.69165193E-03-6.83637866E-06 3  
 5.88297146E-09-1.89767893E-12 8.20538451E+03 9.10829950E+00 9.43531248E+03 4

7487-94-7

HgCl2 (gas) HF298=-146.29 kJ REF=HF298 and Data taken from Webbook 2003 quoting JANAF 1961. No gas phase data available below 1500 K.

HgCl2 T12/03HG 1.CL 2. 0. 0.G 1500.000 6000.000 F 271.49540 1  
 7.39652541E+00 8.32747985E-05-2.47105146E-08 3.02995739E-12-1.23771168E-16 2  
 -1.98011886E+04 1.55281444E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 3  
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00-1.75945426E+04 4

21908-53-2

HgO SOLID HF298=-90.789+/-0.1 kJ HF0=-86.208 kJ REF=JANAF 1962

HgO(s) J 6/62HG 1.O 1. 0. 0.C 300.000 1000.000 B 216.58940 1  
 3.41708660E+00 7.11605700E-03-1.48969960E-06-4.49135480E-09 2.59379240E-12 2  
 -1.22332700E+04-1.30371850E+01 3.41708660E+00 7.11605700E-03-1.48969960E-06 3  
 -4.49135480E-09 2.59379240E-12-1.22332700E+04-1.30371850E+01-1.09189916E+04 4

Table 4 (continued)

14362-44-8

I HF298=106.76+/-0.04 kJ REF=JANAF {HF298=106.756+/-0.04 kJ REF=ATcT A}  
 I J 6/82I 1. 0. 0. 0.G 200.000 6000.000 A 126.90447 1  
 2.61667712E+00-2.66010320E-04 1.86060150E-07-3.81927472E-11 2.52036053E-15 2  
 1.20582790E+04 6.87896653E+00 2.50041683E+00-4.48046831E-06 1.69962536E-08 3  
 -2.67708030E-11 1.48927452E-14 1.20947990E+04 7.49816581E+00 1.28402035E+04 4

15465-40-4

INO2 NITRO-IODINE SIGMA=2 IAIBIC=9.848 E-114 NU=1500,1250,500,400,320(2)  
 HF298=14.4+/-1 kcal REF=estimated by Van den Berg & Troe J. Chem. Phys. 64,  
 (1976),736 Max Lst Sq Error Cp @ 400 K 0.34%  
 INO2 NITRO-IODIN T05/99I 1.N 1.0 2. 0.G 200.000 6000.000 C 172.91001 1  
 7.95621858E+00 2.06254528E-03-8.00706693E-07 1.35937003E-10-8.42239842E-15 2  
 4.51430115E+03-1.11369097E+01 3.03369023E+00 2.20635097E-02-3.60079637E-05 3  
 3.05880596E-08-1.03317241E-11 5.62372932E+03 1.28994935E+01 7.24631999E+03 4

14696-98-1

IO T=0 STATWT=2 BE=0.340206 DE=3.6E-6 WE=681.6004 WEXE=4.3699 ALPHAE=0.0026296  
 T0=2091 STATWT=2 BE=0.340206 DE=3.6E-6 WE=681.6004 WEXE=4.3699 ALPHAE=0.0026296  
 T0=21577.81 STATWT=2 BE=0.27635 DE=3.2E-6 WE=514.57 WEXE=5.52 ALPHAE=0.00273  
 T0=24698 STATWT=2 BE=0.27635 DE=3.2E-6 WE=514.57 WEXE=5.52 ALPHAE=0.00273  
 HF298=126 +/- 18 kJ REF=C.W.Chase JPCRD 25 (1966),1297 Max Lst Sq Error  
 Cp @ 1300 K 0.66%.  
 IO T02/97I 1.0 1. 0. 0.G 200.000 6000.000 A 142.90387 1  
 4.43373036E+00 8.12520620E-04-3.07327741E-07 6.49186840E-11-1.64640359E-15 2  
 1.36225573E+04 2.96744910E+00 2.90243248E+00 5.16413407E-03-6.69836698E-06 3  
 5.78794148E-09-2.15394553E-12 1.41080990E+04 1.10195868E+01 1.51542304E+04 4

184842-55-5

IO2 I-O-O SIGMA=1 STATWT=2 IA=1.1391 IB=33.4021 IC=34.5412 NU=1500,150,  
 275 HF298=116.5+/- 40 kJ REF= C.W.Chase JPCRD 25 (1966),1297 Max Lst Sq Error  
 Cp @ 1300 K 0.22%  
 IO2 O-O-I T02/97I 1.0 2. 0. 0.G 200.000 6000.000 C 158.90327 1  
 5.98554951E+00 1.00992962E-03-3.88836232E-07 6.56594736E-11-4.05315145E-15 2  
 1.20886501E+04 1.04056474E+00 5.01488370E+00 4.03669659E-03-5.27430680E-06 3  
 4.73349091E-09-1.84251518E-12 1.23751572E+04 6.06532665E+00 1.40116495E+04 4

13494-92-3

IO2 O-I-O SIGMA=2 STATWT=2 IA=3.4373 IB=12.1991 IC=16.3491 NU=765,192,  
 800 HF298=159.3+/- 25 kJ REF= C.W.Chase JPCRD 25 (1966),1297 Max Lst Sq Error  
 Cp @ 2300 K 0.13%.  
 IO2 O-I-O T02/97I 1.0 2. 0. 0.G 200.000 6000.000 C 158.90327 1  
 6.34102047E+00 6.83348986E-04-2.69576480E-07 4.62346615E-11-2.88443810E-15 2  
 1.70776899E+04-2.88252557E+00 3.42630811E+00 1.04246908E-02-1.18836503E-05 3  
 5.37825233E-09-5.47457748E-13 1.77689996E+04 1.16760933E+01 1.91592770E+04 4

13870-16-1

IO3 SIGMA=3 STATWT=2 IA=IB=14.7650 IC=16.7280 NU=780,357,809.(2),326.(2)  
 HF298=241.9+/- 50 kJ REF= C.W.Chase JPCRD 25 (1966),1297 Max Lst Sq Error  
 Cp @ 1200 K 0.20%  
 IO3 T02/97I 1.0 3. 0. 0.G 200.000 6000.000 C 174.90267 1  
 8.79038934E+00 1.25737248E-03-4.96749925E-07 8.52803184E-11-5.32401360E-15 2  
 2.61270594E+04-1.59036984E+01 1.87546093E+00 2.97337732E-02-4.73077645E-05 3  
 3.59378000E-08-1.06083014E-11 2.75649245E+04 1.74919459E+01 2.90937169E+04 4

Table 4 (continued)

7553-56-2

I2 IS NOT A REFERENCE ELEMENT. HF298=62.421 kJ and HF=0 ABOVE 457.7 K. REF=JANAF  
 {HF298=62.415+/-0.08 kJ REF=ATcT A>

I2	J 9/61I	2	0	0	OG	300.000	5000.000	B	253.8089	1
0.44710820E+01	0.10020430E-03	-0.14380573E-07	0.27741939E-11	-0.19669640E-15						2
0.61639529E+04	0.58150347E+01	0.41670013E+01	0.14456721E-02	-0.22818415E-05						3
0.17076469E-08	-0.47899533E-12	0.62206616E+04	0.72552216E+01	0.75073722E+04						4

184825-25-0

I2O I-I-O SIGMA=1 STATWT=3 IA=5.1010 IB=112.5438 IC=117.6448 NU=750,100,  
 170 HF298=106.7+/- 40 kJ REF= C.W.Chase JPCRD 25 (1966)1297 Max Lst Sq Error  
 Cp @ 1200 K 0.07%.

I2O	I-I-O	T02/97I	2.0	1.	0.	OG	200.000	6000.000	C	269.80834	1
6.67743067E+00	3.35545667E-04	-1.32620068E-07	2.27738344E-11	-1.42202132E-15						2	
1.07480142E+04	1.43598484E+00	4.83414789E+00	7.77521188E-03	-1.20331147E-05						3	
8.84990542E-09	-2.52444240E-12	1.11361166E+04	1.03678902E+01	1.28329872E+04						4	

39319-71-6

I2O I-O-I SIGMA=2 STATWT=1 IA=2.8860 IB=119.9153 IC=122.8013 NU=475,100,  
 525 HF298=119.5+/- 25 kJ REF= C.W.Chase JPCRD 25 (1966)1297 Max Lst Sq Error  
 Cp @ 700 K 0.17%

I2O	I-O-I	T02/97I	2.0	1.	0.	OG	200.000	6000.000	C	269.80834	1
6.69553230E+00	3.20537584E-04	-1.27603300E-07	2.20163162E-11	-1.37922928E-15						2	
1.22845166E+04	-1.37479980E+00	3.43863289E+00	1.69797854E-02	-3.36137723E-05						3	
3.04801550E-08	-1.03756973E-11	1.28341774E+04	1.36477676E+01	1.43724645E+04						4	

7440-09-7

K(S,L) REFERENCE ELEMENT REF=CODATA 1989, NASA-Glen.

K(cr)	REF ELEMENT CODA89K	1.	0.	0.	0.C	200.000	336.860	B	39.09830	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00						2
0.00000000E+00	0.00000000E+00	-2.08951123E+00	6.16320193E-02	-2.40731903E-04						3
3.27255823E-07	0.00000000E+00	-6.36098059E+02	9.11736910E+00	0.00000000E+00						4
K(L)	REF ELEMENT CODA89K	1.	0.	0.	0.L	336.860	2200.000	B	39.09830	1
4.64954931E+00	-2.79174106E-03	1.80836337E-06	3.41244868E-11	-4.48782184E-15						2
-1.01467797E+03	-1.71767347E+01	4.22910563E+00	-7.06885543E-04	-2.12965848E-06						3
3.36227270E-09	-1.05902602E-12	-9.45117514E+02	-1.52340054E+01	0.00000000E+00						4

7440-09-7

K gas REF=JANAF 1983 HF298=89.0+/-0.4 kJ

K	L 4/93K	1.	0.	0.	OG	200.000	6000.000	B	39.09830	1
2.26026721E+00	5.62341179E-04	-4.48551838E-07	1.36243498E-10	-1.02926268E-14						2
1.00348812E+04	6.31568201E+00	2.50000712E+00	-7.25113166E-08	2.59068481E-10						3
-3.79460911E-13	1.93210641E-16	9.95880307E+03	5.04054517E+00	1.07041786E+04						4

24203-36-9

K+ (ion) REF=JANAF 1983 HF298=514.0 kJ

K+	J12/83K	1.E	-1.	0.	OG	298.150	6000.000	B	39.09775	1
2.50000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00						2
6.10751051E+04	4.34740449E+00	2.50000000E+00	0.00000000E+00	0.00000000E+00						3
0.00000000E+00	0.00000000E+00	6.10751051E+04	4.34740449E+00	6.18204801E+04						4



Table 4 (continued)

N/A

KNO<sub>3</sub> (S,L) Potassium Nitrate REF=McBride, Zehe, Gordon NASA/TP-2002-211556

HF298=-494.0+/-0.5 kJ REF=Gurvich 1982+1991 Max Lst Sq Error Cp @ 300 K 0.03%

KNO <sub>3</sub> (a) Rhombic	G09/02K	1.N	1.O	3.	0.C	200.000	402.000	B	101.10320	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
0.00000000E+00	0.00000000E+00	2.27228768E+02	-3.37546448E+00	1.90895706E-02						3
-4.65580008E-05	4.14595689E-08	-7.10865075E+04	-7.91333595E+02	-5.94142048E+04						4
KNO <sub>3</sub> (b) Hexagonal	G09/02K	1.N	1.O	3.	0.C	402.000	607.700	B	101.10320	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
0.00000000E+00	0.00000000E+00	4.11832358E+03	-3.39709442E+01	1.04795707E-01						3
-1.42778041E-04	7.24825679E-08	-4.55407739E+05	-1.68673429E+04	-5.94142048E+04						4
KNO <sub>3</sub> (L)	G09/02K	1.N	1.O	3.	0.L	607.700	6000.000	B	101.10320	1
1.69583829E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
-6.16499439E+04	-8.01839G52E+01	1.69583829E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00					3
0.00000000E+00	0.00000000E+00	-6.16499439E+04	-8.01839152E+01	-5.94142048E+04						4

N/A

KNO<sub>3</sub>(G) Potassium Nitrate REF=McBride, Zehe, Gordon NASA/TP-2002-211556

HF298=-315.833 kJ REF=Gurvich 1982+1991 Max Lst Sq Error Cp @ 1300 K 0.30%

KNO <sub>3</sub>	T 2/03K	1.N	1.O	3.	0.G	200.000	6000.000	B	101.10324	1
9.83342547E+00	3.24949762E-03	-1.28263805E-06	2.21146538E-10	-1.38801628E-14						2
-4.15640186E+04	-2.06635840E+01	4.62661240E+00	1.20422956E-02	5.33588742E-06						3
-1.98979277E-08	9.90068378E-12	-3.99129238E+04	7.42946290E+00	-3.79857622E+04						4

12136-45-7

K<sub>2</sub>O(g) HF298=-74.09 kJ REF=NASA (Glen) database Originating from Gurvich 1982

Max Lst sq Error Cp @ 400 K 0.16% Cp @ 1300 K 0.13%.

K <sub>2</sub> O	T 1/03K	2.O	1.	0.	0.G	200.000	6000.000	B	94.19600	1
6.85373450E+00	1.20610755E-04	-3.58446400E-08	4.41811547E-12	-1.85943403E-16						2
-1.10138636E+04	-4.75445780E+00	4.46818995E+00	1.27465910E-02	-2.62629170E-05						3
2.45126610E-08	-8.52179219E-12	-1.06216912E+04	6.17284336E+00	-8.91056719E+03						4

17014-71-0

K<sub>2</sub>O<sub>2</sub>(g) HF298=-191.566 kJ REF=NASA (Glen) database Originating from Gurvich

1982 Max Lst sq Error Cp @ 400 K 0.18% Cp @ 1300 K 0.15%.

K <sub>2</sub> O <sub>2</sub>	T 1/03K	2.O	2.	0.	0.G	200.000	6000.000	B	110.19540	1
9.31212268E+00	7.27176294E-04	-2.92192682E-07	5.09662863E-11	-3.22456333E-15						2
-2.60045018E+04	-1.67867684E+01	3.88984198E+00	2.72139924E-02	-5.18905525E-05						3
4.60841100E-08	-1.55025439E-11	-2.50345980E+04	8.51183208E+00	-2.30399627E+04						4

7439-90-9

Kr HF298=0.0 KJ REF=C.E. Moore U.S. Nat. Bur. Stand. NSRDS-NBS 34/35 1970.

Kr	REF ELEMENT	L10/90KR	1.	0.	0.	0.G	200.000	6000.000	B	83.80000	1
2.50000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2	
-7.45375000E+02	5.49095651E+00	2.50000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					3	
0.00000000E+00	0.00000000E+00	-7.45375000E+02	5.49095651E+00	0.00000000E+00	0.00000000E+00					4	

16915-28-9

Kr+ HF298=1356.954 kJ HF0=1350.756 kJ REF=Sugar &amp; Musgrove JPCRD 20, (1991),

1213 {HF298=1356.956+/-9.84E-4 kJ REF=ATcT A} Max Lst Sq Error Cp @ 1300 K 0.49%.

Kr+	g 7/97KR	1.E	-1.	0.	0.G	298.150	6000.000		83.79945	1
2.36497979E+00	1.27777445E-04	3.61872531E-08	-1.73046684E-11	1.53456326E-15						2
1.62522530E+05	7.67137103E+00	2.49760846E+00	1.45839121E-05	-1.92982926E-08						3
-2.15798802E-11	4.18601780E-14	1.62457997E+05	6.88748457E+00	1.63203113E+05						4

Table 4 (continued)

7439-95-4

Mg Magnesium REFERENCE ELEMENT HF298=0 REF=Alcok Chase & Itkin JPCRD 22 (1993)  
1-85 McBride Gordon & Reno NASA TP-3287 (1993) {Mg(L) HF298=4.79 kJ REF=JANAF}

Mg(cr)	L	93MG	1.	0.	0.	0.S	298.150	923.000	A	24.30500	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
0.00000000E+00	0.00000000E+00	1.47884944E+00	9.27430526E-03	-1.95050788E-05							3
1.98215527E-08	-7.04927374E-12	-7.16649299E+02	-6.57222695E+00	0.00000000E+00							4
Mg(L)	L	93MG	1.	0.	0.	0.L	923.000	6000.000	A	24.30500	1
4.12531827E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00						2
-6.58934341E+02	-1.93786894E+01	4.12531827E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00						3
0.00000000E+00	0.00000000E+00	-6.58934341E+02	-1.93786894E+01	0.00000000E+00							4

7439-95-4

Mg Magnesium HF298=147.10+/-0.8 kJ HF0=145.90 kJ REF=JANAF

Mg	J	9/83MG	1.	0.	0.	0.G	200.000	6000.000	A	24.30500	1
2.31664484E+00	3.65866339E-04	-2.33227803E-07	5.37117570E-11	-2.99513065E-15							2
1.70119233E+04	4.63449516E+00	2.50000000E+00	0.00000000E+00	0.00000000E+00							3
0.00000000E+00	0.00000000E+00	1.69465876E+04	3.63433014E+00	1.76919626E+04							4

14581-92-1

Mg+ Magnesium ion HF298=891.047 kJ HF0=883.631+/-1.3 kJ REF=Kaufman &amp; Martin JPCRD 20,(1991),83 Max Lst Sq Error Cp @ 6000 K 0.007%

Mg+	g	6/97MG	1.E	-1.	0.	0.G	298.150	6000.000	A	24.30445	1
2.50436286E+00	-9.52643105E-06	7.12820817E-09	-2.20778708E-12	2.43149667E-16							2
1.06420863E+05	4.30394336E+00	2.50000000E+00	0.00000000E+00	0.00000000E+00							3
0.00000000E+00	0.00000000E+00	1.06422335E+05	4.32744346E+00	1.07167710E+05							4

12068-51-8

MgAl2O4 Magnesium aluminium oxide Solid HF298(S)=-2299.11 kJ HF298(L)=-2106.53 kJ REF=JANAF

MgAl2O4(s)	J12/79MG	1.AL	2.O	4.	0.S	300.000	2408.000	142.26568	1
1.46976790E+01	9.33047970E-03	-3.55225980E-06	1.15505300E-09	-1.43345310E-13					2
-2.81664110E+05	-7.66686850E+01	-6.39126250E+00	1.17188600E-01	-2.13251780E-04					3
1.82774050E-07	-5.88319910E-11	-2.78271410E+05	2.01327010E+01	-2.76518945E+05					4
MgAl2O4(L)	J12/79MG	1.AL	2.O	4.	0.L	2408.000	5000.000	142.26568	1
2.64191880E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
-2.68835360E+05	-1.41985810E+02	2.64191880E+01	0.00000000E+00	0.00000000E+00					3
0.00000000E+00	0.00000000E+00	-2.68835360E+05	-1.41985810E+02	0.00000000E+00					4

14519-11-0

MgBr Magnesium Bromide HF298=-35.34+/-41.8 kJ HF0=-27.7 kJ REF=JANAF

MgBr	J	6/75MG	1.BR	1.	0.	0.G	300.000	5000.000	104.20900	1
4.40998540E+00	1.60217360E-04	-4.15012230E-08	5.93703420E-12	-4.82315730E-17						2
-5.59619090E+03	4.22960309E+00	3.51072850E+00	4.45285100E-03	-8.01240750E-06						3
6.70669000E-09	-2.12327180E-12	-5.43682570E+03	8.43148999E+00	-4.25072458E+03						4

7789-48-2

MgBr2 Solid &amp; Liquid Magnesium dibromide HF298(solid)=-524.26+/-2.1 kJ

HF298(liq)=-490.41 kJ REF=JANAF

MgBr2(s)	J	6/74MG	1.BR	2.	0.	0.C	300.000	984.000	184.11300	1
5.19664220E+00	2.06702530E-02	-3.72539390E-05	3.19375640E-08	-9.95070160E-12						2
-6.52526160E+04	-2.02889100E+01	5.19664220E+00	2.06702530E-02	-3.72539390E-05						3
3.19375640E-08	-9.95070160E-12	-6.52526160E+04	-2.02889100E+01	-6.30552290E+04						4
MgBr2(L)	J	6/74MG	1.BR	2.	0.	0.C	984.000	5000.000	184.11300	1
1.25807370E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00						2
-6.39629820E+04	-5.62554600E+01	1.25807370E+01	0.00000000E+00	0.00000000E+00						3
0.00000000E+00	0.00000000E+00	-6.39629820E+04	-5.62554600E+01	0.00000000E+00						4

Table 4 (continued)

7789-48-2

MgBr<sub>2</sub> Magnesium Dibromide HF298=-302.92+/-10.5 kJ REF=JANAF

MgBr <sub>2</sub>	J 6/74MG 1.BR 2.	0.	0.G	300.000	5000.000	184.11300	1
	7.32151000E+00	2.06437250E-04	-9.24892080E-08	1.82558380E-11	-1.32311700E-15		2
	-3.86713040E+04	-5.67846591E+00	5.71391020E+00	7.73216170E-03	-1.38657930E-05		3
	1.14779000E-08	-3.60578840E-12	-3.83794830E+04	1.86860229E+00	-3.64337335E+04		4

546-93-0

MgCO<sub>3</sub> Solid Magnesium Carbonate HF298=-1111.69+/-8. kJ REF=JANAF

MgCO <sub>3</sub> (s)	J12/66MG 1.C 1.O 3.	0.C	300.000	1000.000	84.31420	1
	1.34919240E+00	3.69341120E-02	-4.44929520E-05	3.18159060E-08	-9.75453000E-12	2
	-1.35416850E+05	-9.06187320E+00	1.34919240E+00	3.69341120E-02	-4.44929520E-05	3
	3.18159060E-08	-9.75453000E-12	-1.35416850E+05	-9.06187320E+00	-1.33707806E+05	4

14989-29-8

MgCl Magnesium Chloride HF298=-43.51+/-42. kJ REF=JANAF

MgCl	J 3/66MG 1.CL 1.	0.	0.G	300.000	5000.000	59.75770	1
	4.37758330E+00	1.88341780E-04	-5.44885920E-08	9.94810310E-12	-6.69496110E-16		2
	-6.58308260E+03	2.98938866E+00	3.38005340E+00	4.28133890E-03	-6.44573330E-06		3
	4.44722910E-09	-1.14217270E-12	-6.38265600E+03	7.78898816E+00	-5.23329928E+03		4

32195-53-2

Magnesium Chloride Cation HF298=652.7+/-84. kJ REF=JANAF

MgCL+	J 6/68MG 1.CL 1.E -1.	0.G	300.000	5000.000	59.75715	1
	6.35123440E+00	-3.79671900E-03	2.47129450E-06	-5.08236530E-10	3.36726250E-14	2
	7.64808790E+04	-8.29036227E+00	3.60122300E+00	3.47918590E-03	-5.13531430E-06	3
	3.44463370E-09	-8.38482060E-13	7.73146880E+04	6.13385933E+00	7.85040728E+04	4

60175-01-1

Magnesium Chloride Fluoride Hf298=-569.02+/-21. kJ REF=JANAF

MgCLF	J 3/66MG 1.CL 1.F 1.	0.G	200.000	6000.000	78.75610	1
	6.57082252E+00	4.48876208E-04	-1.77994819E-07	3.06318205E-11	-1.91554544E-15	2
	-7.05235977E+04	-5.83555414E+00	3.15704293E+00	1.64534790E-02	-3.01126869E-05	3
	2.57974606E-08	-8.42487547E-12	-6.98910040E+04	1.02255402E+01	-6.84374665E+04	4

7786-30-3

MgCl<sub>2</sub> Solid & Liquid HF298(S)=-641.62+/-0.46 kJ HF298(L)=-601.58 kJ REF=JANAF

MgCL2(s)	J12/65MG 1.CL 2.	0.	0.C	300.000	987.000	95.21040	1
	5.44912960E+00	1.67452240E-02	-2.59569070E-05	1.91115730E-08	-5.10590140E-12		2
	-7.93438940E+04	-2.42610840E+01	5.44912960E+00	1.67452240E-02	-2.59569070E-05		3
	1.91115730E-08	-5.10590140E-12	-7.93438940E+04	-2.42610840E+01	-7.71689336E+04		4
MgCL2(L)	J12/65MG 1.CL 2.	0.	0.C	987.000	5000.000	95.21040	1
	1.10710480E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
	-7.62946180E+04	-4.89725880E+01	1.10710480E+01	0.00000000E+00	0.00000000E+00		3
	0.00000000E+00	0.00000000E+00	-7.62946180E+04	-4.89725880E+01	0.00000000E+00		4

7786-30-3

MgCl<sub>2</sub> Magnesium dichloride HF298=-392.46+/-2.1 kJ REF=JANAF

MgCL2	J12/69MG 1.CL 2.	0.	0.G	300.000	5000.000	95.21040	1
	7.24019130E+00	2.88562390E-04	-1.24011870E-07	2.35271010E-11	-1.64432050E-15		2
	-4.94423260E+04	-8.18090146E+00	5.40955290E+00	7.72062810E-03	-1.16200940E-05		3
	7.94178890E-09	-2.02525020E-12	-4.90705370E+04	6.47158084E-01	-4.72024455E+04		4

Table 4 (continued)

14953-28-7

MgF Magnesium MonoFluoride HF298=-236.81+/-8.4 kJ REF=JANAF

MgF	J 6/76MG 1.F 1. 0. 0.G	300.000	5000.000	43.30340	1
4.19221190E+00	4.03626440E-04-1.50976310E-07	2.81692210E-11-1.82758920E-15			2
-2.98137100E+04	2.43696211E+00 2.65707520E+00	6.68261350E-03-1.03311560E-05			3
7.68717660E-09	-2.22450570E-12-2.94948900E+04	9.85508041E+00-2.84827958E+04			4

21308-25-8

Magnesium Fluoride Cation HF298=512.29+/-46. kJ REF=JANAF

MgF+	J12/75MG 1.F 1.E -1. 0.G	300.000	5000.000	43.30285	1
4.36810570E+00	4.11759660E-03-2.93947970E-06	7.27118430E-10-5.98448020E-14			2
5.95360000E+04	-1.34577794E+00 3.43876540E+00	2.22526540E-03-5.46212020E-06			3
1.40842760E-08	-8.07269060E-12 6.05156660E+04	5.77835456E+00 6.16156042E+04			4

7783-40-6

MgF2 Solid and Liquid Magnesium Fluoride HF298(s)=-1124.2+/-1.3 kJ

HF298(L)=-1072.36 kJ REF=JANAF

MgF2(s)	J 6/75MG 1.F 2. 0. 0.S	300.000	1536.000	62.30181	1
-2.10224270E+00	3.50242280E-02-3.97498930E-05	2.04618590E-08-3.95344100E-12			2
-1.35393080E+05	1.10445550E+01 1.60361100E+00	3.17944860E-02-5.26857980E-05			3
4.15877060E-08	-1.26194950E-11-1.36720340E+05	-9.73231710E+00-1.35218306E+05			4
MgF2(L)	J 6/75MG 1.F 2. 0. 0.L	1536.000	5000.000	62.30181	1
1.14167670E+01	0.00000000E+00 0.00000000E+00	0.00000000E+00 0.00000000E+00			2
-1.34084100E+05	-5.74250690E+01 1.14167670E+01	0.00000000E+00 0.00000000E+00			3
0.00000000E+00	0.00000000E+00-1.34084100E+05	-5.74250690E+01 0.00000000E+00			4

7783-40-6

MgF2 Magnesium Fluoride HF298=-726.76+/-16.7 kJ REF=JANAF

MgF2	J 6/75MG 1.F 2. 0. 0.G	300.000	5000.000	62.30181	1
6.36420730E+00	7.26278270E-04-3.22800460E-07	6.33636660E-11-4.57384370E-15			2
-8.94644290E+04	-5.91513079E+00 3.34790580E+00	1.31152970E-02-2.05416070E-05			3
1.53957840E-08	-4.49090410E-12-8.88388740E+04	8.65190211E+00-8.74109410E+04			4

68193-66-8

MgF2+ HF298=592.+/-20.9 kJ REF=JANAF

MgF2+	J12/75MG 1.F 2.E -1. 0.G	300.000	5000.000	62.30126	1
6.89106730E+00	7.17812830E-04-3.29411720E-07	6.58811280E-11-4.58732280E-15			2
6.89931450E+04	-8.71301395E+00 3.52128840E+00	1.52695560E-02-2.51800890E-05			3
1.96354990E-08	-5.90549190E-12 6.96583880E+04	7.39020945E+00 7.12004950E+04			4

14332-53-7

MgH Magnesium monohydride HF298=169.03 kJ REF=JANAF

MgH	J12/66MG 1.H 1. 0. 0.G	300.000	5000.000	25.31294	1
3.46385910E+00	1.24040550E-03-5.02782100E-07	9.81188340E-11-6.61830680E-15			2
1.91763100E+04	2.99775186E+00 3.51023970E+00	-1.23683520E-03 6.42469980E-06			3
-6.60548460E-09	2.20036250E-12 1.92938930E+04	3.37365416E+00 2.03302445E+04			4

14332-62-8

MgI Magnesium Iodide HF298=24.61+/-41.8 kJ REF=JANAF

MgI	J12/74MG 1.I 1. 0. 0.G	200.000	6000.000	151.20947	1
4.41245599E+00	1.78910914E-04-5.22986679E-08	9.68713486E-12-4.67113786E-16			2
1.62581907E+03	5.16451018E+00 3.39596606E+00	6.11494866E-03-1.31544146E-05			3
1.27259311E-08	-4.53414297E-12 1.76933628E+03	9.69586508E+00 2.96042364E+03			4

Table 4 (continued)

10377-58-9

MgI2 Magnesium Diiodide Condensed HF298(S)=-366.94+/-6.3 kJ HF298(L)=-342.25 kJ  
REF=JANAF

MgI2(s)	J12/74MG	1.I	2.	0.	0.C	300.000	907.000	278.11394	1
6.70171590E+00	1.16970220E-02	-1.68363080E-05	1.31438090E-08	-4.00999570E-12					2
-4.65277610E+04	-2.54320430E+01	6.70171590E+00	1.16970220E-02	-1.68363080E-05					3
1.31438090E-08	-4.00999570E-12	-4.65277610E+04	-2.54320430E+01	-4.41344148E+04					4
MgI2(L)	J12/74MG	1.I	2.	0.	0.C	907.000	5000.000	278.11394	1
1.20775070E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
-4.55256600E+04	-5.18835260E+01	1.20775070E+01	0.00000000E+00	0.00000000E+00					3
0.00000000E+00	0.00000000E+00	-4.55256600E+04	-5.18835260E+01	0.00000000E+00					4

10377-58-9

MgI2 Magnesium Diiodide gas HF298=-160.25+/-10.5 kJ REF=JANAF

MgI2	J12/74MG	1.I	2.	0.	0.G	300.000	5000.000	278.11394	1
7.37111620E+00	1.49419540E-04	-6.70677380E-08	1.32575590E-11	-9.62005020E-16					2
-2.15119230E+04	-3.93845663E+00	6.10814260E+00	6.14621180E-03	-1.11665270E-05					3
9.32665250E-09	-2.94871660E-12	-2.12863230E+04	1.97126687E+00	-1.92736169E+04					4

60195-15-5

Magnesium Nitride HF298=288.70+/-25.1 kJ HF0=289.04 kJ REF=JANAF

MgN	J	3/64MG	1.N	1.	0.	0.G	300.000	5000.000	38.31174	1
4.22144170E+00	3.64892400E-04	-1.29957300E-07	2.44189400E-11	-1.69177590E-15					2	
3.33829310E+04	2.73205196E+00	2.88945490E+00	5.17571750E-03	-6.58490160E-06					3	
3.72189330E-09	-7.23059640E-13	3.36810580E+04	9.29758946E+00	3.47214301E+04					4	

1309-48-4

MgO Solid &amp; Liquid Magnesium Oxide HF298(Solid)=-601.24+/-0.63 kJ

HF0(S)=-597.06 kJ HF298(Liq)=-532.61 kJ REF=JANAF

MgO(s)	J12/74MG	1.O	1.	0.	0.C	300.000	3105.000	40.30440	1
5.04486810E+00	1.68982010E-03	-7.56176950E-07	2.02868930E-10	-2.05912710E-14					2
-7.40292850E+04	-2.63288920E+01	-4.54039530E-01	2.78732690E-02	-4.90622470E-05					3
4.04741510E-08	-1.26703440E-11	-7.30579480E+04	-6.35520200E-01	-7.23138995E+04					4
MgO(L)	J12/74MG	1.O	1.	0.	0.C	3105.000	5000.000	40.30440	1
8.05167150E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
-6.98794510E+04	-4.43438250E+01	8.05167150E+00	0.00000000E+00	0.00000000E+00					3
0.00000000E+00	0.00000000E+00	-6.98794510E+04	-4.43438250E+01	0.00000000E+00					4

1309-48-4

MgO Magnesium Oxide HF298=58.16+/-25.1 kJ REF=JANAF

MgO	J12/74MG	1.O	1.	0.	0.G	300.000	5000.000	40.30440	1
7.94944280E+00	-1.26407550E-03	-2.40097300E-07	1.62732770E-10	-1.76119090E-14					2
3.49443840E+03	-2.18011730E+01	5.33534970E+00	-1.33391340E-02	3.56675260E-05					3
-2.60574710E-08	4.98411960E-12	5.73155730E+03	-2.13277681E+00	6.99538853E+03					4

12141-11-6

MgOH Magnesium hydroxide HF298=-164.76+/-37.7 kJ REF=JANAF

MgOH	J12/75MG	1.O	1.H	1.	0.G	300.000	5000.000	41.31234	1
5.26714240E+00	1.67827200E-03	-5.43091730E-07	8.25633490E-11	-4.71335130E-15					2
-2.15093360E+04	-3.39516556E+00	1.76243570E+00	1.91670050E-02	-3.32193180E-05					3
2.71589780E-08	-8.38892750E-12	-2.09491820E+04	1.27344525E+01	-1.98155784E+04					4

Table 4 (continued)

60172-61-4

MgOH+ Magnesium Hydroxide Cation HF298=584.42+/-62.8 kJ REF=JANAF

MgOH+	J12/75MG	1.O	1.H	1.E	-1.G	300.000	5000.000	41.31179	1
5.28244790E+00	1.66404370E-03	-5.40166510E-07	8.34678240E-11	-5.00361680E-15					2
6.85958160E+04	-4.15038863E+00	1.78314210E+00	1.92285270E-02	-3.35031430E-05					3
2.74913640E-08	-8.51510070E-12	6.91505840E+04	1.19305236E+01	7.02911854E+04					4

1309-42-8

MgO2H2(S) Magnesium hydroxide HO-Mg-OH HF298(S)=-924.66+/-2.1 kJ REF=JANAF

MgO2H2(s)	J12/75MG	1.O	2.H	2.	0.C	300.000	1000.000	58.31968	1
-4.16642480E+00	7.68449870E-02	-1.37207670E-04	1.14268590E-07	-3.59258370E-11					2
-1.12384340E+05	1.35926370E+01	-4.16642480E+00	7.68449870E-02	-1.37207670E-04					3
1.14268590E-07	-3.59258370E-11	-1.12384340E+05	1.35926370E+01	-1.11214407E+05					4

1309-42-8

MgO2H2 Magnesium hydroxide HO-Mg-OH HF298=-572.37+/-33.5 kJ REF=JANAF

MgO2H2	J12/75MG	1.O	2.H	2.	0.G	300.000	5000.000	58.31968	1
8.51783840E+00	3.37913800E-03	-1.10220330E-06	1.71111790E-10	-1.03022860E-14					2
-7.16267310E+04	-1.76294649E+01	1.54947500E+00	3.82704800E-02	-6.65093280E-05					3
5.45362940E-08	-1.68913380E-11	-7.05167540E+04	1.44170361E+01	-6.88415815E+04					4

12032-36-9

MgS Magnesium Sulfide SOLID HF298(S)=-345.72+/-4.2 kJ REF=JANAF

MgS(s)	J 9/77MG	1.S	1.	0.	0.C	300.000	3000.000	56.37100	1
5.35012290E+00	1.34336550E-03	-6.29050000E-07	1.98198580E-10	-2.25916480E-14					2
-4.32385480E+04	-2.48378310E+01	4.09728770E+00	6.92978580E-03	-9.20292860E-06					3
5.63293350E-09	-1.21703300E-12	-4.30407590E+04	-1.89960010E+01	-4.15818955E+04					4

12032-36-9

MgS Magnesium Sulfide HF298=-145.23+/-66.9 kJ REF=JANAF

MgS	J 9/77MG	1.S	1.	0.	0.G	300.000	5000.000	56.37100	1
1.03585650E+01	-5.53070850E-03	2.09511990E-06	-3.52248380E-10	2.22827360E-14					2
1.33293460E+04	-3.31905223E+01	7.80892150E+00	-3.24935950E-02	9.25172570E-05					3
-9.09652030E-08	2.97256310E-11	1.59322900E+04	-1.10479053E+01	1.74679365E+04					4

748-88-9

MgSO4 Magnesium Sulfate Condensed HF298(S)=-1261.79+/-20.9 kJ

HF298(L)=-1246.59 kJ REF=JANAF

MgSO4(s)	L 7/76MG	1.S	1.O	4.	0.S	300.000	1400.000	120.36860	1
-6.44769200E+01	2.63753170E-01	-3.24918840E-04	1.82572340E-07	-3.86907670E-11					2
-1.40661070E+05	3.21883890E+02	2.15340590E+00	4.87565320E-02	-7.36650300E-05					3
5.94277870E-08	-1.84337080E-11	-1.56809620E+05	-1.30284440E+01	-1.54542596E+05					4
MgSO4(L)	L 7/76MG	1.S	1.O	4.	0.L	1400.000	5000.000	120.36860	1
1.91227200E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
-1.60928760E+05	-1.01804650E+02	1.91227200E+01	0.00000000E+00	0.00000000E+00					3
0.00000000E+00	0.00000000E+00	-1.60928760E+05	-1.01804650E+02	0.00000000E+00					4

Table 4 (continued)

13776-74-4

MgSiO<sub>3</sub> Magnesium Silicate Condensed HF298(S)=-1548.92+/-4.2 kJ

HF298(L)=-1494.86+/-20.9 kJ REF=JANAF

MgSiO <sub>3</sub> (I)	J12/67MG	1.SI	1.0	3.	0.S	300.000	903.000	100.38870	1
1.33777790E+00	4.44532220E-02	-6.59737530E-05	4.74142570E-08	-1.23310980E-11					2
-1.88172260E+05	-1.01789360E+01	1.33777790E+00	4.44532220E-02	-6.59737530E-05					3
4.74142570E-08	-1.23310980E-11	-1.88172260E+05	-1.01789360E+01	-1.86292592E+05					4
MgSiO <sub>3</sub> (II)	J12/67MG	1.SI	1.0	3.	0.S	903.000	1258.000	100.38870	1
1.44738860E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
-1.91621720E+05	-7.66594640E+01	1.44738860E+01	0.00000000E+00	0.00000000E+00					3
0.00000000E+00	0.00000000E+00	-1.91621720E+05	-7.66594640E+01	0.00000000E+00					4
MgSiO <sub>3</sub> (III)	J12/67MG	1.SI	1.0	3.	0.S	1258.000	1850.000	100.38870	1
1.47255010E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
-1.91741990E+05	-7.82992980E+01	1.47255010E+01	0.00000000E+00	0.00000000E+00					3
0.00000000E+00	0.00000000E+00	-1.91741990E+05	-7.82992980E+01	0.00000000E+00					4
MgSiO <sub>3</sub> (L)	J12/67MG	1.SI	1.0	3.	0.L	1850.000	5000.000	100.38870	1
1.76130310E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
-1.88025790E+05	-9.51257310E+01	1.76130310E+01	0.00000000E+00	0.00000000E+00					3
0.00000000E+00	0.00000000E+00	-1.88025790E+05	-9.51257310E+01	0.00000000E+00					4

12032-30-3

MgTiO<sub>3</sub> Magnesium Titanate Condensed HF298(S)=-1572.56+/-6.3 kJ

HF298(L)=-1497.63+/-6.3 kJ REF=JANAF

MgTiO <sub>3</sub> (s)	J 6/67MG	1.TI	1.0	3.	0.S	300.000	1953.000	120.18320	1
1.02882240E+01	1.03437300E-02	-7.40121790E-06	2.79288240E-09	-3.95324480E-13					2
-1.92811680E+05	-5.29580880E+01	-1.57777430E-01	6.20183970E-02	-1.04805960E-04					3
8.49409250E-08	-2.63672950E-11	-1.91077380E+05	-4.66165350E+00	-1.89138441E+05					4
MgTiO <sub>3</sub> (L)	J 6/67MG	1.TI	1.0	3.	0.L	1953.000	5000.000	120.18320	1
1.96259490E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
-1.90918120E+05	-1.06562040E+02	1.96259490E+01	0.00000000E+00	0.00000000E+00					3
0.00000000E+00	0.00000000E+00	-1.90918120E+05	-1.06562040E+02	0.00000000E+00					4

12032-35-8

MgTi<sub>2</sub>O<sub>5</sub> Magnesium Ditungsten Pentoxide Condensed HF298(S)=-2509.36+/-10.5 kJ

HF298(L)=-2382.31+/-8.4 kJ REF=JANAF

MgTi <sub>2</sub> O <sub>5</sub> (s)	J 6/67MG	1.TI	2.0	5.	0.S	300.000	1963.000	200.06200	1
1.67766080E+01	1.22377910E-02	-6.30131600E-06	2.40194880E-09	-3.54129300E-13					2
-3.07546550E+05	-8.32933900E+01	1.27163110E+00	9.26637940E-02	-1.63695020E-04					3
1.39033730E-07	-4.45132320E-11	-3.05116130E+05	-1.24221020E+01	-3.01810872E+05					4
MgTi <sub>2</sub> O <sub>5</sub> (L)	J 6/67MG	1.TI	2.0	5.	0.L	1963.000	5000.000	200.06200	1
3.14015190E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
-3.04100010E+05	-1.68586490E+02	3.14015190E+01	0.00000000E+00	0.00000000E+00					3
0.00000000E+00	0.00000000E+00	-3.04100010E+05	-1.68586490E+02	0.00000000E+00					4

29904-79-8

Magnesium dimer HF298=287.63+/-0.8 kJ REF=JANAF

Mg <sub>2</sub>	J 9/83MG	2.	0.	0.	0.G	200.000	6000.000	48.61000	1
1.55499308E+00	3.13771932E-03	-3.15497401E-06	1.11815199E-09	-1.08539001E-13					2
3.41094885E+04	1.94547704E+01	5.66548917E+00	-1.81207983E-02	4.05706233E-05					3
-4.00720091E-08	1.45040463E-11	3.34280753E+04	5.33095711E-01	3.45979248E+04					4

58790-40-3

Mg<sub>2</sub>F<sub>4</sub> Magnesium Fluoride HF298=-1718.37+/-37.7 kJ REF=JANAF

Mg <sub>2</sub> F <sub>4</sub>	J12/75MG	2.F	4.	0.	0.G	300.000	5000.000	124.60361	1
1.46720160E+01	1.52993180E-03	-6.83471170E-07	1.34604690E-10	-9.73833980E-15					2
-2.11437660E+05	-4.42782440E+01	4.22990530E+00	4.92908490E-02	-8.64496720E-05					3
7.04593710E-08	-2.18871100E-11	-2.09492990E+05	5.00323615E+00	-2.06675889E+05					4

Table 4 (continued)

10034-94-3

Mg<sub>2</sub>SiO<sub>4</sub> Condensed HF298(S)=-2176.94+/-4.2 kJ HF298(L)=-2113.88+/-20.9 kJ  
REF=JANAF

Mg <sub>2</sub> SiO <sub>4</sub> (s)	J12/67MG 2.SI 1.O 4.	0.S	300.000	2171.000	140.69310	1
1.57526790E+01	6.80046500E-03	-1.62039510E-06	7.73681120E-12	6.33375730E-14		2
-2.67299550E+05	-8.14579920E+01	1.34289820E+00	6.68665880E-02	-9.64456250E-05		3
6.64239600E-08	-1.71839900E-11	-2.64469010E+05	-1.23991620E+01	-2.61825552E+05		4
Mg <sub>2</sub> SiO <sub>4</sub> (L)	J12/67MG 2.SI 1.O 4.	0.L	2171.000	5000.000	140.69310	1
2.46582440E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
-2.66925490E+05	-1.34615100E+02	2.46582440E+01	0.00000000E+00	0.00000000E+00		3
0.00000000E+00	0.00000000E+00	-2.66925490E+05	-1.34615100E+02	0.00000000E+00		4

12032-52-9

Mg<sub>2</sub>TiO<sub>4</sub> Magnesium Titanium Oxide Condensed HF298(S)=-2164.38+/-6.3 kJ  
HF298(L)=-2046.33 kJ REF=JANAF

Mg <sub>2</sub> TiO <sub>4</sub> (s)	J 6/67MG 2.TI 1.O 4.	0.S	300.000	2013.000	160.48760	1
1.47725770E+01	1.08241470E-02	-4.99075600E-06	1.74079440E-09	-2.53981950E-13		2
-2.65390780E+05	-7.39337100E+01	-5.04411560E-02	8.80864240E-02	-1.56837890E-04		3
1.34018470E-07	-4.31237870E-11	-2.63078650E+05	-6.25375070E+00	-2.60319690E+05		4
Mg <sub>2</sub> TiO <sub>4</sub> (L)	J 6/67MG 2.TI 1.O 4.	0.L	2013.000	5000.000	160.48760	1
2.74763290E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
-2.61535590E+05	-1.47458370E+02	2.74763290E+01	0.00000000E+00	0.00000000E+00		3
0.00000000E+00	0.00000000E+00	-2.61535590E+05	-1.47458370E+02	0.00000000E+00		4

1344-43-0

MnO Manganese Oxide Data from Barin Database 1989 HF298(S)=-385.221 kJ

MnO (S)	B /89MN 1.O 1.	0.	0.S	298.150	2115.000	C 70.93745	1
1.35627103E+01	-2.23122322E-02	2.45011706E-05	-1.09793320E-08	1.74986515E-12			2
-5.02522690E+04	-6.60188273E+01	2.56643455E+00	1.55785511E-02	-2.79738618E-05			3
2.42198962E-08	-7.86883817E-12	-4.75857738E+04	-1.10409128E+01	-4.63311729E+04			4
MnO (L)	B /89MN 1.O 1.	0.	0.L	2115.000	2500.000	C 70.93745	1
-2.63748329E+01	5.81346781E-02	-3.75984688E-05	1.07961809E-08	-1.16134596E-12			2
-2.88800210E+04	1.56912584E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00			3
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	-4.63311729E+04			4

1313-13-9

MnO<sub>2</sub> Manganese Dioxide Data from Barin Database 1989 HF298(S)=-520.029 kJ

MnO <sub>2</sub> (S)	B /89MN 1.O 2.	0.	0.S	298.150	800.000	C 86.93685	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			2
0.00000000E+00	0.00000000E+00	-4.79951256E+00	7.20358836E-02	-1.55128177E-04			3
1.55651945E-07	-5.93342269E-11	-6.32245896E+04	1.78855218E+01	-6.25447561E+04			4

18820-29-6

MnS Manganese Monosulfide (Green) Data from Barin HF298(S)=-214.414 kJ

MnS Solid	B /89MN 1.S 1.	0.	0.S	298.150	1803.000	C 87.00405	1
5.73936431E+00	9.01938576E-04	3.02740651E-11	1.69143122E-12	-5.47133193E-16			2
-2.75139333E+04	-2.35653794E+01	5.73590949E+00	9.12003512E-04	-1.77463767E-08			3
2.06928531E-11	-8.38201915E-15	-2.75127688E+04	-2.35470661E+01	-2.57621916E+04			4
MnS Liquid	B /89MN 1.S 1.	0.	0.L	1803.000	2200.000	C 87.00405	1
7.36336543E+00	1.36969500E-03	-1.02073380E-06	3.37546304E-10	-4.17948179E-14			2
-2.67980686E+04	-3.37306895E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00			3
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	-2.57621916E+04			4



Table 4 (continued)

12125-23-4

MnS2 Manganese Disulfide Data from Barin Database HF298(S)=-223.844 kJ

MnS2 (S)	B	/89MN 1.S	2.	0.	0.S	298.150	700.000	C	119.07005	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
0.00000000E+00	0.00000000E+00	4.48568512E+00	2.44442175E-02	-5.26856546E-05						3
5.76754423E-08	-2.41568621E-11	-2.89830667E+04	-1.89489535E+01	-2.69220916E+04						4

1317-34-6

Mn2O3 Dimanganese Trioxide Data from Barin Database 1989. HF298(S)=-959.0 kJ

Mn2O3 (S)	B	/89MN 2.O	3.	0.	0.S	298.150	1400.000	C	157.87430	1
4.13175143E+00	2.94925699E-02	-2.97408107E-05	1.57530821E-08	-3.14027515E-12						2
-1.17345192E+05	-1.71563396E+01	3.73625576E+00	4.53603719E-02	-7.84795848E-05						3
6.79682080E-08	-2.20889333E-11	-1.17901390E+05	-1.85906447E+01	-1.15340772E+05						4

1317-35-7

Mn3O4 Trimanganese Tetraoxide Data from Barin 1989. HF298(S)=-1434.191 kJ

Mn3O4 Solid-A	B	/89MN 3.O	4.	0.	0.S	298.150	1445.000	C	228.81175	1
9.24690980E+00	3.03097632E-02	-2.77876351E-05	1.42175100E-08	-2.74343370E-12						2
-1.70540047E+05	-4.13240828E+01	5.30992963E+00	6.45031044E-02	-1.12103682E-04						3
9.70819405E-08	-3.15481785E-11	-1.70549547E+05	-2.65839957E+01	-1.66912903E+05						4
Mn3O4 Solid-B	B	/89MN 3.O	4.	0.	0.S	1445.000	1835.000	C	228.81175	1
2.18396178E+01	8.24501377E-03	-7.43602439E-06	2.97586871E-09	-4.45964303E-13						2
-1.74631781E+05	-1.12000838E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00						3
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	-1.66912903E+05						4

12033-08-8

Mn5N2 Pentamanganese Dinitride Data from Barin 1989 HF298(S)=-204.2 kJ

Mn5N2 (S)	B	/89MN 5.N	2.	0.	0.S	298.150	800.000	C	302.70373	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
0.00000000E+00	0.00000000E+00	1.53753139E+01	1.93066443E-02	5.09039170E-08						3
-6.55123649E-11	3.04082415E-14	-3.00020762E+04	-7.08162751E+01	-2.45594749E+04						4

7439-98-7

Mo Molibden REFERENCE ELEMENT HF298(S)=0.0 REF=JANAF

Mo(cr) REF ELEMENTJ	3/78MO	1.	0.	0.	0.S	200.000	2896.000	B	95.94000	1
5.38432823E+00	-6.01622180E-03	6.01482526E-06	-2.32962338E-09	3.52007808E-13						2
-1.62657220E+03	-2.62488891E+01	1.32884141E+00	9.82553689E-03	-2.10929825E-05						3
2.09509528E-08	-7.60703244E-12	-6.84364789E+02	-6.29286538E+00	0.00000000E+00						4
Mo(L)	J	3/78MO	1.	0.	0.L	2896.000	6000.000	B	95.94000	1
4.52894999E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
2.02140667E+03	-2.28074752E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		3
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		4

12011-97-1

MoC Molibdenum Monocarbide Gamma Data from Barin 1989 HF298(S)=-28.451 kJ

MoC Solid-C	B	/89C 1.MO	1.	0.	0.S	298.150	1400.000	C	107.95100	1
1.95688580E+00	7.45582204E-03	-4.92462131E-06	1.16731721E-09	5.69099576E-14						2
-4.30569462E+03	-8.78043176E+00	1.75407212E+00	8.17609975E-03	-5.89254003E-06						3
1.74969447E-09	-7.50126171E-14	-4.25959002E+03	-7.77690797E+00	-3.42184927E+03						4

18868-43-4

MoO2 Molibdenum Dioxide Solid Data from Barin 1989 HF298(S)=-588.94 kJ

MoO2 Solid	B	/89MO 1.O	2.	0.	0.S	298.150	2000.000	C	127.93880	1
5.57003335E+00	7.01737124E-03	-4.11649672E-06	1.48282458E-09	-1.41613677E-13						2
-7.28178014E+04	-2.82261435E+01	6.56226971E-01	3.36489565E-02	-5.76641545E-05						3
4.88255458E-08	-1.56544560E-11	-7.21036803E+04	-6.04322444E+00	-7.08327971E+04						4

Table 4 (continued)

18868-43-4

MoO2 Molybdenum Dioxide Gas Data from Barin Database 1989 HF298=-8.314 kJ

MoO2	B	/89MO	1.O	2.	0.	0.G	298.150	3000.000	C	127.93880	1	
							4.14494627E+00	7.05834738E-04	-5.16986528E-07	1.86466769E-10	-2.22683845E-14	2
							-2.29247521E+03	6.46991922E+00	2.90286012E+00	6.65546290E-03	-1.14989921E-05	3
							9.33240931E-09	-2.89374741E-12	-2.07672445E+03	1.22605433E+01	-9.99938661E+02	4

12069-89-5

Mo2C DiMolybdenum Carbide Data from Barin Database 1989 HF298(S)=-53.137 kJ

Mo2C(S)	B	/89MO	2.C	1.	0.	0.S	298.150	1400.000	C	203.89100	1	
							2.63292301E+00	1.91409016E-02	-1.95825211E-05	8.67987123E-09	-1.10539752E-12	2
							-7.76509118E+03	-1.17561621E+01	2.42024100E+00	2.50702462E-02	-3.73749151E-05	3
							2.75982039E-08	-7.94799883E-12	-7.94734639E+03	-1.19156150E+01	-6.39087571E+03	4

17778-88-0

N REF=C.E. Moore "Selected Tables of Atomic Spectra" NSRDS-NBS Sec 5 1975

p. A7 I. HF298=472.68 kJ REF=CODATA Key Values 1989 p.22. {HF298=472.459+/-0.04 kJ REF=ATcT A}

N	L	6/88N	1	0	0	OG	200.000	6000.000	A	14.00674	1	
							0.24159429E+01	0.17489065E-03	-0.11902369E-06	0.30226244E-10	-0.20360983E-14	2
							0.56133775E+05	0.46496095E+01	0.25000000E+01	0.00000000E+00	0.00000000E+00	3
							0.00000000E+00	0.00000000E+00	0.56104638E+05	0.41939088E+01	0.56850013E+05	4

15123-00-9

ND T0=0 STATWT=3 Be=8.993 WE=2422 WEXE=50.6 ALFAE=0.252 REF=JANAF

Calculated from the JANAF table. HF0 calculated from NASA TM-83800, 1985 p2.

HF0(ND) = HF0(NH) + HF0(D) - HF0(H) + E0(ND) - E0(NH) HF0(NH) = 357. +/- 1. kJ

E0 = .5\*(we - .5wexe + .25weye) \*1.438769\*8.31451 J/mol

E0(NH) = (3282.09 - 78.3/2)/2 = 1621.47 cm-1 = 19.3971 kJ/mol

E0(ND) = (2422. - 50.6/2)/2 = 1198.35 cm-1 = 14.3355 kJ/mol

HF0(D) = 219.807 kJ/mol HF0(H) = 216.035 kJ/mol REF= NASA Glenn.

HF0(ND) = 357. + 219.807 - 216.035 - 19.3971 + 14.3355 = 355.7104 kJ/mol

HF298=355.739 kJ Max Lst Sq Error Cp @ 6000 K 0.26%.

ND	g	4/01N	1.D	1.	0.	0.G	200.000	6000.000	B	16.02084	1	
							2.92141593E+00	1.46824830E-03	-5.06132450E-07	8.16389936E-11	-4.88173770E-15	2
							4.18711786E+04	5.51040842E+00	3.53318513E+00	-1.16333934E-04	-5.33442392E-07	3
							2.54879097E-09	-1.47191074E-12	4.17374216E+04	2.42706696E+00	4.27852991E+04	4

15117-75-6

NDH Deuterated Amidogen SIGMA=1 STATWT=2 A0=19.35545 B0=8.037364

C0=5.67911 Nu=3365,2450,1405 T0=11122.6 STATWT=2 SIGMA=1 REF=Burcat G3B3 calc

HF0(NDH) = HF0(NH2) + 2[hf0(D)-HF0(H)] + E000(ND2) - E000(NH2)

HF0(NH2) = 189.1 +/- 1. kJ/mol E0 = .5\*Sum(freqs in ground state)

E0(NH2) = (3219.37+1497.32+3301.11)/2 = 4008.9 cm-1 = 47.9571 kJ/mol

E0(NDH) = (3365.+2450.+1405)/2 = 3610. cm-1 = 43.1852 kJ/mol

HF0(D) = 219.807 kJ/mol HF0(H) = 216.035 kJ/mol REF= NASA Glenn.

HF0(NDH) = 189.1 + (219.807-216.035) + 43.1852 - 47.9571 = 188.1001 kJ/mol

HF298=185.159 kJ Max Lst Sq Error Cp @ 6000 K 0.43%

NHD	A	1/05N	1.H	1.D	1.	0.G	200.000	6000.000	B	17.02878	1	
							2.99345271E+00	3.20175498E-03	-1.05832428E-06	1.69569103E-10	-1.03556752E-14	2
							2.12466567E+04	6.78901866E+00	4.24787376E+00	-2.74853399E-03	9.03939336E-06	3
							-7.36770381E-09	2.12506752E-12	2.10587078E+04	1.00378371E+00	2.22693532E+04	4

Table 4 (continued)

15117-84-7

ND2 Amidogen D2 SIGMA=2 STATWT=1 A0=13.342 B0=6.488 C0=4.290  
 NU=2440,2502,1490,1150,1108.75 T0=11122.6 STATWT=2 SIGMA=2 Nu=2520,430,2584  
 IAIBIC=0.0194

Hf0(ND2) = Hf0(NH2) + 2 [Hf0(D)-Hf0(H)] + E000(ND2) - E000(NH2)  
 Hf0(NH2) = 189.1 +/- 1. kJ/mol E0 = .5\*Sum(freqs in ground state)  
 E0(NH2) = (3219.37+1497.32+3301.11)/2 = 4008.9 cm-1 = 47.9571 kJ/mol  
 E0(ND2) = (2440.+1108.75+2502)/2 = 3025.375 cm-1 = 36.1915 kJ/mol  
 Hf0(D) = 219.807 kJ/mol Hf0(H) = 216.035 kJ/mol REF= NASA Glenn.  
 Hf0(ND2) = 189.1 + 2(219.807-216.035) + 36.1915 - 47.9571 = 184.8784 kJ/mol  
 HF298=181.94+/-4 kJ REF=Jacox NIST + McBride NASA Max Lst Sq Error Cp @  
 1300 K 0.58%.

ND2	g	4/01N	1.D	2.	0.	0.G	200.000	6000.000	B	18.03494	1
3.39344029E+00	3.09430279E-03	-1.07944873E-06	1.82615632E-10	-1.16377076E-14							2
2.06724522E+04	4.23145961E+00	4.08174416E+00	-1.72293187E-03	8.47237526E-06							3
-7.55764433E-09	2.30572906E-12	2.06804160E+04	1.51889257E+00	2.18818150E+04							4

13780-28-4

ND2H SIGMA=1 STATWT=1 IA=0.3843 IB=0.5288 IC=0.7394 Nu=945,1314,1544,  
 2509,2634,3527 REF=BURCAT G3B3 calc HF298=-52.748 kJ HF0=-45.684 kJ Max  
 Lst Sq Error Cp @ 6000 K 0.50%

ND2H	A12/04N	1.D	2.H	1.	0.G	200.000	6000.000	B	19.04288	1
2.86769974E+00	6.12085160E-03	-2.14513316E-06	3.40381895E-10	-2.01260754E-14						2
-7.55372452E+03	6.89502363E+00	4.27750279E+00	-4.94603206E-03	2.36611000E-05						3
-2.44173647E-08	8.58846789E-12	-7.56444563E+03	1.42064991E+00	-6.34409833E+03						4

84796-14-5

ND3 DEUTERATED AMONIA SIGMA=3 STATWT=1 IAIBIC=0.25775E-117 NU=2652(2),2495,  
 1225(2),793 REF=Gurvich 89 HF298=-54.583+/-0.4 kJ HF0=-47.546 kJ REF=NH3  
 Max Lst Sq Error Cp @ 6000 K 0.57%.

ND3	g	4/01N	1.D	3.	0.	0.G	200.000	6000.000	B	20.04905	1
3.74049272E+00	5.66468659E-03	-1.95157691E-06	2.98615230E-10	-1.71464955E-14							2
-8.10768376E+03	1.17487971E+00	3.79962127E+00	-1.34158180E-03	1.95137187E-05							3
-2.28145952E-08	8.57790808E-12	-7.75948499E+03	2.59569454E+00	-6.55489091E+03							4

13967-06-1

NF CALCULATED FROM ORIGINAL DATA REF=Gurvich 1989 HF0=233.+/-3 KJ Max Lst Sq  
 Error Cp @ 6000 K 0.41%.

NF	RUS 89N	1.F	1.	0.	0.G	200.000	6000.000	B	33.00514	1
4.06042292E+00	3.50654850E-04	-6.95721815E-08	1.45925454E-11	-1.56372401E-15						2
2.66711982E+04	2.08774805E+00	3.59927999E+00	-2.18190788E-03	1.14106853E-05						3
-1.40068494E-08	5.53332638E-12	2.69702525E+04	5.35573603E+00	2.80221438E+04						4

3744-07-8

NF2 RADICAL SIGMA=2 STATWT=2 A0=2.35149 B0=.396015 C0=.338116 NU=1074,573,  
 931 TAAA=-.000259 TBBB=-2.7E-6 TAAB=9.9E-6 TABA=-4.2E-6 TCCC=-1.3E-6  
 TAAC=1.9E-6 TBBC=-1.8E-6 HF0=37+/-5. KJ REF=Gurvich 1989 Max Lst Sq Error  
 Cp @ 400 K 0.33%

NF2	L	5/95N	1F	2	0	OG	200.000	6000.000	B	52.00355	1
0.58364792E+01	0.12115300E-02	-0.46827522E-06	0.79997253E-10	-0.49773112E-14							2
0.21075383E+04	-0.41367038E+01	0.30383609E+01	0.66254958E-02	0.16160965E-05							3
-0.98870122E-08	0.52618129E-11	0.29422774E+04	0.10741500E+02	0.41398711E+04							4

Table 4 (continued)

7783-54-2

NF3 SIGMA=3 STATWT=1 A0=0.1948 B0=C0=0.35628 NU=1032,647,908(2),493(2)  
 X11=-2.8 X12=-3.5 X13=-9.9 X14=-2.3 X22=-2.5 X23=-6.5 X24=-2.4 X33=-3.5  
 X34=-1.5 X44=-0.6 ALFAA1=9.8E-4 ALFAA2=.000573 ALFAA3=9.22E-4 ALFAA4=6.51E-4  
 ALFAB1=-.001438 ALFAB2=.001288 ALFAB3=.0002629 ALFAB4=.0001493  
 ALFAC1=-.001438 ALFAC2=.001288 ALFAC3=.0002629 ALFAC4=.0001493  
 DJ=4.85E-7 DK=3.27E-7 DJK=-7.475E-7 REF=Gurvich 89 HF298=-131.7+/-1. KJ  
 Max Lst Sq Error Cp @ 400 K 0.3%  
 NF3 L 5/95N 1F 3 0 OG 200.000 6000.000 A 71.00195 1  
 0.80969263E+01 0.22248772E-02-0.73845724E-06 0.13242062E-09-0.82140433E-14 2  
 -0.18767390E+05-0.16378386E+02 0.13184910E+01 0.23460985E-01-0.23520025E-04 3  
 0.82591366E-08 0.18896563E-12-0.17084267E+05 0.17841863E+02-0.15839779E+05 4

13774-92-0

NH REF=TSIV 78 (Error found in H-H0 of Gurvich 1989). HF298=358.78+/-0.37 kJ  
 REF=ATcT A {HF298=357+/-1. kJ REF=Anderson J.Phys. Chem. 93 (1989), 530}  
 Max Lst Sq Error Cp @ 6000 K 0.28%  
 NH ATcT/AN 1.H 1. 0. 0.G 200.000 6000.000 A 15.01468 1  
 2.78372644E+00 1.32985888E-03-4.24785573E-07 7.83494442E-11-5.50451310E-15 2  
 4.23461945E+04 5.74084863E+00 3.49295037E+00 3.11795720E-04-1.48906628E-06 3  
 2.48167402E-09-1.03570916E-12 4.21059722E+04 1.84834973E+00 4.31525130E+04 4

19067-62-0

NH+ GENERETED FROM ORIGINAL VALUES HF0=1656.3 KJ REF= Gurvich 1989 Max Lst  
 Sq Error Cp @ 6000 K 0.22%  
 NH+ L 2/89N 1.H 1.E -1. 0.G 298.150 6000.000 B 15.01413 1  
 2.95918980E+00 1.34991719E-03-4.61487782E-07 8.26977666E-11-5.55758913E-15 2  
 1.99524505E+05 5.59978021E+00 4.61611136E+00-3.13435677E-03 2.91705130E-06 3  
 2.57384848E-10-7.31431347E-13 1.99085043E+05-2.92758460E+00 2.00347960E+05 4

13824-71-0

NHF RADICAL STATWT=2 SIGMA=1 IAIBIC=1.221 NU=3200,1000,1432 T0=20141.26  
 STATWT=2 SIGMA=1 HF298=112.+/-15 kJ REF=Gurvich 1989 Max Lst Sq Error Cp @  
 6000 K 0.29%  
 NHF RUS 89N 1H 1F 1 OG 200.000 6000.000 B 34.01308 1  
 0.38957856E+01 0.26972954E-02-0.96413416E-06 0.15656481E-09-0.93275479E-14 2  
 0.12097631E+05 0.45781245E+01 0.41481642E+01-0.33379936E-02 0.17632209E-04 3  
 -0.20570502E-07 0.79043064E-11 0.12263155E+05 0.45024858E+01 0.13470427E+05 4

10405-27-3

NHF2 SIGMA=1 IAIBIC=109.9 NU=3193,1424,1307,970,888,500 REF=Gurvich 1989  
 HF298=-103 KJ Max Lst Sq Error Cp @ 6000 K 0.38%  
 NHF2 RUS 89N 1H 1F 2 OG 200.000 6000.000 B 53.01149 1  
 0.56498758E+01 0.39393919E-02-0.14331458E-05 0.23343765E-09-0.14065134E-13 2  
 -0.14562287E+05-0.36451783E+01 0.33212629E+01 0.35048001E-02 0.16269284E-04 3  
 -0.25711192E-07 0.10991340E-10-0.13632111E+05 0.99205457E+01-0.12387982E+05 4

13770-40-6

NH2 AMIDOGEN RADICAL SIGMA=2 STATWT=2 A=23.693 B=12.952 C=8.173 NU=3219,  
 1497,3301 T0=11123. SIGMA=2 STATWT=2 REF=The polynomials were calculated from  
 the original tables of Martin et al JCP 97 (1992),3530 HF298=186.2+/-1.0 KJ  
 HF0=189.1+/-1 kJ REF= Ruscic et al JPCRD 2003 IUPAC {HF298=186.422+/-0.20 kJ  
 REF=ATcT A} Max Lst Sq Error Cp @ 1600 K 0.18%  
 NH2 AMIDOGEN RAD IU3/03N 1.H 2. 0. 0.G 200.000 3000.000 A 16.02258 1  
 2.59263049E+00 3.47683597E-03-1.08271624E-06 1.49342558E-10-5.75241187E-15 2  
 2.15738340E+04 7.90565351E+00 4.19198016E+00-2.04602827E-03 6.67756134E-06 3  
 -5.24907235E-09 1.55589948E-12 2.11864310E+04-9.04785244E-02 2.23946872E+04 4

Table 4 (continued)

13587-49-0

NH2D SIGMA=1 STATWT=1 IA=0.2952 IB=0.4424 IC=0.5895 NU=1043,1473,1692,2565,3484,3568 REF=BURCAT G3B3 calc HF298=-48.697 kJ HF0=41.752 kJ REF=NH3  
Max Lst Sq Error Cp @ 6000 K 0.43%.

NH2D	A12/04N	1.H	2.D	1.	0.G	200.000	6000.000	B	18.03672	1
	2.46696436E+00	6.15154392E-03	-2.08150811E-06	3.22155216E-10	-1.87071378E-14					2
	-6.87576021E+03	8.88442382E+00	4.42403751E+00	-5.80703730E-03	2.35306405E-05					3
	-2.33891265E-08	8.08193402E-12	-7.08323343E+03	3.96548654E-01	-5.85682560E+03					4

15861-05-9

NH2F SIGMA=1 IAIBIC=3.06 NU=3260,3210,1620,1500,1280,910 HF298=-75. KJ  
REF=Gurvich 1989 Max Lst Sq Error Cp @ 6000 K 0.47%.

NH2F	RUS 89N	1H	2F	1	0G	200.000	6000.000	B	35.02102	1
	0.34379333E+01	0.56345867E-02	-0.19763269E-05	0.31384602E-09	-0.18569992E-13					2
	-0.10454484E+05	0.60423912E+01	0.44307579E+01	-0.70044845E-02	0.32429410E-04					3
	-0.35524163E-07	0.13059948E-10	-0.10252553E+05	0.32967779E+01	-0.90203752E+04					4

7664-41-7

NH3 AMONIA RRHO SIGMA=3 STATWT=1 A=9.7713479 B=9.7703061 C=6.3292427  
Nu=3568(2),3436,1727(2),1132 HF298=-45.567 KJ HF0=-38.574 REF=Burcat G3B3  
{HF298=-45.567+/-0.030 kJ REF=ATcT A; HF298=-45.94+/-0.35 kJ REF=Gurvich 89}  
Max Lst Sq Error Cp @ 6000 K 0.34%.

NH3	RRHO	G3B3	T12/04H	3.N	1.	0.	0.G	200.000	6000.000	B	17.03056	1
	2.09566674E+00	6.14750045E-03	-2.00328925E-06	3.01334626E-10	-1.71227204E-14						2	
	-6.30945436E+03	9.59574081E+00	4.46075151E+00	-5.68781763E-03	2.11411484E-05						3	
	-2.02849980E-08	6.89500555E-12	-6.70753514E+03	-1.34450793E+00	-5.48041917E+03						4	

7664-41-7

NH3 AMONIA Anharmonic SIGMA=3 STATWT=1 HF298=-45.567 KJ HF0=-38.574  
REF=Burcat G3B3 Calculations performed from Gurvich's & Lester Haar J. Res.  
Nat. Bur. Stand. 72A,(1968),207 original tables. Gurvich's data include  
anharmonic calculations. {HF298=-45.567+/-0.030 kJ REF=ATcT A;  
HF298=-45.94+/-0.35 kJ REF=Gurvich 89} Max Lst Sq Error Cp @ 6000 K 0.30%.

NH3	Anharmonic	RUS 89N	1.H	3.	0.	0.G	200.000	6000.000	A	17.03056	1
	2.71709692E+00	5.56856338E-03	-1.76886396E-06	2.67417260E-10	-1.52731419E-14					2	
	-6.58451989E+03	6.09289837E+00	4.30177808E+00	-4.77127330E-03	2.19341619E-05					3	
	-2.29856489E-08	8.28992268E-12	-6.74806394E+03	-6.90644393E-01	-5.52528050E+03					4	

7803-49-8

NH2OH HYDROXYLAMINE STATWT=1 SIGMA=1 A0=6.370312 B0=.841238 C0=.839105  
NU=3620,3297,1605,1357,1115,895,3350,765,386 T0=3800. STATWT=1 REF=Gurvich 89  
HF298=-43.95+/-0.55 kJ REF=ATcT A {HF298=-50+/-10 kJ REF=Gurvich} Max Lst  
Sq Error Cp @ 0.39%

NH2OH	RUS 78N	1H	3O	1	0G	200.000	6000.000	B	33.02996	1
	0.38808544E+01	0.81574618E-02	-0.28263348E-05	0.43796511E-09	-0.25274751E-13					2
	-0.75876998E+04	0.37931250E+01	0.32101336E+01	0.61970334E-02	0.11058271E-04					3
	-0.19665010E-07	0.88242437E-11	-0.73091267E+04	0.79330377E+01	-0.60135835E+04					4

14798-03-9

NH4+ AMONIUM ION SIGMA=12 STATWT=1 IAIBIC=.106E-117 NU=3250,1700(2),  
3350(3),1430(3) HF298=644.9 KJ REF=TSIV

NH4+	RUS 78N	1H	4E	-1	0G	298.150	6000.000	C	18.03795	1
	0.13156479E+01	0.96493541E-02	-0.32905419E-05	0.51205492E-09	-0.29850594E-13					2
	0.76727757E+05	0.12093408E+02	0.50221425E+01	-0.11710230E-01	0.39760767E-04					3
	-0.36942723E-07	0.12026708E-10	0.76303001E+05	-0.42054342E+01	0.77563825E+05					4

Table 4 (continued)

7790-98-9

NH<sub>4</sub>ClO<sub>4</sub> (I) and (II) Amonium Perchlorate crystal REF=JANAF HF298=-70.69 kcal

NH <sub>4</sub> ClO <sub>4</sub> (I)	J12/62N	1.H	4.CL	1.O	4.S	200.000	513.150	C	117.48880	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2
0.00000000E+00	0.00000000E+00	6.35703886E+00	4.13638533E-02	-5.92805489E-05						3
8.96504531E-08	-4.96854073E-11	-3.89362027E+04	-2.44599186E+01	-3.55723861E+04						4
NH <sub>4</sub> ClO <sub>4</sub> (II)	J12/62N	1.H	4.CL	1.O	4.S	513.150	1500.000	C	117.48880	1
1.55208289E+02	-1.85584191E-01	7.02879745E-05	0.00000000E+00	0.00000000E+00						2
-1.10827457E+05	-8.51152444E+02	2.57678288E+03	-1.79847751E+01	4.36807324E-02						3
-4.44267613E-05	1.61939332E-08	-3.01717712E+05	-1.08243913E+04	-3.55723861E+04						4

10102-43-9

NO GENERATED FROM ORIGINAL VALUES HFO=82.09 KJ REF=Gurvich 1989

{HF298=91.097+/-0.085 kJ REF=ATcT A}. Max Lst Sq Error Cp @ 1300 K 0.30%

NO	RUS 89N	1.O	1.	0.	0.G	200.000	6000.000	A	30.00614	1
3.26071234E+00	1.19101135E-03	-4.29122646E-07	6.94481463E-11	-4.03295681E-15						2
9.92143132E+03	6.36900518E+00	4.21859896E+00	-4.63988124E-03	1.10443049E-05						3
-9.34055507E-09	2.80554874E-12	9.84509964E+03	2.28061001E+00	1.09770882E+04						4

14452-93-8

NO+ GENERATED FROM ORIGINAL VALUES HFO=982.137 KJ REF=Gurvich 1989

NO+	RUS 89N	1.O	1.E	-1.	0.G	298.150	6000.000	A	30.00559	1
2.94587702E+00	1.40325260E-03	-4.95503196E-07	7.95948973E-11	-4.72076668E-15						2
1.18244340E+05	6.70644634E+00	3.69301231E+00	-1.34229158E-03	2.67343395E-06						3
-1.02609308E-09	-6.95610492E-14	1.18103055E+05	3.09126691E+00	1.19166025E+05						4

2696-92-6

NOCl SIGMA=1 STATWT=1 A0=2.9145 B0=.19139 C0=.17933 NU=1800,596,332

X11=-17.8 X12=0. X13=-.6 X22=-2.6 X23=-4.3 X33=-1. ALFAA1=.04016

ALFAA2=-.03888 ALFAA3=-.01061 ALFAB1=-.00033 ALFAB2=.00053 ALFAB3=-.0016

ALFAC1=-.00013 ALFAC2=.00069 ALFAC3=.00153 TAAA=-.00057778 TBBB=-9.75E-7

TAAB=8.5222E-6 TABA=-3.6732E-6 TCCC=-.7.032E-7 TAAC=5.2943E-6

TBBC=-8.2374E-7 T0=10000. STATWT=3 SIGMA=1 T0=16000. STATWT=1 SIGMA=1

REF=Gurvich 1989 HF298=52.524+/-0.09 kJ REF=ATcT A {HFO=54.6+/-0.5 kJ

REF=Gurvich 89} Max Lst Sq Error Cp @ 1300 0.66%.

NOCL	L 5/95N	1O	1CL	1	OG	200.000	6000.000	A	65.45884	1
0.61799190E+01	0.28500775E-03	0.17276529E-06	-0.30166754E-10	0.90192767E-15						2
0.56327606E+04	-0.43234813E+01	0.32325533E+01	0.11886435E-01	-0.21070873E-04						3
0.19552938E-07	-0.69926270E-11	0.63635546E+04	0.10277271E+02	0.77048343E+04						4

7789-25-5

NOF SIGMA=1 A0=3.175188 B0=.395080 C0=.350519 NU=1844,756,520 X11=-17.5

X12=1.5 X13=2. X22=-4.7 X23=-2. X33=-1.5 ALFAA1=.0345 ALFAA2=-.01912

ALFAA3=-.01354 ALFAB1=-.00014 ALFAB2=.00166 ALFAB3=.00484 ALFAC1=.00024

ALFAC2=.00184 ALFAC3=.0047 TAAA=-.00052 TBBB=-3.32E-6 TAAB=.000014

TABA=-9.66E-6 TCCC=-1.89E-6 TAAC=4.68E-6 TBBC=-2.46E-6 T0=15000. SIGMA=1

STATWT=3 HF298=-65.+/-2.0 kJ REF=Gurvich 1989 Max Lst Sq Error Cp @ 6000 K 0.40%.

NOF	L 5/95N	1O	1F	1	OG	200.000	6000.000	A	49.00454	1
0.52530781E+01	0.19000792E-02	-0.75667187E-06	0.15514137E-09	-0.10897571E-13						2
-0.96262527E+04	-0.98536249E+00	0.28886971E+01	0.10359580E-01	-0.13880734E-04						3
0.10416535E-07	-0.32433490E-11	-0.90357928E+04	0.10837381E+02	-0.78176585E+04						4

Table 4 (continued)

13847-65-9

NOF3 SIGMA=3 STATWT=1 IAIBIC=3250. NU=1689,740,542,884(2),528(2),398(2)  
 HF298=-187.+/-7 kJ REF=Gurvich 1989 Max Lst Sq Error Cp @ 1200 K 0.34%  
 NOF3 RUS 89N 1O 1F 3 OG 200.000 6000.000 B 87.00135 1  
 0.10122162E+02 0.29210198E-02-0.11381315E-05 0.19369199E-09-0.12021234E-13 2  
 -0.26123657E+05-0.26256953E+02-0.15692449E+00 0.44229130E-01-0.68789152E-04 3  
 0.52715545E-07-0.15911878E-10-0.23898778E+05 0.23733541E+02-0.22490802E+05 4

1012-44-0

NO2 STATWT=2 SIGMA=2 A0=8.002509 B0=.4336646 C0=.4104926 NU=1320,750,1616  
 X11=-8.1 X12=-9.7 X13=-29.8 X22=-.5 X23=-2.7 X33=-15.6 ALFAA1=-.0753  
 ALFAA2=-.364 ALFAA3=.2208 TAAA=-.11367E-1 TBBB=-.14180E-5 TCCC=-.89140E-6  
 TAAB=.6906E-4 TAAC=.31970E-4 TBBC=-.10890E-5 TABA=-.8215E-5 ALFAB1=.002354  
 ALFAB3=.002718 ALFAC1=.00282 ALFAC2=-.00095 ALFAC3=.00264 TO=11956.  
 STATWT=2. T0=14744. STATWT=2 T0=26000. STATWT=4 T0=27000. STATWT=4  
 T0=31000. STATWT=2 T0=40125 STATWT=2 HF0=37.0+/-0.5 kJ REF= Gurvich 1989.  
 {HF298=34.025+/-0.085 REF=ATcT A} Max Lst Sq Error Cp @ 1300 K 0.48%.  
 NO2 L 7/88N 1° 2 0 OG 200.000 6000.000 A 46.00554 1  
 0.48847540E+01 0.21723955E-02-0.82806909E-06 0.15747510E-09-0.10510895E-13 2  
 0.23164982E+04-0.11741695E+00 0.39440312E+01-0.15854290E-02 0.16657812E-04 3  
 -0.20475426E-07 0.78350564E-11 0.28966180E+04 0.63119919E+01 0.41124701E+04 4

14797-65-0

NO2- STATWT=1 SIGMA=2 IA=.649 IB=5.907 IC=6.556 NU=1330,810,1245  
 HF298=-200.035 KJ REF= Gurvich 1989. Max Lst Sq Error Cp @ 1300 K 0.34%  
 NO2- RUS 89N 1O 2E 1 OG 298.150 6000.000 B 46.00609 1  
 0.50533023E+01 0.20755476E-02-0.87000155E-06 0.16107454E-09-0.10344873E-13 2  
 -0.25904369E+05-0.15407134E+01 0.30978573E+01 0.37047376E-02 0.59296511E-05 3  
 -0.10949983E-07 0.46273153E-11-0.25179837E+05 0.94822771E+01-0.24058613E+05 4

13444-90-1

NO2CL SIGMA=2 STATWT=1 A0=.44334 B0=.172637 C0=.1240691 NU=1286,793,370,  
 1685,408,652 TAAA=-2.04E-6 TBBB=-.59E-6 TAAB=.28E-6 TABA=-.86E-6  
 TCCC=-.15E-6 TAAC=-.17E-7 TBBC=-.284E-6 REF=Gurvich 1989 HF298=12.5+/-1 kJ  
 Max Lst Sq Error Cp @ 1300 K 0.38 %  
 NO2CL L 5/95N 1O 2CL 1 OG 200.000 6000.000 A 81.45824 1  
 0.73973930E+01 0.26288293E-02-0.10108361E-05 0.17126196E-09-0.10596506E-13 2  
 -0.11593163E+04-0.10963487E+02 0.23950579E+01 0.19208111E-01-0.23484888E-04 3  
 0.15177254E-07-0.41194825E-11 0.11500810E+03 0.14274389E+02 0.15033959E+04 4

10022-50-1

NO2F SIGMA=2 STATWT=1 A0=.440348 B0=.3818057 C0=.2041075 NU=1310,822,568,  
 1792,560,742 TAAA=-1.328E-6 TBBB=-2.623E-6 TCCC=-.224E-6 TAAB=.415E-6  
 TABA=-1.63E-6 TAAC=-.167E-6 TBBC=-.66E-6 HF298=-109.+/-20 kJ REF=Gurvich 89  
 Max Lst Sq Error Cp @ 1300 K 0.40%.  
 NO2F L 5/95N 1O 2F 1 OG 200.000 6000.000 A 65.00394 1  
 0.70399495E+01 0.29695800E-02-0.11442077E-05 0.19364501E-09-0.11972566E-13 2  
 -0.15731594E+05-0.10688099E+02 0.18781432E+01 0.17625040E-01-0.15399750E-04 3  
 0.47606145E-08 0.18294737E-12-0.14326397E+05 0.15869654E+02-0.13109612E+05 4

Table 4 (continued)

12033-49-7

NO3 SIGMA=6 STATWT=2 IA=IB=6.4277 IC=12.8555 NU=1158(2),940,704(2),765  
 HF298=74.628+/-0.69 kJ REF=ATcT A {HF298=71.13 kJ REF=JANAF} Max Lst Sq  
 Error Cp @ 2300 K 0.34%.

NO3	J12/64N	1.0	3.	0.	0.G	200.000	6000.000	C	62.00494	1
7.48347734E+00	2.57772041E-03	-1.00945831E-06	1.72314072E-10	-1.07154015E-14						2
5.70919428E+03	-1.41618155E+01	2.17359310E+00	1.04902697E-02	1.10472650E-05						3
-2.81561854E-08	1.36583958E-11	7.39219877E+03	1.46022098E+01	8.55492386E+03						4

14797-55-8

NO3- ION STATWT=1 SIGMA=6 IAIBIC=480.E-117 NU=1055,830,1370(2),720(2)  
 HF0=-298.0 kJ REF=Gurvich 1989

NO3-	RUS 89N	1.0	3.E	1.	0.G	298.150	6000.000	B	62.00549	1
6.88404739E+00	3.16062982E-03	-1.23048782E-06	2.09257989E-10	-1.29795471E-14						2
-4.00548152E+04	-1.17087097E+01	1.21258521E+00	1.71545193E-02	-1.05270457E-05						3
-1.16074097E-09	2.33114998E-12	-3.84077713E+04	1.79933865E+01	-3.73779731E+04						4

7789-26-6

NO3F SIGMA=1 IAIBIC=3300. IR=1.709 ROSYM=2. POT. BARRIER V(2)=3510. cm-1  
 NU=1759,1301,928,804,663,455,303,709 HF298=15. kJ REF=Gurvich 1989 Max Lst  
 Sq Error Cp @ 1300 K 0.52%

NO3F	RUS 89N	1.0	3F	1	0G	200.000	5000.000	B	81.00334	1
0.98118818E+01	0.35639389E-02	-0.15419861E-05	0.27634191E-09	-0.17658973E-13						2
-0.18356434E+04	-0.22945174E+02	0.23251747E+01	0.26601706E-01	-0.29142030E-04						3
0.15590927E-07	-0.32832597E-11	0.15666889E+03	0.15244961E+02	0.18040750E+04						4

7727-37-9

N2 HF298= 0.0 kJ REF=TSIV Max Lst Sq Error Cp @ 6000 K 0.29%

N2	REF ELEMENT	G 8/02N	2.	0.	0.	0.G	200.000	6000.000	A	28.01340	1
2.95257637E+00	1.39690040E-03	-4.92631603E-07	7.86010195E-11	-4.60755204E-15						2	
-9.23948688E+02	5.87188762E+00	3.53100528E+00	-1.23660988E-04	-5.02999433E-07						3	
2.43530612E-09	-1.40881235E-12	-1.04697628E+03	2.96747038E+00	0.00000000E+00						4	

66511-78-2

N2D2-cis STATWT=1 SIGMA=2 IA=.5832 IB=2.1780 IC=2.7612 NU=2300,1490,1058,  
 2400,1150,750 REF=JANAF HF298=202.857 kJ HF0=209.788 kJ REF=HF0 of N2H2  
 Max Lst Sq Error Cp @ 1300 K 0.58

N2D2,cis	g 6/01N	2.D	2.	0.	0.G	200.000	6000.000	B	32.04168	1
4.51455406E+00	5.18901136E-03	-1.93684182E-06	3.20575724E-10	-1.95208436E-14						2
2.25118040E+04	-9.52667764E-01	3.87335926E+00	-2.62328993E-03	2.63075876E-05						3
-3.13008811E-08	1.18110027E-11	2.31835992E+04	4.74949032E+00	2.43979898E+04						4

10578-16-2

N2F2 ISOMERS CIS AND TRANS WERE MIXED BY INCLUDING THEM AS EXCITED STATES. 1 IS  
 CIS AND 2 IS TRANS SIGMA=2 IAIBIC=668.2 NU=1525,896,341,300,952,737 T0=470.  
 SIGMA=2 IAIBIC=390. NU=1523,1018,603,362,990,422 HF0=67.+/-10. kJ  
 REF=Gurvich 89 Max Lst Sq Error Cp @ 1300 K 0.31%.

N2F2	RUS 89N	2F	2	0	0G	200.000	6000.000	B	66.01029	1
0.79266250E+01	0.21002389E-02	-0.81722252E-06	0.13894835E-09	-0.86178747E-14						2
0.47212571E+04	-0.14265182E+02	0.26944269E+01	0.19996317E-01	-0.25239401E-04						3
0.15967248E-07	-0.40786186E-11	0.60030677E+04	0.11933973E+02	0.75018251E+04						4



Table 4 (continued)

10036-47-2

N2F4 EQUILIBRIUM MIXTURE OF TRANS AND GAUCHE ISOMERS. SIGMA=2 STATWT=1  
 IAIBIC=13800. NU=1039,719,601,354,962,252,131,873,999,542,494,467 T0=100.  
 SIGMA=2 STATWT=1 IAIBIC=11800. NU=1027,946,733,587,423,298,115,1012,931,515,  
 288,242 HF298=-22.+/-10. kJ REF=Gurvich 1989 Max Lst Sq Error Cp @ 1300 0.27%  
 N2F4 RUS 89N 2F 4 0 OG 200.000 6000.000 B 104.00709 1  
 0.13251312E+02 0.28400333E-02-0.11179520E-05 0.19147494E-09-0.11934318E-13 2  
 -0.73226616E+04-0.39550630E+02 0.13352845E+01 0.47397540E-01-0.66795981E-04 3  
 0.45073083E-07-0.11856992E-10-0.46441011E+04 0.19044610E+02-0.26459767E+04 4

36882-13-0

N2H (NNH) STATWT=2 IA=0.131 IB=1.789419 IC=1.92025 NU=1129,1484,2926  
 REF=C.Melius BAC/MP4 Calculations, Private Communication HF298=\*59.636+/-3.24\*  
 KCAL Max Lst Sq Error Cp @ 6000 K 0.38%  
 N2H T07/93N 2H 1 0 OG 200.000 6000.000 B 29.02142 1  
 0.37667545E+01 0.28915081E-02-0.10416620E-05 0.16842594E-09-0.10091896E-13 2  
 0.28650697E+05 0.44705068E+01 0.43446927E+01-0.48497072E-02 0.20059459E-04 3  
 -0.21726464E-07 0.79469538E-11 0.28791973E+05 0.29779411E+01 0.30009829E+05 4

3618-05-1

N2H2 SIGMA=2 STATWT=1 A0=10.00021 B0=1.304194 C0=1.149861 NU=1286,  
 1529,1583,3120.3,3131,1300 T0=3000. STATWT=1 SIGMA=2 IAIBIC=1.46E-117  
 NU=1390,1470,1670,3040,3090,1100 T0=6000. STATWT=3 IAIBIC=1.58E-117 NU=1360,  
 1485,1580,3330,3380,1200 T0=6700. STATWT=1 T0=14000. STATWT=3 T0=20700.  
 STATWT=3 T0=17400. STATWT=1 HF298=211.86 kJ HF0=219.0 kJ REF= Gurvich 1989.  
 {HF0=198.32+/-4.6 kJ REF=Ruscic & Berkowitz JCP 95 (1991),4378} Max Lst Sq  
 Error Cp @ 6000 K 0.32%  
 N2H2 L 5/90N 2H 2 0 OG 200.000 6000.000 A 30.02936 1  
 0.13111509E+01 0.90018727E-02-0.31491187E-05 0.48144969E-09-0.27189798E-13 2  
 0.24786417E+05 0.16409109E+02 0.49106602E+01-0.10779187E-01 0.38651644E-04 3  
 -0.38650163E-07 0.13485210E-10 0.24224273E+05 0.91027970E-01 0.25480756E+05 4

7782-94-7

NH2NO2 NITRAMIDE SIGMA=1 STATWT=1 A0=0.422182 B0=0.396691 C0=0.205612  
 Nu=3280,1613,1370,1175,1050,783,716,3400,1540,800,596,350 HF298= -26.0+/-10 kJ  
 REF=Gurvich 1989 {HF298=-3. kJ??? REF= Dorofeeva & Tolmach. Thermochim. Acta  
 240, (1994),47-66}. Max Lst Sq Error Cp @ 6000 0.44 %.  
 NH2NO2 NITRAMIDE tpis89N 2.H 2.O 2. O.G 200.000 6000.000 B 62.02816 1  
 7.38890844E+00 7.65188287E-03-2.75087184E-06 4.44623197E-10-2.66488354E-14 2  
 -6.21766970E+03-1.32736914E+01 2.17310160E+00 1.43162238E-02 1.09031816E-05 3  
 -2.76714916E-08 1.29868784E-11-4.45906123E+03 1.53831146E+01-3.12706341E+03 4

13598-46-4

N2H3 Hydrazine Radical STATWT=2 SIGMA=1 IA=0.4194 IB=2.7615 IC=3.1149  
 NU=3601,3441,3373,1695,1513,1238,1162,740,648 HF298=220.58+/-1.34 REF=ATcT A  
 {HF298=54.62 kcal HF0=57.19 kcal WRONG! REF=Burcat G3B3 Calc.:  
 HF298=53.79+/-17.0 KCAL HF0=55.3+/-0.3 kcal REF=Ruscic Berkowitz JCP 95 (1991),  
 4378} Max Lst Sq Error Cp @ 6000 K 0.40%  
 N2H3 Hydrazine R A05/05H 3.N 2. 0. O.G 200.000 6000.000 B 31.03730 1  
 4.04483566E+00 7.31130186E-03-2.47625799E-06 3.83733021E-10-2.23107573E-14 2  
 2.48098603E+04 2.88423392E+00 3.42125505E+00 1.34901590E-03 2.23459071E-05 3  
 -2.99727732E-08 1.20978970E-11 2.53056139E+04 7.83176309E+00 2.65295249E+04 4

Table 4 (continued)

302-01-2

N2H4 liquid Hydrazine REF=JANAF HF298=50.38 kJ REF=Gurvich 1989

{HF298=50.690+/-0.18 kJ REF=ATcT A} Max Lst Sq Error H-H0 @ 300 K 0.60%

N2H4(L) Hydrazin	J12/65N	2.H	4.	0.	0.L	200.000	800.000	B	32.04524	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			2
0.00000000E+00	0.00000000E+00	1.20310475E+01	-1.58854987E-02	7.53502039E-05						3
-9.15945394E-08	4.07674892E-11	2.67428635E+03	-5.18137624E+01	6.05923187E+03						4

302-01-2

N2H4 HYDRAZINE STATWT=1 SIGMA=1 IAIBIC=7.0E-117 Ir=0.146 ROSYM=2

V(2)=1700. cm-1 NU=3280,3325,1587,1275,1098,780,3314,3350,1628,1275,937.2

HF298= 95.18+/-4.2 KJ REF=Gurvich 1989. {HF0=109.32+/-0.5 kJ REF=Ruscic & Berkowitz JCP 95 (1991),4378; HF298=95.417+/-0.18 kJ REF=ATcT A} Max Lst Sq Error Cp @ 6000 K 0.42%.

N2H4 HYDRAZINE	L 5/90N	2.H	4.	0.	0.G	200.000	6000.000	B	32.04524	1
4.93957357E+00	8.75017187E-03	-2.99399058E-06	4.67278418E-10	-2.73068599E-14						2
9.28265548E+03	-2.69439772E+00	3.83472149E+00	-6.49129555E-04	3.76848463E-05						3
-5.00709182E-08	2.03362064E-11	1.00893925E+04	5.75272030E+00	1.14474575E+04						4

6484-52-2

NH4NO3 Amonium Nitrate solid and liquid. HF298=-365.6+/-1.0 kJ Generated and corrected by McBride from original values by Gurvich et al. Vol 1. 1989.

{HF298=-365.102+/-0.18 kJ REF=ATcT A}

NH4NO3 (IV)	G10/02N	2.H	4.O	3.	0.C	256.200	298.150	B	80.04344	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			2
0.00000000E+00	0.00000000E+00	-1.29547150E+02	1.81866355E+00	-8.94421296E-03						3
2.02563499E-05	-1.74314429E-08	-3.89655352E+04	4.67032673E+02	-4.39713224E+04						4
NH4NO3 (IV)	G10/02N	2.H	4.O	3.	0.C	298.150	305.380	B	80.04344	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			2
0.00000000E+00	0.00000000E+00	5.86564933E+00	3.64302887E-02	0.00000000E+00						3
0.00000000E+00	0.00000000E+00	-4.73393723E+04	-2.61436244E+01	-4.39713224E+04						4
NH4NO3 (III)	G10/02N	2.H	4.O	3.	0.C	305.380	357.250	B	80.04344	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			2
0.00000000E+00	0.00000000E+00	7.23313821E+00	2.33327039E-02	0.00000000E+00						3
0.00000000E+00	0.00000000E+00	-4.69417938E+04	-2.92985169E+01	-4.39713224E+04						4
NH4NO3 (II)	G10/02N	2.H	4.O	3.	0.C	357.250	399.000	B	80.04344	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			2
0.00000000E+00	0.00000000E+00	6.02320522E+01	-1.76799354E-01	0.00000000E+00						3
4.52882972E-07	0.00000000E+00	-5.47863351E+04	-2.75780621E+02	-4.39713224E+04						4
NH4NO3 (I)	G10/02N	2.H	4.O	3.	0.C	399.000	442.850	B	80.04344	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			2
0.00000000E+00	0.00000000E+00	1.29532588E+01	1.56353170E-02	0.00000000E+00						3
0.00000000E+00	0.00000000E+00	-4.78370128E+04	-5.84851082E+01	-4.39713224E+04						4
NH4NO3 (L)	G10/02N	2.H	4.O	3.	0.L	442.850	900.000	B	80.04344	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00			2
0.00000000E+00	0.00000000E+00	1.93637388E+01	0.00000000E+00	0.00000000E+00						3
0.00000000E+00	0.00000000E+00	-4.84379330E+04	-8.90300528E+01	-4.39713224E+04						4

Table 4 (continued)

10024-97-2

N2O NNO STATWT=1 B0=.4190113 NU=1277,589,2224 X11=-3.842 X12=.182  
 X13=-27.352 X22=-.271 X23=-14.672 X33=-15.155 G22=.366 Y111=-.021  
 Y112=-.152 Y122=-.030 Y222=-.007 Y113=-.338 Y133=.124 Y123=.390  
 Y223=.059 Y233=.029 Y333=-.002 W0=29.55 ALFAB1=.001917 ALFAB2=-.000577  
 ALFAB3=.003481 D0=17.59E-8 HF298= 81.6 KJ REF= Gurvich 1989.  
 {HF298=82.58+/-0.1 kJ REF=ATcT A}

N2O	L 7/88N	2O	1	0	OG	200.000	6000.000	A	44.01288	1
0.48230729E+01	0.26270251E-02	-0.95850872E-06	0.16000712E-09	-0.97752302E-14						2
0.80734047E+04	-0.22017208E+01	0.22571502E+01	0.11304728E-01	-0.13671319E-04						3
0.96819803E-08	-0.29307182E-11	0.87417746E+04	0.10757992E+02	0.98141682E+04						4

12269-46-4

N2O+ ION STATWT=2 B0=.411407 NU=1737,461(2),1126 T0=132.4 STATWT=2 T0=28229.  
 STATWT=2 HF=1333.399+/-0.63 KJ REF=JANAF

N2O+	J12/70N	2O	1E	-1	OG	298.150	6000.000	B	44.01233	1
0.55285660E+01	0.19596138E-02	-0.75377712E-06	0.12704886E-09	-0.78022397E-14						2
0.15842390E+06	-0.44187923E+01	0.32869103E+01	0.74022215E-02	-0.48666444E-05						3
0.73292750E-09	0.29823434E-12	0.15910253E+06	0.74013737E+01	0.16037012E+06						4

10544-73-7

N2O3 STATWT=1 SIGMA=1 IAIBIC=3562E-117 IR=1.124 ROT. BARRIER V(2)=490. cm-1  
 ROSYM=2 NU=1832,1630,1305,773,414,260,160,337 T0=14100. STATWT=1  
 HF0=91.2 KJ REF= Gurvich 1989. {HF298=86.090+/-0.18 kJ REF=ATcT A}

N2O3	L 4/90N	2.O	3.	0.	O.G	200.000	6000.000	B	76.01168	1
9.08583845E+00	3.37756330E-03	-1.31583890E-06	2.30762329E-10	-1.47151267E-14						2
7.27160146E+03	-1.55361904E+01	5.81083964E+00	1.43330962E-02	-1.96208597E-05						3
1.73060735E-08	-6.46553954E-12	8.19184453E+03	1.20461321E+00	1.04192062E+04						4

10544-72-6

N2O4 STATWT=1 SIGMA=4 IAIBIC=10500.E-117 IR=3.22 ROSYM=2 POTENTIAL BARRIER  
 V(2)=1600.cm-1 ROT LEVELS=187 NU=1373,812,260,751,1710,480,430,675,1758,270,  
 1264 HF0=20.4 KJ REF= Gurvich 1989. {HF298=10.785+/-0.17 kJ REF=ATcT A}

N2O4	RUS 89N	2O	4	0	OG	200.000	6000.000	B	92.01108	1
1.15752899E+01	4.01616086E-03	-1.57178323E-06	2.68274309E-10	-1.66922019E-14						2
-2.92191226E+03	-3.19488439E+01	3.02002308E+00	2.95904321E-02	-3.01342458E-05						3
1.42360407E-08	-2.44100049E-12	-6.40040162E+02	1.18059606E+01	1.33632866E+03						4

10102-03-1

N2O5 O2N-O-NO2 STATWT=1 SIGMA=2 IAIBIC=29700.E-117 Ir=4.8 V(2)=660. cm-1  
 ROSYM=2 ROT. LEVELS=187 (TWO EQUIVALENT ROTORS) NU= 1728,353(2),1338,1247,860,  
 743(2),85,645,614,577,1728,353 HF298= 13.3 KJ REF= Gurvich 1989.  
 {HF298=15.437+/-0.74 kJ REF=ATcT A}

N2O5	L 4/90N	2.O	5.	0.	O.G	200.000	6000.000	B	108.01048	1
1.31108082E+01	4.87435791E-03	-1.87548389E-06	3.16374121E-10	-1.95926845E-14						2
-3.11634700E+03	-3.46877692E+01	3.68767444E+00	3.92120798E-02	-5.53770029E-05						3
4.20097833E-08	-1.31260710E-11	-8.30291184E+02	1.21967866E+01	1.59961321E+03						4

12596-60-0

N3 AZIDE SIGMA=2 STATWT=2 B0=.43113 NU=1400,737(2),2150 T0=71.9 STATWT=2  
 REF=Gurvich 1989 HF298=453.54+/-3.5 kJ HF0=456.97 kJ REF=ATcT A  
 {HF298=436.0+/-15. KJ REF=Gurvich 1989.} Max Lst Sq Error Cp @ 1300 K 0.44%.

N3	ATcT/AN	3.	0.	0.	O.G	200.000	6000.000	B	42.02022	1
4.64110774E+00	2.76960647E-03	-1.04917579E-06	1.75340743E-10	-1.07482727E-14						2
5.28079884E+04	-9.40233115E-01	2.86063087E+00	4.24883043E-03	5.14574004E-06						3
-1.01478684E-08	4.41879795E-12	5.34787743E+04	9.11586663E+00	5.45480131E+04						4

Table 4 (continued)

7782-79-8

N3H SIGMA=1 STATWT=1 A0=20.380639 B0=.4014156 C0=.3929878 NU=3340,2140,  
 1264,1150.5,534,607 DJ=1.64E-7 DJK=2.63E-5 DK=7.67E-3 REF=Gurvich 89  
 HF298=453.54+/-3.5 kJ REF=ATcT A {HF298=294.0+/-4. KJ REF= Gurvich 1989}.  
 HF298(s)=261.59+/-0.77 kJ REF=ATcT A Max Lst Sq Error Cp @ 6000 K 0.38%.  
 N3H ATcT/AN 3.H 1. 0. 0.G 200.000 6000.000 B 43.02816 1  
 5.14700198E+00 4.30561405E-03-1.52704650E-06 2.46295940E-10-1.47144292E-14 2  
 3.31533377E+04-2.25528569E+00 2.88510835E+00 9.44343949E-03-3.87921021E-06 3  
 -1.89401832E-09 1.60183173E-12 3.38421425E+04 9.71687992E+00 3.50848096E+04 4

12164-94-2

N4H4 NH4N3 HF298 cr =114.14+/-0.94 kJ HF298(g)=179,7 kJ?? REF=Finch,Gardner,  
 Head,Xiaoping J. Chem Therm. 22,(1990),301-5. Note! Probably does not exist in  
 gas phase but dissociate to NH3 + HN3

7440-01-9

Ne HF298= 0.0 KJ REF=McBride, HeimeI, Ehlers & Gordon "Thermodynamic Proper-  
 ties to 6000 K..." NASA SP-3001 1963.  
 NE REF ELEMENT L10/90NE 100 000 000 0G 200.000 6000.000 B 20.1797 1  
 0.25000000E 01 0.00000000E 00 0.00000000E 00 0.00000000E 00 0.00000000E 00 2  
 -0.74537500E 03 0.33553227E 01 0.25000000E 01 0.00000000E 00 0.00000000E 00 3  
 0.00000000E 00 0.00000000E 00-0.74537498E 03 0.33553227E 01 0.00000000E+00 4

14782-23-1

Ne+ HF298=2086.966 kJ HF0=2080.662 kJ REF=C.E. Moore U.S. Nat. Bur. Stand.  
 NSRDS-NBS 34 1970 {HF298=2086.966+/-0.00132 kJ REF=ATcT A} Max Lst Sq Error  
 Cp @ 1300 K 0.14%.  
 Ne+ g 3/97NE 1.E -1. 0. 0.G 298.150 6000.000 A 20.17915 1  
 2.89659836E+00-3.51984734E-04 1.26030599E-07-2.02696042E-11 1.20889482E-15 2  
 2.50144008E+05 2.60525287E+00 1.94150245E+00 4.40493934E-03-8.59235286E-06 3  
 7.02349108E-09-2.12599650E-12 2.50291271E+05 6.98897045E+00 2.51002879E+05 4

7440-02-0

Ni REFERENCE ELEMENT Condensed Phase HF298(S)=0.0 kJ REF=JANAF  
 Ni(cr) J12/76NI 1. 0. 0. 0.S 200.000 631.000 B 58.69340 1  
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2  
 0.00000000E+00 0.00000000E+00 3.92097614E+00-2.34184719E-02 1.34230145E-04 3  
 -2.75971639E-07 1.98530861E-10-8.62387206E+02-1.56856186E+01 0.00000000E+00 4  
 Ni(cr) J12/76NI 1. 0. 0. 0.S 631.000 1728.000 B 58.69340 1  
 9.58208572E+00-1.78945122E-02 1.97185112E-05-9.11957952E-09 1.58728609E-12 2  
 -2.61782185E+03-4.74612393E+01 4.85484877E+02-2.30395380E+00 4.10622634E-03 3  
 -3.23350101E-06 9.49617381E-10-8.11709085E+04-2.25428960E+03 0.00000000E+00 4  
 Ni(L) J12/76NI 1. 0. 0. 0.L 1728.000 6000.000 B 58.69340 1  
 4.67989094E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2  
 -3.22238346E+02-2.33517797E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 3  
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 4

1313-99-1

NiO Nickel Oxide Data from Barin Database 1989 HF298(S)=-239.70 kJ  
 NiO Solid-A B /89NI 1.0 1. 0. 0.S 298.150 525.000 C 74.689 1  
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2  
 0.00000000E+00 0.00000000E+00-1.57324752E+01 1.79860646E-01-5.57051845E-04 3  
 7.23393852E-07-2.80704261E-10-6.79031544E+02 5.95039043E+01-9.99938661E+02 4  
 NiO Solid-B B /89NI 1.0 1. 0. 0.S 525.000 565.000 C 74.689 1  
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2  
 0.00000000E+00 0.00000000E+00-4.05614678E+00 2.02539491E-02 0.00000000E+00 3  
 0.00000000E+00 0.00000000E+00-1.82561755E+02 2.29564525E+01-9.99938661E+02 4

Table 4 (continued)

NiO Solid-C	B /89NI 1.O 1. 0. 0.S	565.000 2228.000 C 74.689	1
8.54519666E+00-6.01462324E-03	5.06266530E-06-1.02231132E-09-5.77542484E-14		2
-3.39816451E+03-4.28164283E+01	5.32267831E+00 7.63070044E-03-1.69937025E-05		3
1.50561208E-08-4.50262391E-12-2.77681950E+03-2.74214599E+01-9.99938661E+02			4
NiO Liquid	B /89NI 1.O 1. 0. 0.L	2228.000 2500.000 C 74.689	1
6.50276297E+00 4.91821956E-05-2.06203183E-08	2.87842575E-12 0.00000000E+00		2
4.43423749E+03-2.91641267E+01 0.00000000E+00	0.00000000E+00 0.00000000E+00		3
0.00000000E+00 0.00000000E+00 0.00000000E+00	0.00000000E+00-9.99938661E+02		4
16812-54-7			
NiS Nickel Sulfide Condensed phase	REF=JANAF HF298(S)=-87.86+/-6.3 kJ		
NiS(b) Crystal	J12/76NI 1.S 1. 0. 0.S	300.000 652.000 B 90.75940	1
2.51505130E+00 1.98108790E-02-4.47517130E-05	5.35527360E-08-2.47391510E-11		2
-1.18972750E+04-1.22988050E+01 2.51505130E+00	1.98108790E-02-4.47517130E-05		3
5.35527360E-08-2.47391510E-11-1.18972750E+04-1.22988050E+01-1.05681072E+04			4
NiS(a) Crystal	J12/76NI 1.S 1. 0. 0.S	652.000 1249.000 B 90.75940	1
-2.16882770E+00 2.04672610E-02-1.52390680E-05	4.52420390E-09 0.00000000E+00		2
-9.25397310E+03 1.60189760E+01 1.59778550E+00	1.62791590E-02-2.39592640E-05		3
1.96652470E-08-5.99935920E-12-1.06051920E+04-4.99884140E+00	0.00000000E+00		4
NiS(L) Liquid	J12/76NI 1.S 1. 0. 0.L	1249.000 5000.000 B 90.75940	1
9.23426080E+00 0.00000000E+00 0.00000000E+00	0.00000000E+00 0.00000000E+00		2
-1.10536520E+04-4.57697360E+01 9.23426080E+00	0.00000000E+00 0.00000000E+00		3
0.00000000E+00 0.00000000E+00-1.10536520E+04-4.57697360E+01	0.00000000E+00		4
12035-51-7			
NiS2 Condensed Phase	REF=JANAF HF298(S)=-131.376 +/- 16.7 kJ		
NiS2(s)	J 3/77NI 1.S 2. 0. 0.C	300.000 1280.000 C 122.82540	1
5.27426400E+00 9.08709310E-03-5.82010990E-06	1.70500810E-09 0.00000000E+00		2
-1.75287250E+04-2.33922190E+01 7.74493490E+00	2.53517140E-03-9.97675870E-08		3
1.07829500E-10-4.19129410E-14-1.82225390E+04-3.62243880E+01-1.58013948E+04			4
NiS2(L)	J 3/77NI 1.S 2. 0. 0.C	1280.000 5000.000 C 122.82540	1
1.09452410E+01 0.00000000E+00 0.00000000E+00	0.00000000E+00 0.00000000E+00		2
-1.23449250E+04-4.97206240E+01 1.09452410E+01	0.00000000E+00 0.00000000E+00		3
0.00000000E+00 0.00000000E+00-1.23449250E+04-4.97206240E+01	0.00000000E+00		4
12035-72-2			
Ni3S2 Condensed phase	REF=JANAF HF298(S)=-216.31 +/- 5. kJ		
Ni3S2(I)	J12/76NI 3.S 2. 0. 0.S	300.000 829.000 C 240.21220	1
6.92383000E+00 4.04466800E-02-7.30739570E-05	7.10070760E-08-2.62218590E-11		2
-2.93621960E+04-3.27350520E+01 6.92383000E+00	4.04466800E-02-7.30739570E-05		3
7.10070760E-08-2.62218590E-11-2.93621960E+04-3.27350520E+01-2.60177884E+04			4
Ni3S2(II)	J12/76NI 3.S 2. 0. 0.S	829.000 1062.000 C 240.21220	1
2.26855850E+01 0.00000000E+00 0.00000000E+00	0.00000000E+00 0.00000000E+00		2
-2.93134790E+04-1.11689780E+02 2.26855850E+01	0.00000000E+00 0.00000000E+00		3
0.00000000E+00 0.00000000E+00-2.93134790E+04-1.11689780E+02	0.00000000E+00		4
Ni3S2(L)	J12/76NI 3.S 2. 0. 0.L	1062.000 5000.000 C 240.21220	1
2.30680390E+01 0.00000000E+00 0.00000000E+00	0.00000000E+00 0.00000000E+00		2
-2.73444020E+04-1.12118110E+02 2.30680390E+01	0.00000000E+00 0.00000000E+00		3
0.00000000E+00 0.00000000E+00-2.73444020E+04-1.12118110E+02	0.00000000E+00		4
12137-12-1			
Ni3S4 Solid	REF=JANAF HF298(S)=-301.11 +/- 25.1 kJ		
Ni3S4(s)	J 3/77NI 3.S 4. 0. 0.C	300.000 1100.000 C 304.34420	1
1.46738180E+01 1.72757180E-02 0.00000000E+00	0.00000000E+00 0.00000000E+00		2
-4.13600010E+04-6.63291620E+01 1.46711930E+01	1.72771640E-02-2.75692840E-09		3
1.02338580E-11-6.29839560E-15-4.13584790E+04-6.63129390E+01-3.62163568E+04			4

Table 4 (continued)

17778-80-2

O HF298=249.175+/-0.1 KJ REF=C.E. Moore "Selected Tables of Atomic Spectra"  
NSRDS-NBS Sec 7 1976 p. A8 I {HF298=249.229+/-0.02 kJ REF=ATcT A}

O	L 1/900	1.	0.	0.	0.G	200.000	6000.000	A	15.99940	1
2.54363697E+00	-2.73162486E-05	-4.19029520E-09	4.95481845E-12	-4.79553694E-16						2
2.92260120E+04	4.92229457E+00	3.16826710E+00	-3.27931884E-03	6.64306396E-06						3
-6.12806624E-09	2.11265971E-12	2.91222592E+04	2.05193346E+00	2.99687009E+04						4

14337-01-0

O- OXYGEN ION HF0=95.093 KJ REF=Gurvich 89

O-	RUS 890	1.E	1.	0.	0.G	298.150	6000.000	B	15.99995	1
2.54474868E+00	-4.66695419E-05	1.84912310E-08	-3.18159131E-12	1.98962894E-16						2
1.14822713E+04	4.52131018E+00	2.90805921E+00	-1.69804907E-03	2.98069956E-06						3
-2.43835127E-09	7.61229313E-13	1.14138341E+04	2.80339097E+00	1.22272740E+04						4

7782-44-7

O2 CALCULATED FROM ORIGINAL VALUES HF298=0 KJ REF=Gurvich 1989.

02	REF ELEMENT	RUS 890	2	0	0	0G	200.000	6000.000	A	31.99880	1
	3.66096083E+00	6.56365523E-04	-1.41149485E-07	2.05797658E-11	-1.29913248E-15						2
	-1.21597725E+03	3.41536184E+00	3.78245636E+00	-2.99673415E-03	9.84730200E-06						3
	-9.68129508E-09	3.24372836E-12	-1.06394356E+03	3.65767573E+00	0.00000000E+00						4

12185-07-8

O2+ CALCULATED FROM ORIGINAL VALUES HF0=1165.0 KJ REF=Gurvich 1989.

O2+	RUS 890	2.E -1.	0.	0.G	298.150	6000.000	A	31.99825	1
3.31675922E+00	1.11522244E-03	-3.83492556E-07	5.72784687E-11	-2.77648381E-15					2
1.39876823E+05	5.44726469E+00	4.61017167E+00	-6.35951952E-03	1.42425624E-05					3
-1.20997923E-08	3.70956878E-12	1.39742229E+05	-2.01326941E-01	1.40937762E+05					4

11062-77-4

O2- CALCULATED FROM ORIGINAL VALUES HF0=-42.5 KJ REF=Gurvich 1989.

Q2-	L 4/890	2.E	1.	0.	0.G	298.150	6000.000	A	31.99935	1
	3.95666294E+00	5.98141823E-04	-2.12133905E-07	3.63267581E-11	-2.24989228E-15					2
	-7.06287229E+03	2.27871017E+00	3.66442522E+00	-9.28741138E-04	6.45477082E-06					3
	-7.74703380E-09	2.93332662E-12	-6.87076983E+03	4.35140681E+00	-5.77639825E+03					4

10028-15-6

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O3   OZONE      SIGMA=2  STATWT=1  A0=3.553664  B0=.4452762  C0=.394758  NU=1103,
701,1042  X11=-4.9  X12=-9.1  X13=-34.8  X22=-1.0  X23=-17.  X33=-10.6
ALFAA1=-.002981  ALFAA2=-.053415  ALFAA3=.053118  ALFAB1=.002554  ALFAB2=.001269
ALFAB3=.003992  ALFAC1=.002319  ALFAC2=.002307  ALFAC3=.003613  W=-27.05
TAAA=-8.1429E-6  TBBB=-2.3864E-6  TCCC=-1.2694E-6  TAAB=16.947E-6  TAAC=3.2717E-6
TBBC=-1.6665E-6  TABA=-9.2093E-6  T0=10000.  STATWT=3  SIGMA=2  IAIBIC=48.
NU=600(2),350  T0=12500.  STATWT=3  SIGMA=2  IAIBIC=51.  NU=600(2),350
T0=13000.  STATWT=1  SIGMA=6  IAIBIC=32.  NU=850,500(2)  T0=13500.  STATWT=3
SIGMA=2  IAIBIC=48.  NU=600(2),350  HF298=141.8 KJ  REF= Gurvich 1989.
{HF298=141.733+/-0.039 kJ  REF=ATcT A}

```

O3	L 5/900	3	0	0	OG	200.000	6000.000	A	47.99820	1
	1.23302914E+01	-1.19324783E-02	7.98741278E-06	-1.77194552E-09	1.26075824E-13					2
	1.26755831E+04	-4.08823374E+01	3.40738221E+00	2.05379063E-03	1.38486052E-05					3
	-2.23311542E-08	9.76073226E-12	1.58644979E+04	8.28247580E+00	1.70545228E+04					4

Table 4 (continued)

7723-14-0

P HF298=-316.39+/-1.0 kJ REF=JANAF

P	J12/82P	1.	0.	0.	0.G	200.000	6000.000	B	30.97376	1
	2.80721555E+00-5.30841988E-04	2.44543046E-07-2.05708252E-11-2.94546619E-16								2
	3.71892748E+04	3.67764723E+00	2.50004278E+00-4.38968637E-07	1.58131741E-09						3
	-2.33900457E-12	1.20510940E-15	3.73073754E+04	5.38414719E+00	3.80527536E+04					4

7719-12-2

PCL3 SIGMA=3 STATWT=1 IA=IB=32.3918 IC=57.6799 NU=510,507(2),259,187(2)

HF298=-288.70+/-5.4 kJ REF=JANAF

PCL3	J 6/70P	1.CL	3.	0.	0.G	300.000	5000.000	B	137.33186	1
	9.45661160E+00	6.02784010E-04-2.58468780E-07	4.89042800E-11-3.40832850E-15							2
	-3.77045574E+04-1.69296498E+01	5.25905370E+00	1.78805660E-02-2.73175850E-05							3
	1.88982400E-08-4.87384960E-12-3.68644304E+04	3.25232968E+00-3.47080119E+04								4

16027-92-2

PF SIGMA=1 T0(STATWT)=0(3) BE=0.5665 WE=846.75 WEXE=4.489 ALFAE=0.00456

T0(STATWT)=7090.41(2) BE=0.5699 WE=858.79 WEXE=4.438 ALFAE=0.00467

T0(STATWT)=13353.91(1) BE=0.5725 WE=866.14 WEXE=4.51 ALFAE=0.0045

T0(STATWT)=29338.69(2) BE=0.4632 WE=436 WEXE=1.5 ALFAE=0.004

T0(STATWT)=29481.80(2) BE=0.4663 WE=436 WEXE=1.5 ALFAE=0.0038

T0(STATWT)=29623.06(2) BE=0.4693 WE=436 WEXE=1.5 ALFAE=0.0037

T0(STATWT)=35812.29(2) BE=0.4848 WE=413 WEXE=1.5 ALFAE=0.0062

HF298=-52.25+/-20.9 kJ REF=JANAF

PF	J 6/77P	1.F	1.	0.	0.G	300.000	5000.000	A	49.97217	1
	4.28444030E+00	4.65131920E-05	1.29231550E-07-3.54596860E-11	2.93086420E-15						2
	-7.67566495E+03	2.40196395E+00	2.67608630E+00	5.57221620E-03-7.28377960E-06						3
	4.58194390E-09-1.11881060E-12-7.28916135E+03	1.04341832E+01-6.29944377E+03								4

13873-52-4

PF2 SIGMA=2 T0(STATWT)=0(2),25000(2),28000(2),30000(2) IA=2.9836 IB=9.1077

IC=12.0913 NU=852,831,353 HF298=-488.256+/-20.9 kJ REF=JANAF

PF2	J 6/77P	1.F	2.	0.	0.G	300.000	5000.000	C	68.97057	1
	6.09265880E+00	1.03133240E-03-4.53710200E-07	8.70455830E-11-5.97140520E-15							2
	-6.07553254E+04-3.78513004E+00	2.44285260E+00	1.51863310E-02-2.21969240E-05							3
	1.56489320E-08-4.32983720E-12-5.99609804E+04	1.40371170E+01-5.87248863E+04								4

7783-55-3

PF3 SIGMA=3 STATWT=1 IA=IB=10.8265 IC=17.6633 NU=892,860(2),487,344(2)

HF298=-958.441+/-3.8 kJ REF=JANAF

PF3	J12/69P	1.F	3.	0.	0.G	300.000	5000.000	B	87.96897	1
	8.43477330E+00	1.73939200E-03-7.51198080E-07	1.43442470E-10-1.00939790E-14							2
	-1.18180783E+05-1.64636020E+01	2.36218780E+00	2.28200450E-02-2.76566420E-05							3
	1.44909620E-08-2.46023600E-12-1.16776903E+05	1.36864320E+01-1.15275206E+05								4

7647-19-0

PF5 SIGMA=6 STATWT=1 IA=2.23 IB=IC=269 NU=1025(2),947(5),817,640,575,

532(2),514(2),179(2) HF298=-1594.409+/-2.9 kJ REF=JANAF

PF5	J12/69P	1.F	5.	0.	0.G	300.000	5000.000	B	125.96578	1
	1.28461840E+01	3.51044850E-03-1.51986040E-06	2.91019040E-10-2.05347080E-14							2
	-1.96362263E+05-3.94755420E+01	1.05232490E+00	4.44540040E-02-5.39014290E-05							3
	2.84166860E-08-4.91432680E-12-1.93632313E+05	1.90890100E+01-1.91765100E+05								4

Table 4 (continued)

13967-14-1

PH SIGMA=1 T0(STATWT)=0(3),7650(2),15150(1),29560(6),38110(2),57490(1)  
 BE=8.412 WE=2380 WEXE=55 ALFAE=0.28 REF=JANAF Polynomials calculated from  
 original Gurvich tables HF298=230.7+/-33.5 kJ HF0=231.698 kJ (HF298=253.55 kJ  
 REF=JANAF) Max Lst Sq Error Cp @ 1300 K 0.39%.

PH	tpis89P	1.H	1.	0.	0.G	200.000	6000.000	B	31.98170	1
	3.19038459E+00	9.44379562E-04	-1.75369338E-07	2.21554014E-11	-1.74345542E-15					2
	2.67435431E+04	5.14131630E+00	3.55305265E+00	-2.82506559E-04	-3.86398145E-08					3
	2.02508720E-09	-1.27718672E-12	2.67030973E+04	3.44583231E+00	2.77529408E+04					4

13765-43-0

PH2 Phosphino Radical SIGMA=2 STATWT=2 IA=0.3124 IB=0.3521 IC=0.6645  
 Nu=2383,2371,1154 T0=18276.6 SIGMA=2 STATWT=2 HF298=135.47 kJ HF0=139.33+/-8  
 kJ REF=Burcat G3B3 calc {HF298=119.553 kJ REF=Gurvich 89; HF298=125.94 kJ  
 REF=JANAF 63} Max Lst Sq Error Cp @ 6000 K 0.47%

PH2	A 5/05P	1.H	2.	0.	0.G	200.000	6000.000	B	32.98964	1
	3.21773792E+00	3.49542717E-03	-1.29980152E-06	2.17194645E-10	-1.32490322E-14					2
	1.51316700E+04	6.15415960E+00	4.16964428E+00	-2.45830485E-03	1.00971169E-05					3
	-8.78319734E-09	2.59205016E-12	1.50866950E+04	2.18270208E+00	1.62936842E+04					4

PH2- SIGMA=2 STATWT=1 IAIBIC=0.49 Nu=2650,2600,1200 REF=Gurvich 89 estim.  
 HF298=-9.265 kJ HF0=0.800 kJ REF=McBride 01 {HF298=27+/-9.2 REF=Webbook 04}  
 Max Lst Sq Error Cp @ 6000 K 0.43.

PH2-	tpis89P	1.H	2.E	1.	0.G	298.150	6000.000	C	32.99019	1
	3.03027756E+00	3.49534162E-03	-1.24425876E-06	1.99400556E-10	-1.18681640E-14					2
	-2.17226020E+03	6.42905285E+00	3.95759446E+00	-7.28833868E-04	5.13055397E-06					3
	-3.73171703E-09	8.41295283E-13	-2.30028023E+03	2.15722543E+00	-1.11436729E+03					4

7803-51-2

PH3 PHOSPHINE RRHO SIGMA=3 STATWT=1 IA=IB=0.6264 IC=0.7201 NU=2328(2),  
 2323,1122(2),992 REF=JANAF HF298=11.786+/-8 kJ HF0=19.75 kJ REF=Burcat G3B3  
 {HF298=5.439+/-1.7 kJ REF=JANAF} Max Lst Sq Error Cp @ 1300 K 0.62%.

PH3 RRHO	A 6/05P	1.H	3.	0.	0.G	200.000	6000.000	B	33.99758	1
	3.71229298E+00	5.85959002E-03	-2.16607791E-06	3.56195511E-10	-2.15913467E-14					2
	-1.88863997E+02	1.92781913E+00	4.17009763E+00	-5.06487157E-03	2.86027846E-05					3
	-3.13123782E-08	1.13447768E-11	2.03144445E+02	2.02004617E+00	1.41752190E+03					4

17739-47-8

PN PHOSPHORUS NITRIDE SIGMA=1 STATWT=1 BE=0.7862 WE=1337.24 WEXE=6.983  
 ALFAE=0.00557 HF298=104.78+/-5.0 kJ REF=JANAF

PN	J 9/62P	1.N	1.	0.	0.G	300.000	5000.000	B	44.98050	1
	3.64192260E+00	9.44606720E-04	-3.89234800E-07	7.32158260E-11	-5.09616320E-15					2
	1.13936880E+04	4.19044189E+00	3.37552390E+00	-4.10093860E-04	5.12651510E-06					3
	-5.94788980E-09	2.12135820E-12	1.15788400E+04	6.10290619E+00	1.26017849E+04					4

14452-66-5

PO SIGMA=1 T0(STATWT)=0(2),224(2),30696(2),32884(4),38055(4),40485(2),43629(2),  
 47251(2),48580(4) BE=0.7337 WE=1233.3 WEXE=6.56 ALFAE=0.0056  
 HF298=-29.597+/-4.2 kJ REF=Lewis (JANAF'S HF298=23.55 kJ is erroneous).

PO	J 6/71P	1.O	1.	0.	0.G	300.000	5000.000	B	46.97316	1
	3.84279220E+00	7.23644560E-04	-2.89341990E-07	5.30135540E-11	-3.54953730E-15					2
	-4.79945495E+03	4.55237735E+00	3.96130800E+00	-2.12353990E-03	7.52012190E-06					3
	-7.59509120E-09	2.56375910E-12	-4.69896895E+03	4.58369215E+00	-3.55964877E+03					4



Table 4 (continued)

12164-97-5

PO2 SIGMA=2 STATWT=2 IA=0.8775 IB=9.9337 IC=10.8112 NU=1044,980,515

HF298=-314.524 kJ REF=JANAF

PO2	J 9/62P	1.0	2.	0.	0.G	300.000	5000.000	C	62.97256	1
		5.69132780E+00	1.48068660E-03	-6.54256920E-07	1.27932310E-10	-9.20992770E-15				2
		-3.97947254E+04	-2.81972206E+00	2.33452730E+00	1.25021000E-02	-1.43361950E-05				3
		7.67621660E-09	-1.54016940E-12	-3.89688654E+04	1.40544350E+01	-3.78293636E+04				4

12185-09-0

P2 SIGMA=2 STATWT=1 BE=0.30327 WE=780.43 WEXE=2.804 ALFAE=0.00142

HF298=143.65+/-2.1 kJ REF=JANAF

P2	J 6/61P	2.	0.	0.	0.G	300.000	5000.000	B	61.94752	1
		4.16117330E+00	3.96208000E-04	-1.55803390E-07	2.90934740E-11	-2.00424580E-15				2
		1.59468693E+04	2.24109239E+00	2.83911070E+00	4.82661930E-03	-5.49474880E-06				3
		2.58005070E-09	-3.22364530E-13	1.62597073E+04	8.84241009E+00	1.72771170E+04				4

12185-10-3

P4 SIGMA=12 STATWT=1 IA=IB=IC=25.1209 NU=606,464.5(3),363

HF298=58.9+/-2.1 kJ REF=JANAF

P4	J 6/61P	4.	0.	0.	0.G	300.000	5000.000	B	123.89505	1
		9.22627890E+00	8.68941280E-04	-3.77583380E-07	7.23796660E-11	-5.10661090E-15				2
		4.09054959E+03	-1.96417049E+01	3.53533000E+00	2.41252920E-02	-3.64627590E-05				3
		2.49169060E-08	-6.32985630E-12	5.23553359E+03	7.75589569E+00	7.08599199E+03				4

10248-58-5

P4O6 (P2O3)2 SIGMA=12 STATWT=1 IAIBIC=483801.7E-117 NU=1029(2),919(2),643(3),636(3),613(2),465(2),407(3),370(3),302(3) HF298=-2144.519+/-33.5 kJ

REF=McBride (JANAF's HF298=-2214.31 is erroneous).

P4O6	J12/62P	4.0	6.	0.	0.G	300.000	5000.000	B	219.89145	1
		2.23829590E+01	6.41271290E-03	-2.84877920E-06	5.58964390E-10	-4.03341410E-14				2
		-2.65985440E+05	-9.04488339E+01	-5.41216630E+00	1.22358190E-01	-1.95002050E-04				3
		1.48292330E-07	-4.37707920E-11	-2.60299220E+05	4.33724011E+01	-2.66312810E+05				4

16752-60-6

P4O10 (P2O5)2 SIGMA=12 STATWT=1 IA=IB=IC=143.243 NU=1417,1390(3),1015(3),952(2),764(3),750(3),721,650(2),573(3),470(3),424,329(3),278(2),257(3),170(3)

HF298=-2904.08+/-8.9 kJ REF=JANAF

P4O10	J12/65P	4.0	10.	0.	0.G	300.000	5000.000	B	283.88905	1
		2.89396590E+01	1.24520960E-02	-5.48543200E-06	1.07047430E-09	-7.69568570E-14				2
		-3.60148633E+05	-1.23859447E+02	-4.41428830E+00	1.37590810E-01	-1.92685980E-04				3
		1.32720680E-07	-3.63113780E-11	-3.52629523E+05	4.01782260E+01	-3.49287392E+05				4

16752-60-6

P4O10(s)	J12/65P	4.0	10.	0.	0.S	300.000	1500.000	C	283.88905	1
		-4.33006250E+01	2.15673760E-01	-1.76863440E-04	6.76428520E-08	-9.91087100E-12				2
		-3.53461393E+05	2.26054720E+02	3.95560990E-01	1.13338170E-01	-1.24099820E-04				3
		9.77156010E-08	-3.41078390E-11	-3.66256443E+05	-3.80906970E+00	-3.62020394E+05				4

Table 4 (continued)

7439-92-1

Pb REFERENCE ELEMENT Calculated from Gurvich's 1991 data, solid and liquid.

Pb(cr)	TPIS91PB 1.	0.	0.	0.C	200.000	600.650	B 207.20000	1
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
	0.00000000E+00	0.00000000E+00	3.36014248E+00	-4.31525514E-03	2.10404411E-05			3
	-3.35897357E-08	1.91850988E-11	-9.38593007E+02	-1.07408687E+01	0.00000000E+00			4
Pb(L)	TPIS91PB 1.	0.	0.	0.C	600.650	3600.000	B 207.20000	1
	4.18191355E+00	-9.84150979E-04	3.55339809E-07	-1.75808349E-11	-3.23884419E-15			2
	-7.56065769E+02	-1.51099545E+01	3.40679935E+00	2.03221927E-03	-4.17417470E-06			3
	3.08397022E-09	-8.16531438E-13	-5.92027769E+02	-1.13377955E+01	0.00000000E+00			4

7439-92-1

Pb (gas) HF298=195.2+/-0.8 kJ HF0=195.88 REF=JANAF &amp; Gurvich

Pb	J 3/83PB 1.	0.	0.	0.G	200.000	6000.000	207.20000	1
	4.16342379E+00	-3.49637723E-03	2.28263170E-06	-4.76749242E-10	3.22223800E-14			2
	2.21687499E+04	-2.13525305E+00	2.50229005E+00	-2.44053643E-05	9.17082578E-08			3
	-1.42817771E-10	7.83762196E-14	2.27314919E+04	6.84009322E+00	2.34770299E+04			4

15576-47-3

PbBr Bromyl Lead Calc. From original Tables Gurvitch 1991 with B. McBride's correct. HF298=64.821+/-20. kJ HF0=73.805 kJ {HF298=70.92 kJ REF=JANAF 1973}

Max Lst Sq Error Cp @ 6000 K 0.28%

PbBr	tpis91PB 1.BR 1.	0.	0.G	200.000	6000.000	B 287.10400	1
	4.88335727E+00	-7.86114204E-04	5.80804002E-07	-1.28047000E-10	8.75460006E-15		2
	6.31394151E+03	5.06201066E+00	3.91081467E+00	3.42699379E-03	-7.50571408E-06		3
	7.38045812E-09	-2.65379783E-12	6.53082034E+03	9.77305103E+00	7.79616863E+03		4

10031-22-8

PbBr2 DiBromo Lead SIGMA=2 STATWT=1 IAIBIC=645.E-114 Nu=200,64,189

REF=Gurvich B.McBride's correct. HF298=-103.908+/-7. kJ HF0=-87.54 kJ

{HF298=-104.39 REF=JANAF 1973} Max Lst Sq Error Cp @ 400 K 0.13%.

PbBr2	tpis91PB 1.BR 2.	0.	0.G	200.000	6000.000	B 367.00800	1
	6.94157005E+00	6.21326203E-05	-2.48772114E-08	4.30873672E-12	-2.70637013E-16		2
	-1.45807339E+04	1.25545062E+00	5.86671307E+00	6.50942993E-03	-1.45793024E-05		3
	1.43718900E-08	-5.18586713E-12	-1.44328266E+04	6.01742022E+00	-1.24971962E+04		4

99260-59-0

PbBr3 TriBromo Lead SIGMA=3 STATWT=2 IAIBIC=43.E-112 Nu=210,110,220(2), 90(4) REF=Gurvich 1991 HF298=-104.011+/-80. kJ HF0=-80.330 kJ Max Lst Sq Error Cp @ 400 K 0.19%

PbBr3	tpis91PB 1.BR 3.	0.	0.G	200.000	6000.000	B 446.91200	1
	9.87687123E+00	1.30906478E-04	-5.24079767E-08	9.07642769E-12	-5.70073979E-16		2
	-1.54839306E+04	-1.00395521E+01	7.63531090E+00	1.35414085E-02	-3.02742328E-05		3
	2.98094808E-08	-1.07480912E-11	-1.51742765E+04	-1.01579232E-01	-1.25095715E+04		4

13701-91-2

PbBr4 TetraBromo Lead SIGMA=12 STATWT=1 IAIBIC=14.E-111 Nu=210,55(2), 240(3),70(3) REF=Gurvich 1991 HF298=-182.436+/-80. kJ HF0=-152.397 kJ

{HF298=-456.36 kJ REF=JANAF 1973} Max Lst Sq Error Cp @ 400 K 0.19%

PbBr4	tpis91PB 1.BR 4.	0.	0.G	200.000	6000.000	B 526.81600	1
	1.28293030E+01	1.81406972E-04	-7.26097179E-08	1.25732708E-11	-7.89625085E-16		2
	-2.58086915E+04	-2.17938757E+01	9.79363830E+00	1.82325847E-02	-4.05892151E-05		3
	3.98579771E-08	-1.43451011E-11	-2.53855692E+04	-8.31284551E+00	-2.19418235E+04		4

Table 4 (continued)

13931-84-5

PbCl Chloro Lead Calc. From original Tables Gurvitch 1991 with B. McBride's corrections. HF298=8.819+/-12. kJ HF0=10.493 kJ {HF298=15.06 kJ REF=JANAF 1973} Max Lst Sq Error Cp @ 1200 K 0.22%

PbCL	tpis91PB 1.CL 1.	0.	0.G	200.000	6000.000	B 242.65270	1
	4.77878516E+00-5.76185892E-04	4.16285656E-07-7.78043957E-11	4.41848596E-15				2
	-3.99310196E+02 4.22241249E+00	3.43346577E+00 5.91645117E-03	-1.27643042E-05				3
	1.23644948E-08-4.40460852E-12	-1.35548782E+02 1.05680311E+01	1.06069005E+03				4

7758-95-4

PbCl2 DiChloro Lead SIGMA=2 STATWT=1 IAIBIC=56.E-114 Nu=315,100,300 REF=Gurvich 1991 + McBride's correct. HF298=-175.046+/-5. HF0=-173.5 kJ {HF298=-174.05 kJ REF=JANAF 1973} Max Lst Sq Error Cp @ 400 K 0.23%

PbCL2	tpis91PB 1.CL 2.	0.	0.G	200.000	6000.000	B 278.10540	1
	6.86386584E+00 1.44418948E-04	-5.77475949E-08 9.99307033E-12	-6.27298781E-16				2
	-2.31956081E+04-1.26438369E+00	4.67246881E+00 1.28333505E-02	-2.80322378E-05				3
	2.71928111E-08-9.70648954E-12	-2.28783788E+04 8.53709056E+00	-2.11133874E+04				4

99260-58-9

PbCl3 TriChloro Lead SIGMA=3 STATWT=2 IAIBIC=27.E-113 Nu=320,150,310(2), 140(2) REF=Gurvich 1991 HF298=-177.654+/-80. kJ HF0=-175.268 kJ Max Lst Sq Error Cp @ 400 K 0.30%

PbCL3	tpis91PB 1.CL 3.	0.	0.G	200.000	6000.000	B 313.55810	1
	9.75449943E+00 2.60511450E-04	-1.04184055E-07 1.80305836E-11	-1.13191790E-15				2
	-2.43386827E+04-1.34988839E+01	5.73329673E+00 2.36645015E-02	-5.18850552E-05				3
	5.04554082E-08-1.80404257E-11	-2.37606703E+04 4.46241013E+00	-2.13666839E+04				4

13463-30-4

PbCl4 TetraChloro Lead SIGMA=12 STATWT=1 IAIBIC=8.E-112 Nu=331,90(2), 352(3),103(3) REF=Gurvich 1991 + McBride's correct. HF298=-327.43+/-80. kJ HF0=-325.648 kJ {HF298=-552.41 kJ REF=JANAF 1973} Max Lst Sq Error Cp @ 400 K 0.28%.

PbCL4	tpis91PB 1.CL 4.	0.	0.G	200.000	6000.000	B 349.01080	1
	1.26456229E+01 3.75600343E-04	-1.50109809E-07 2.59670773E-11	-1.62965193E-15				2
	-4.32462623E+04-2.64535498E+01	7.20271123E+00 3.15039589E-02	-6.81959986E-05				3
	6.57680628E-08-2.33832835E-11	-4.24447601E+04-2.02928080E+00	-3.93805963E+04				4

14986-72-2

PbF Fluoro Lead Calc. From original Tables Gurvitch 1991 with B. McBride's corrections. HF298=-98.072+/-10. kJ HF0=-96.853 kJ {HF298=-80.27 kJ REF=JANAF 1973} Max Lst Sq Error Cp @ 1200 K 0.19%

PbF	tpis91PB 1.F 1.	0.	0.G	200.000	6000.000	B 226.19840	1
	4.62469521E+00-3.57182851E-04	2.96708600E-07-5.23626254E-11	2.70488402E-15				2
	-1.33304718E+04 3.63389401E+00	2.78063887E+00 8.11843060E-03	-1.57616127E-05				3
	1.41586145E-08-4.78150801E-12	-1.29673501E+04 1.23847920E+01	-1.18909941E+04				4

7783-46-2

PbF2 DiFluoro Lead SIGMA=2 STATWT=1 IAIBIC=3430. Nu=545,170,520 REF=Gurvich 1991 + McBride's corrections. HF298=-443.427+/-11. kJ HF0=-440.305 kJ {HF298=-435.14 kJ REF=JANAF 1973} Max Lst sq Error Cp @ 700 K 0.17%.

PbF2	tpis91PB 1.F 2.	0.	0.G	200.000	6000.000	B 245.19681	1
	6.64915005E+00 3.68964558E-04	-1.46786420E-07 2.53152951E-11	-1.58542811E-15				2
	-5.54201768E+04-3.14761847E+00	3.09009719E+00 1.82755848E-02	-3.56644939E-05				3
	3.20090682E-08-1.08151983E-11	-5.48084139E+04 1.33318334E+01	-5.33317526E+04				4

Table 4 (continued)

41547-50-6

PbF3 TriFluoro Lead SIGMA=3 STATWT=2 IAIBIC=14000. Nu=550,520(2),240,230(2)  
 HF298=-489.573+/-60. kJ HF0=-485.0 kJ REF=Gurvich 1991. Max Lst Sq Error Cp  
 @ 700 K 0.29%

PbF3	tpis91PB 1.F 3.	0.	0.G	200.000	6000.000	B 264.19521	1
	9.39298592E+00	6.39307274E-04	-2.54559542E-07	4.39277645E-11	-2.75218204E-15		2
	-6.18612634E+04	-1.60342079E+01	2.60791365E+00	3.60809169E-02	-7.27567333E-05		3
	6.68990558E-08	-2.30122438E-11	-6.07414884E+04	1.51122184E+01	-5.88817156E+04		4

7783-59-7

PbF4 TetraFluoro Lead SIGMA=12 STATWT=1 IAIBIC=38000. Nu=590(3),580,180(3),  
 160(2) REF=Gurvich 1991 HF298=-799.925+/-60. kJ HF0=-795.031 kJ  
 {HF298=-1133.45 REF=JANAF 1973} Max Lst Sq Error Cp @ 700 K 0.20%.

PbF4	tpis91PB 1.F 4.	0.	0.G	200.000	6000.000	B 283.19361	1
	1.21140354E+01	9.30014166E-04	-3.69586454E-07	6.36943618E-11	-3.98701941E-15		2
	-1.00086052E+05	-2.99293752E+01	3.78352540E+00	4.20272805E-02	-8.06350471E-05		3
	7.15285812E-08	-2.39701696E-11	-9.86220071E+04	8.82112974E+00	-9.62083363E+04		4

13779-93-6

PbI Lead Iodide Calc. From original Tables Gurvitch 1991 with B. McBride's  
 corrections. HF298=108.904+/-4. kJ HF0=112.033 kJ {HF298=107.74 kJ REF=JANAF  
 1973} Max Lst Sq Error Cp @ 6000 K 0.60%

PbI	tpis91PB 1.I 1.	0.	0.G	200.000	6000.000	B 334.10447	1
	4.77908801E+00	-6.13423042E-04	5.04852546E-07	-1.21025192E-10	8.86739199E-15		2
	1.16616491E+04	6.57802286E+00	4.12154865E+00	2.24055372E-03	-4.90143238E-06		3
	4.84068166E-09	-1.74299193E-12	1.18042403E+04	9.75337209E+00	1.30981049E+04		4

10101-63-0

PbI2 Lead Diiodide SIGMA=2 STATWT=1 IAIBIC=306.E-113 Nu=178,49,177  
 REF=Gurvich 1991 HF298=-10.253+/-5. kJ HF0=-5.434 kJ {HF298=-3.18 kJ  
 REF=JANAF 1973} Max Lst Sq Error Cp @ 400 K 0.11%.

PbI2	tpis91PB 1.I 2.	0.	0.G	200.000	6000.000	B 461.00894	1
	6.95171958E+00	5.13521190E-05	-2.05634944E-08	3.56191178E-12	-2.23741341E-16		2
	-3.31710200E+03	2.76237665E+00	6.05113168E+00	5.47268122E-03	-1.22876373E-05		3
	1.21318468E-08	-4.38217601E-12	-3.19383480E+03	6.74835176E+00	-1.23310093E+03		4

99260-54-5

PbI3 Lead TriIodide SIGMA=3 STATWT=2 IAIBIC=26.E-111 Nu=170(2),160,80,60(2)  
 REF=Gurvich + McBride's correct. HF298=21.755+/-80 kJ HF0=27.35 kJ Max Lst  
 Sq Error Cp @ 400 K 0.12%.

PbI3	tpis91PB 1.I 3.	0.	0.G	200.000	6000.000	B 587.91341	1
	9.92779040E+00	7.68212140E-05	-3.07661461E-08	5.32960773E-12	-3.34797849E-16		2
	-3.60146434E+02	-7.12646213E+00	8.56169127E+00	8.33054851E-03	-1.87515559E-05		3
	1.85434528E-08	-6.70529633E-12	-1.74186170E+02	-1.08625004E+00	2.61655973E+03		4

13779-98-1

PbI4 TeraIodo Lead SIGMA=12 STATWT=1 IAIBIC=86.E-111 Nu=170(3),140,50(3),  
 40(2) REF=Gurvich 1991 HF298=-41.281+/-80. kJ HF0=-35.485 kJ {HF298=-224.47  
 kJ REF=JANAF 1973} Max Lst Sq Error Cp @ 400 K 0.11%.

PbI4	tpis91PB 1.I 4.	0.	0.G	200.000	6000.000	B 714.81788	1
	1.29129326E+01	9.26271909E-05	-3.70961452E-08	6.42613508E-12	-4.03679383E-16		2
	-8.82855657E+03	-1.78594578E+01	1.12667107E+01	1.00373100E-02	-2.25910309E-05		3
	2.23388514E-08	-8.07735499E-12	-8.60441382E+03	-1.05803790E+01	-4.95837506E+03		4

Table 4 (continued)

1317-36-8

PbO Lead Oxide Calc. From original Tables Gurvitch 1991 with B. McBride's corrections. HF298=68.187+/-4.5 kJ HF0=70.385 kJ {HF298=70.29 kJ REF=JANAF 1971} Max Lst Sq Error Cp @ 2400 K 0.27%

PbO	tpis91PB	1.0	1.	0.	0.G	200.000	6000.000	B	223.19940	1
3.74571756E+00	1.33518192E-03	-8.10893018E-07	2.07121667E-10	-1.53836080E-14						2
7.01602960E+03	7.13168301E+00	2.85133114E+00	5.17778949E-03	-6.43570894E-06						3
3.48236131E-09	-6.14028475E-13	7.16496994E+03	1.13376006E+01	8.19496374E+03						4

1309-60-0

PbO2 Lead Dioxide SIGMA=2 STATWT=1 IB=20.2 Nu=695,670,200(2)  
REF=Gurvich 1991 HF298=136.153+/-100. kJ HF0=139.452 kJ Max Lst Sq Error Cp  
1200 K 0.14%.

PbO2	tpis91PB	1.0	2.	0.	0.G	200.000	6000.000	B	239.19880	1
6.94193300E+00	5.82749417E-04	-2.30857663E-07	3.97035999E-11	-2.48173068E-15						2
1.41387466E+04	-8.65827135E+00	2.99335677E+00	1.80665365E-02	-3.11442238E-05						3
2.53517658E-08	-7.93638862E-12	1.49086505E+04	1.01365456E+01	1.63753166E+04						4

1314-87-0

PbS Lead Sulfide Calc. From original Tables Gurvitch 1991 with B. McBride's corrections. HF298=127.945+/-1.5 kJ HF0=129.797 kJ {HF298=131.8 kJ REF=JANAF 1973} Max Lst Sq Error Cp @ 2300 K 0.25%

PbS	tpis91PB	1.S	1.	0.	0.G	200.000	6000.000	B	239.26600	1
3.89380257E+00	1.22928158E-03	-8.24356293E-07	2.27321235E-10	-1.79568342E-14						2
1.42107593E+04	7.78220190E+00	2.94557080E+00	7.91150277E-03	-1.62640747E-05						3
1.52039470E-08	-5.28885362E-12	1.42744762E+04	1.16955085E+01	1.53881964E+04						4

12137-74-5

PbS2 Lead Disulfide SIGMA=2 STATWT=1 IB=58.8 Nu=415,400,110(2)  
REF=Gurvich 1991 HF298=244.049+/-10. kJ HF0=245.722 kJ Max Lst Sq Error Cp  
@ 400 K 0.24%.

PbS2	tpis91PB	1.S	2.	0.	0.G	200.000	6000.000	B	271.33200	1
7.27167091E+00	2.41481526E-04	-9.63891316E-08	1.66603078E-11	-1.04497984E-15						2
2.71195711E+04	-7.22166521E+00	4.14428219E+00	1.75558694E-02	-3.70831339E-05						3
3.51874702E-08	-1.23721092E-11	2.76001912E+04	6.92971803E+00	2.93521813E+04						4

7704-34-9

S(S) REFERENCE ELEMENT DATA from Gurvich 1989 HF298=0. kJ Max Lst Sq Error  
H @ 200 K & 388 K 0.0325%

S(a)	tpis89S	1.	0.	0.	0.C	200.000	368.300	B	32.06600	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00						2
0.00000000E+00	0.00000000E+00	3.71369513E-01	1.53373501E-02	-3.35441107E-05						3
2.89249499E-08	0.00000000E+00	-5.53213850E+02	-1.59624498E+00	0.00000000E+00						4
S(b)	tpis89S	1.	0.	0.	0.C	368.300	388.360	B	32.06600	1
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00						2
0.00000000E+00	0.00000000E+00	2.08033146E+00	2.44137555E-03	0.00000000E+00						3
0.00000000E+00	0.00000000E+00	-6.85306695E+02	-8.60715486E+00	0.00000000E+00						4

7704-34-9

S(liquid) OLD JANAF DATA. For Newer Data from Gurvich 89 See the NASA 9 term  
polynomial database at <http://cea.grc.nasa.gov>

S(L) REF ELEMENT	J	9/77S	10	00	00	0L	388.360	5000.000	A	
32.0660	1									
0.33906200E+01	0.71182514E-03	-0.39087832E-06	0.87327456E-10	-0.68755181E-14						2
-0.63358440E+03	-0.14788307E+02	-0.38449885E+02	0.25707392E+00	-0.55555365E-03						3
0.51325813E-06	-0.17253650E-09	0.42933552E+04	0.16753043E+03	0.00000000E+00						4

Table 4 (continued)

7704-34-9

S HF298=276.98+/-0.25 kJ REF=JANAF

S	J 9/82S	1.	0.	0.	0.G	200.000	6000.000	B	32.06600	1
		2.87936498E+00	-5.11050388E-04	2.53806719E-07	-4.45455458E-11	2.66717362E-15				2
		3.25013791E+04	3.98140647E+00	2.31725616E+00	4.78018342E-03	-1.42082674E-05				3
		1.56569538E-08	-5.96588299E-12	3.25068976E+04	6.06242434E+00	3.33128471E+04				4

14989-32-3

SCL SIGMA=1 T0(STATWT)=0(2),400(2),25000(4) BE=0.2406 WE=536 WEXE=2.08

ALFAE=0.00126 HF298=156.46+/-16.7 kJ REF=JANAF

SCL	J 6/78S	1.CL	1.	0.	0.G	300.000	5000.000	C	67.51870	1
		4.59472600E+00	-5.97717860E-05	4.52264950E-08	-9.37184350E-12	8.07357270E-16				2
		1.74524260E+04	2.37985153E+00	3.70558800E+00	5.27186230E-03	-1.13718200E-05				3
		1.04978270E-08	-3.53184080E-12	1.75611590E+04	6.27945123E+00	1.88189067E+04				4

10545-99-0

SCL2 SIGMA=2 T0(STATWT)=0(1),25810(1),29762(1) IA=5.8026 IB=29.1706

IC=34.9733 NU=528,525,205 HF298=-17.57+/-3.3 kJ REF=JANAF

SCL2	J 6/78S	1.CL	2.	0.	0.G	300.000	5000.000	B	102.97140	1
		6.62714620E+00	4.27470190E-04	-1.88168810E-07	3.57611550E-11	-2.38494000E-15				2
		-4.20002190E+03	-4.23237025E+00	3.59663710E+00	1.43271930E-02	-2.51991970E-05				3
		2.05728820E-08	-6.39769080E-12	-3.63758370E+03	1.00605557E+01	-2.11344531E+03				4

16068-96-5

SF SIGMA=1 T0(STATWT)=0(2),398(2),24991(2),25601(2) BE=0.55427 WE=830

WEXE=4.7 ALFAE=0.0042 HF298=12.97+/-6.3 kJ REF=JANAF

SF	J 6/76S	1.F	1.	0.	0.G	300.000	5000.000	C	51.06440	1
		4.36908850E+00	1.92044240E-04	-6.66303650E-08	1.24485900E-11	-7.65374940E-16				2
		2.20185260E+02	2.07596854E+00	3.42081750E+00	4.55111980E-03	-7.93725640E-06				3
		6.50047110E-09	-2.02896650E-12	3.96095030E+02	6.54700574E+00	1.56005789E+03				4

13814-25-0

SF2 SIGMA=2 STATWT=1 IA=3.1377 IB=9.1367 IC=12.2744 NU=840,809,357

HF298=-296.646+/-16.7 kJ REF=JANAF

SF2	J 6/76S	1.F	2.	0.	0.G	300.000	5000.000	C	70.06281	1
		6.11941960E+00	1.00514240E-03	-4.46533130E-07	8.76240100E-11	-6.32365120E-15				2
		-3.77142410E+04	-4.55717403E+00	2.41030560E+00	1.55901210E-02	-2.31780180E-05				3
		1.65834970E-08	-4.64657610E-12	-3.69163730E+04	1.35066804E+01	-3.56790061E+04				4

30937-38-3

SF3 SIGMA=2 T0(STATWT)=0(2),25000(2) IA=5.8076 IB=17.0895 IC=22.8971

NU=850,725,550,450,350,300 HF298=-503.03+/-33.5 kJ REF=JANAF

SF3	J 6/77S	1.F	3.	0.	0.G	300.000	5000.000	C	89.06121	1
		8.80768970E+00	1.36716760E-03	-6.08083330E-07	1.18830220E-10	-8.44709150E-15				2
		-6.34404940E+04	-1.67648869E+01	1.87777280E+00	3.12340350E-02	-5.15713790E-05				3
		4.02473220E-08	-1.21105940E-11	-6.20679390E+04	1.63694361E+01	-6.05016370E+04				4

7783-60-0

SF4 SIGMA=2 STATWT=1 IA=12.5525 IB=20.5464 IC=26.0707 NU=891.5,867,728,558.4,532.5,475,353,233,228

HF298=-763.162+/-20.9 kJ REF=JANAF

SF4	J 6/76S	1.F	4.	0.	0.G	300.000	5000.000	B	108.05961	1
		1.11243830E+01	2.14579940E-03	-9.54524440E-07	1.87461110E-10	-1.35359530E-14				2
		-9.55816690E+04	-2.88756477E+01	1.28196450E+00	4.35698990E-02	-7.01251680E-05				3
		5.36772440E-08	-1.59143560E-11	-9.35867010E+04	1.84198703E+01	-9.17889260E+04				4

Table 4 (continued)

10546-01-7

SF5 PENTAFLUOROSULFUR SIGMA=4 T0 (STATWT)=0 (2), 10000 (2), 20000 (2), 25000 (2), 30000 (2) IA=30.7102 IB=IC=21.4728 NU=812 (2), 800, 600, 552 (2), 550 (2), 450, 400, 350 (2) HF298=-908.447+/-15.1 kJ REF=JANAF

SF5	J12/77S	1.F	5.	0.	0.G	300.000	5000.000	C	127.05802	1
1.36105630E+01	2.65231300E-03	-1.16914630E-06	2.42451320E-10	-1.83147180E-14						2
-1.14002930E+05	-4.30151012E+01	-1.71476620E+00	6.87160080E-02	-1.14079330E-04						3
8.93363790E-08	-2.69404290E-11	-1.10961780E+05	3.02724678E+01	-1.09262883E+05						4

15607-89-3

SF5Br SIGMA=4 STATWT=1 IA=32.145 IB=IC=71.9835 NU=892 (2), 848, 694, 621, 597, 580 (2), 502, 423 (2), 325, 279, 225 (2) HF298=-972.8+/-59 kJ REF=JANAF

SF5BR	J12/77S	1F	5BR	1	0G	200.000	6000.000	C	206.96202	1
0.16222709E+02	0.28929217E-02	-0.11443577E-05	0.19662531E-09	-0.12282470E-13						2
-0.12263690E+06	-0.54750256E+02	-0.19908752E+01	0.82938683E-01	-0.14215649E-03						3
0.11560301E-06	-0.36238714E-10	-0.11904847E+06	0.32112843E+02	-0.11700028E+06						4

13780-57-9

SF5Cl SIGMA=4 STATWT=1 IA=30.9468 IB=IC=46.3888 NU=909 (2), 855, 707, 625, 602, 579 (2), 505, 441 (2), 402, 332, 287 (2) HF298=-1038.9+/-10.5 kJ REF=JANAF

SF5CL	J12/77S	1F	5CL	1	0G	200.000	6000.000	B	162.51072	1
0.16068448E+02	0.30531997E-02	-0.12076664E-05	0.20749336E-09	-0.12960964E-13						2
-0.13058312E+06	-0.55651991E+02	-0.31561325E+01	0.87699695E-01	-0.15063852E-03						3
0.12275611E-06	-0.38552637E-10	-0.12680072E+06	0.36001021E+02	-0.12495024E+06						4

2551-62-4

SF6 HEXAFLUOROSULFUR SIGMA=24 STATWT=1 IA=IB=IC=30.8679 NU=947.5 (3), 773.1, 641.7 (2), 615.3 (3), 525 (3), 347 (3) HF298=-1220.473 +/-0.8 kJ REF=JANAF

SF6	J 6/76S	1.F	6.	0.	0.G	300.000	5000.000	B	146.05642	1
1.51629500E+01	4.38423180E-03	-1.94863370E-06	3.82471960E-10	-2.76050500E-14						2
-1.52268010E+05	-5.44157194E+01	-3.83880880E+00	8.32217210E-02	-1.31816890E-04						3
9.96361540E-08	-2.92487670E-11	-1.48364770E+05	3.71611426E+01	-1.46791868E+05						4

12033-56-6

SN SIGMA=1 T0 (STATWT)=0 (2), 223 (2) BE=0.7762 WE=1220 WEXE=7.75 ALFAE=0.0064 HF298=263.6+/-105 kJ REF=JANAF

SN	J 6/61S	1.N	1.	0.	0.G	300.000	5000.000	C	46.07274	1
3.84939760E+00	7.27567880E-04	-2.93702030E-07	5.50136280E-11	-3.81235510E-15						2
3.04599620E+04	4.43127355E+00	3.94229710E+00	-2.00355150E-03	7.35346440E-06						3
-7.51685600E-09	2.55910980E-12	3.05639490E+04	4.58030805E+00	3.17016142E+04						4

13827-32-2

SO	T0 (STATWT)=0 (3)	BE=0.72082	WE=1148.19	WEXE=6.12	ALFAE=0.00574
T0 (STATWT)=6350 (2)	BE=0.7119	WE=1148.19	WEXE=6.12	ALFAE=0.00574	
T0 (STATWT)=10510 (1)	BE=0.70261	WE=1067.66	WEXE=7.8	ALFAE=0.00635	
T0 (STATWT)=38292 (2)	BE=0.6067	WE=415.2	WEXE=1.6	ALFAE=0.0194	
T0 (STATWT)=38455 (2)	BE=0.6107	WE=413.3	WEXE=1.6	ALFAE=0.0194	
T0 (STATWT)=38616 (2)	BE=0.6164	WE=412.7	WEXE=1.7	ALFAE=0.0204	
T0 (STATWT)=41629 (3)	BE=0.502	WE=630.4	WEXE=4.8	ALFAE=0.0062	
T0 (STATWT)=42200 (6)	BE=0.5	WE=170	WEXE=0	ALFAE=0	

HF298=5.01+/-1.3 kJ REF=JANAF

SO	J 6/77S	1.O	1.	0.	0.G	300.000	5000.000	A	48.06540	1
4.01428730E+00	2.70228170E-04	8.28966670E-08	-3.43237410E-11	3.11214440E-15						2
-7.10519560E+02	3.49973505E+00	3.14902330E+00	1.18393470E-03	2.57406860E-06						3
-4.44434190E-09	1.87351590E-12	-4.04075710E+02	8.31987915E+00	6.02271219E+02						4

Table 4 (continued)

7783-42-8  
 SOF2 THYONYL FLUORIDE SIGMA=1 STATWT=1 IA=9.7369 IB=10.0399 IC=16.9332  
 NU=1330,808.2,747,530.4,392.5,377.8 HF298=-543.92+/-105 kJ REF=JANAF  
 SOF2 J 6/72S 1.0 1.F 2. 0.G 300.000 5000.000 B 86.06221 1  
 8.08742120E+00 2.10957160E-03-9.08669120E-07 1.73448340E-10-1.22141580E-14 2  
 -6.82381590E+04-1.38555915E+01 2.47490660E+00 2.09524260E-02-2.41642770E-05 3  
 1.21203770E-08-1.93387310E-12-6.68976020E+04 1.41973405E+01-6.54188894E+04 4

7446-09-5  
 SO2 O-S-O SIGMA=2 STATWT=1 IA=1.38 IB=8.131 IC=9.534  
 NU=1361.76,1151.38,517.69 HF298=-296.842+/-0.21 kJ REF=JANAF  
 SO2 J 6/61S 1.0 2. 0. 0.G 300.000 5000.000 B 64.06480 1  
 5.24513640E+00 1.97042040E-03-8.03757690E-07 1.51499690E-10-1.05580040E-14 2  
 -3.75582270E+04-1.07404892E+00 3.26653380E+00 5.32379020E-03 6.84375520E-07 3  
 -5.28100470E-09 2.55904540E-12-3.69081480E+04 9.66465108E+00-3.57007867E+04 4

13637-84-8  
 SO2ClF SULFURYL CHLORIDE FLUORIDE SIGMA=1 STATWT=1 IA=16.4743 IB=29.0842  
 IC=29.3031 NU=1467,1228,824,629,510,474,423,308,300 HF298=-556.5+/-21 kJ  
 REF=JANAF  
 SO2ClF J 6/71S 1.0 2.CL 1.F 1.G 300.000 5000.000 B 118.51590 1  
 1.01182860E+01 3.14889940E-03-1.34715140E-06 2.55803100E-10-1.79382560E-14 2  
 -7.05092910E+04-2.31278508E+01 2.98175280E+00 2.64491670E-02-2.92001820E-05 3  
 1.39576110E-08-2.03044870E-12-6.87614970E+04 1.27316812E+01-6.69282620E+04 4

7791-25-5  
 SO2Cl2 SULFURYL CHLORIDE SIGMA=2 STATWT=1 IA=24.052 IB=36.0706 IC=43.8672  
 NU=1434,1205,586,577,406,388,363,209,208 HF298=-354.80+/-2.1 kJ REF=JANAF  
 SO2Cl2 J 6/71S 1.0 2.CL 2. 0.G 300.000 5000.000 B 134.97020 1  
 1.05509370E+01 2.67343010E-03-1.14282300E-06 2.16862000E-10-1.51991510E-14 2  
 -4.62950560E+04-2.43078570E+01 4.38516770E+00 2.32121570E-02-2.65321120E-05 3  
 1.34999230E-08-2.28192810E-12-4.48029740E+04 6.57867880E+00-4.26726368E+04 4

2699-79-8  
 SO2F2 SULFURYL FLUORIDE SIGMA=2 STATWT=1 IA=16.3467 IB=16.5727 IC=16.5756  
 NU=1502,1269,885,848,553,544,539,388,384 HF298=-758.559+/-8.4 kJ REF=JANAF  
 SO2F2 J 6/71S 1.0 2.F 2. 0.G 300.000 5000.000 B 102.06161 1  
 9.60788850E+00 3.71110260E-03-1.58991140E-06 3.02324640E-10-2.12285770E-14 2  
 -9.47547680E+04-2.28489419E+01 1.73246800E+00 2.85017600E-02-2.94537980E-05 3  
 1.24013000E-08-1.17155330E-12-9.27813930E+04 1.69484101E+01-9.12343116E+04 4

7446-11-9  
 SO3 SIGMA=6 STATWT=1 IA=IB=8.1493 IC=16.2987 NU=1391,1068,529,495  
 HF298=-395.765+/-0.71 kJ REF=JANAF  
 SO3 J 9/65S 1.0 3. 0. 0.G 300.000 5000.000 B 80.06420 1  
 7.07573760E+00 3.17633870E-03-1.35357600E-06 2.56309120E-10-1.79360440E-14 2  
 -5.02113760E+04-1.11875176E+01 2.57803850E+00 1.45563350E-02-9.17641730E-06 3  
 -7.92030220E-10 1.97094730E-12-4.89317530E+04 1.22651384E+01-4.75978348E+04 4



Table 4 (continued)

23550-45-0  
S2 T0 (STATWT)=0 (3) BE=0.2946 WE=724.67 WEXE=2.836 ALFAE=0.00157 DE=2.134E-7  
T0 (STATWT)=4700 (2) BE=0.2923 WE=702.35 WEXE=3.09 ALFAE=0.0017 DE=2.04E-7  
T0 (STATWT)=8500 (1) BE=0.29 WE=700.87 WEXE=3.47 ALFAE=0.0016 DE=2.0E-7  
T0 (STATWT)=21855 (6) BE=0.2284 WE=488.6 WEXE=2.63 ALFAE=0.0014 DE=1.996E-7  
HF298=128.60+/-0.3 kJ REF=JANAF  
S2 J 9/77S 2. 0. 0. 0.G 300.000 5000.000 A 64.13200 1  
3.98860690E+00 5.57750510E-04-5.01892780E-08-1.54703190E-11 2.66617710E-15 2  
1.41980150E+04 4.49119159E+00 2.85857540E+00 5.17583550E-03-6.54934340E-06 3  
3.39986430E-09-4.01567660E-13 1.44124020E+04 9.89127849E+00 1.54434020E+04 4

39594-91-7  
S2C1 (S-S-Cl) SIGMA=1 T0 (STATWT)=0 (2), 23000 (2), 26000 (2), 30000 (2) IA=5.0613  
IB=26.8624 IC=31.9237 NU=550,500,200 HF298=78.6+/-8.4 kJ REF=JANAF  
S2CL J 6/78S 2.CL 1. 0. 0.G 300.000 5000.000 C 99.58470 1  
6.62294250E+00 4.37477870E-04-1.94304060E-07 3.66970150E-11-2.30912150E-15 2  
7.36474510E+03-2.94188157E+00 3.62917020E+00 1.41777000E-02-2.49191780E-05 3  
2.03331190E-08-6.32030790E-12 7.91952490E+03 1.11746042E+01 9.44875520E+03 4

10025-67-9  
S2C12 (Cl-S-S-Cl) SIGMA=2 IA=68.8282 IB=60.6645 IC=15.2331 IR=5.487  
ROTATION BARRIER V0=8387. V2=-3917. V3=-490. cm-1 HF298=-4.0 kcal REF=JANAF  
S2CL2 L 4/93S 2.CL 2. 0. 0.G 200.000 6000.000 B 135.03740 1  
9.46841020E+00 1.12186352E-03-6.92784280E-07 1.38654463E-10-9.29397839E-15 2  
-5.05019524E+03-1.52950441E+01 3.47905708E+00 3.25370028E-02-6.63904620E-05 3  
6.21124845E-08-2.17112325E-11-4.02225567E+03 1.22791824E+01-2.01286666E+03 4

101947-30-2  
S2F2 THIOTHIONYL FLUORIDE S-S-F2 SIGMA=1 T0 (STATWT)=0 (1), 34000 (1)  
IA=10.2965 IB=21.0146 IC=27.5332 NU=760.5, 718.5, 692.3, 411.2, 330, 274  
HF298=-401.413+/-41.8 kJ REF=JANAF  
S2F2 (SSF2) J 6/76S 2.F 2. 0. 0.G 300.000 5000.000 B 102.11681 1  
8.82958920E+00 1.34072340E-03-5.96153210E-07 1.16854000E-10-8.40610860E-15 2  
-5.12234920E+04-1.60942430E+01 1.92539690E+00 3.10520790E-02-5.11986690E-05 3  
3.98812160E-08-1.19774150E-11-4.98547610E+04 1.69255960E+01-4.82791800E+04 4

13709-35-8  
S2F2 FLUORODISULFANE FS-SF IA=7.3579 IB=30.4921 IC=32.6808 NU=717,680.8,  
614.6,319.8,301,182.5 HF298=-336.435+/-41.6 kJ REF=JANAF  
FS2F J 6/76F 2.S 2. 0. 0.G 300.000 5000.000 B 102.11681 1  
9.03087760E+00 1.11307760E-03-4.96295140E-07 9.76154130E-11-7.05574520E-15 2  
-4.34215640E+04-1.69373960E+01 2.84494960E+00 2.82028400E-02-4.73576220E-05 3  
3.73947520E-08-1.13467000E-11-4.22164310E+04 1.25369140E+01-4.04641320E+04 4

5714-22-7  
S2F10 SIGMA=8 STATWT=1 IA=61.4204 IB=IC=119.3402 IR=15.354 INT ROT BARRIER  
V=8.0 kcal NU=938,913,860 (2), 826 (2), 728 (2), 690,684,642,634 (2), 624 (2), 571,  
544 (2), 509 (2), 425 (2), 410 (2), 247,188 (2), 150 (2) HF298=-2064.386+/-29.3 kJ  
REF=JANAF  
S2F10 J12/77S 2F 10 0 0G 200.000 6000.000 B 254.11603 1  
0.28671327E+02 0.57615941E-02-0.24727206E-05 0.44061086E-09-0.28058011E-13 2  
-0.25862467E+06-0.12091379E+03-0.67788927E+01 0.15100498E+00-0.24103120E-03 3  
0.18355215E-06-0.54374282E-10-0.25118529E+06 0.50552882E+02-0.24828715E+06 4

Table 4 (continued)

20901-21-7										
S2O	S-S-O	SIGMA=1	STATWT=1	IA=2.0209	IB=16.6326	IC=18.6536	NU=1165,			
679,388	HF298=-56.48+/-33.5 kJ	REF=JANAF								
S2O	J 9/65S	2.0	1.	0.	0.G	300.000	5000.000	B	80.13140	1
5.90375240E+00	1.23699750E-03	-5.45707900E-07	1.06598420E-10	-7.66882430E-15						2
-8.77520900E+03	-2.26999836E+00	2.84142570E+00	1.21884100E-02	-1.60002410E-05						3
1.03092890E-08	-2.64491200E-12	-8.06030150E+03	1.29180736E+01	-6.79363039E+03						4
10544-50-0										
S8	SIGMA=8	STATWT=1	IA=IB=1.28594	IC=2.36042	NU=475(3),471(2),437(2),411,					
248(2),243,218,191(2),152(2),56(2)	HF298=100.42+/-0.63 kJ	REF=JANAF								
S8	J 9/77S	8.	0.	0.	0.G	200.000	6000.000	B	256.52800	1
2.07249521E+01	1.34686111E-03	-5.37225946E-07	9.28122853E-11	-5.81951340E-15						2
5.53344324E+03	-6.74805287E+01	4.19700496E+00	9.15503597E-02	-1.91263611E-04						3
1.80177196E-07	-6.30393695E-11	8.12071691E+03	7.58043917E+00	1.20776811E+04						4
7440-21-3										
Si	Silicon	REFERENCE ELEMENT	HF298=0. kJ	REF=Gurvich 1991						
Si(cr)	RUS 91SI	1.	0.	0.	0.S	200.000	1690.000	B	28.08550	1
1.75547382E+00	3.17285497E-03	-2.78236402E-06	1.26458065E-09	-2.17128464E-13						2
-6.28657363E+02	-8.55341177E+00	-1.29176912E-01	1.47203139E-02	-2.76510160E-05						3
2.41878251E-08	-7.93452912E-12	-4.15516417E+02	-3.59570008E-01	0.00000000E+00						4
Si(L)	RUS 91SI	1.	0.	0.	0.L	1690.000	6000.000	B	28.08550	1
3.27138941E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00						2
4.88286795E+03	-1.32665477E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00						3
0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00						4
409-21-2										
SiC	Silicon Carbide	REF=JANAF								
SiC(b)	J 3/67SI	1.C	1.	0.	0.S	300.000	4000.000	B	40.09650	1
3.79748090E+00	3.18728860E-03	-1.45023340E-06	3.15497440E-10	-2.61589910E-14						2
-1.02919370E+04	-2.10677910E+01	-2.47159070E+00	3.06937830E-02	-4.92630850E-05						3
3.86263890E-08	-1.17616210E-11	-9.06912600E+03	8.80092140E+00	-8.80624423E+03						4
19165-34-5										
SiCL3	Trichlorosilyl Radical	SIGMA=3	STATWT=2	IA=IB=33.7539	IC=64.6554					
Nu=582(2),470,254,176(2)	REF=JANAF 1977	HF298=-317.98+/-6.6 kJ	REF=Ho & Melius							
JPC 94,(1990),5120	{HF298=-390.37 kJ	REF=JANAF 1977}	Updated old polynomial.							
SiCL3	TT8/03SI	1.CL	3.	0.	0.G	300.000	5000.000	B	134.44360	1
9.35946310E+00	7.38348380E-04	-3.29940490E-07	6.49899730E-11	-4.70232410E-15						2
-4.12236020E+04	-1.56480110E+01	4.26270270E+00	2.40508690E-02	-4.21848820E-05						3
3.43739300E-08	-1.06744620E-11	-4.02747388E+04	8.40523855E+00	-3.824444593E+04						4
10026-04-7										
SiCL4	TetraChloroSilane	SIGMA=12	STATWT=1	IA=IB=IC=63.8879	Nu=620(3),435,					
220(3),149(2)	HF298=-662.75+/-4.2 kJ	HF0=-660.57 kJ	REF=JANAF 1970;	Reference						
compound taken by Ho & Melius	JPC 94 (1990),5123									
SiCL4	J12/70SI	1.CL	4.	0.	0.G	300.000	5000.000	B	169.89630	1
1.20896550E+01	1.01907350E-03	-4.41678650E-07	8.44815730E-11	-5.94915800E-15						2
-8.35902500E+04	-2.99269336E+01	6.10400100E+00	2.49331140E-02	-3.67032630E-05						3
2.44487480E-08	-6.03701550E-12	-8.23592730E+04	-9.76400498E-01	-7.97099719E+04						4

Table 4 (continued)

13966-66-0

SiF2 Difluorosilicon SIGMA=2 STATWT=1 IA=2.8256083 IB=9.3347931  
 IC=12.160355 Nu=343,843,855 REF=JACOX HF298=-149.86+/-4. kcal HF0=149.67  
 kcal REF=Ho & Melius JPC 94, (1990), 5120 Max Lst Sq Error Cp @ 6000 K 0.17%  
 SiF2 T 8/03SI 1.F 2. 0. 0.G 200.000 6000.000 B 66.08231 1  
 6.19390519E+00 8.33925041E-04-3.28508545E-07 5.62901775E-11-3.50955198E-15 2  
 -7.74832375E+04-5.09916171E+00 2.97179653E+00 1.12488760E-02-1.21015308E-05 3  
 4.86338012E-09-2.30419482E-13-7.67006540E+04 1.10843008E+01-7.54120495E+04 4

14835-14-4

SiF3 Trifluorosilicon Radical SIGMA=3 STATWT=2 IA=IB=11.219989 IC=20.422257  
 Nu=290(2), 406,834,954(2) REF=Jacox Webbook 2003 HF298=-237.42+/-1.9 kcal  
 HF0=-236.73 kcal REF=Ho & Melius JPC 94, (1990), 5120 Max Lst Sq Error Cp @  
 1300 K 0.22%  
 SiF3 T 8/03SI 1.F 3. 0. 0.G 200.000 6000.000 B 85.08071 1  
 8.53373721E+00 1.51373466E-03-5.95570184E-07 1.01971950E-10-6.35433845E-15 2  
 -1.22404807E+05-1.58446010E+01 2.73118713E+00 2.17689381E-02-2.75719554E-05 3  
 1.60951524E-08-3.47580296E-12-1.21042135E+05 1.30072861E+01-1.19473701E+05 4

7783-61-1

SiF4 Tetrafluorosilicon SIGMA=12 STATWT=1 IA=IB=IC=20.395102 Nu=268(2),  
 389(3), 800,1032(3). REF=Shimanouchi (Webbook) HF298=-385.99+/-1 kcal  
 HF0=-384.78 kcal REF=Ho & Melius JPC 94, (1990), 5120 Max Lst Sq Error Cp @  
 1300 K 0.27%  
 SiF4 T 8/03SI 1.F 4. 0. 0.G 200.000 6000.000 B 104.07911 1  
 1.07428193E+01 2.32397079E-03-9.12894519E-07 1.56145418E-10-9.72346468E-15 2  
 -1.98002728E+05-2.89723090E+01 2.32194412E+00 3.25987937E-02-4.37937019E-05 3  
 2.84077065E-08-7.23442490E-12-1.96043612E+05 1.27516051E+01-1.94236601E+05 4

10025-78-2

SiHCL3 Trichlorosilane SIGMA=3 STATWT=1 IA=IB=34.3279 IC=64.4220 Nu=2261,  
 811(2), 600(2), 499,254,176(2) HF298=-490.11+/-4.2 kJ REF=Ho & Melius JPC 94,  
 (1990), 5120 {HF298=496.22 kJ REF=JANAF 1976} Corrected Old Polynomial  
 SiHCL3 TT8/03SI 1.H 1.CL 3. 0.G 300.000 5000.000 B 135.45154 1  
 9.93356350E+00 3.24812200E-03-1.37871710E-06 2.62660730E-10-1.85748860E-14 2  
 -5.69608490E+04-2.04720585E+01 2.67420420E+00 3.43803850E-02-5.49538560E-05 3  
 4.31033320E-08-1.31570120E-11-5.54917230E+04 1.43335095E+01-5.89467880E+04 4

13465-71-9

SiHF3 Trifluorosilane SIGMA=3 STATWT=1 IA=IB=11.689916 IC=20.337374  
 Nu=306(2), 425,844(2), 858,998(2), 2316 REF=Shimanouchi (Webbook) HF298=-288.64  
 +/-1.3 kcal HF0=286.96 kcal REF=Ho & Melius JPC 94, (1990), 5120 Max Lst Sq  
 Error Cp @ 1300 K 0.34%  
 SiHF3 T 8/03SI 1.F 3.H 1. 0.G 200.000 6000.000 B 86.08865 1  
 9.16502323E+00 3.75614479E-03-1.43309291E-06 2.40660850E-10-1.48026591E-14 2  
 -1.48632262E+05-2.10748370E+01 1.96239441E+00 2.53209108E-02-2.32513149E-05 3  
 6.98460431E-09 6.97338685E-13-1.46767690E+05 1.55974888E+01-1.45248458E+05 4

13765-44-1

SiH3 Silyl Radical SIGMA=3 STATWT=2 IAIBIC=0.36E-117 Nu=1999(2), 1995,996,  
 925(2) REF=Gurvich 1979 HF298=198.45+/-4.2 kJ REF=Ho & Melius JPC 94(1990), 5120  
 {HF298=209.38 kJ REF=Gurvich} Corrected Old Polynomial  
 SiH3 TT8/03SI 1.H 3. 0. 0.G 298.150 5000.000 B 31.10932 1  
 4.12703760E+00 6.18388660E-03-2.61220960E-06 4.95796950E-10-3.49605200E-14 2  
 1.24968010E+04 1.51808423E-01 3.05068070E+00 3.31032830E-03 1.10939970E-05 3  
 -1.44834900E-08 5.18803540E-12 1.31414240E+04 7.29482068E+00 2.38675610E+04 4

Table 4 (continued)

7803-62-5

SiH<sub>4</sub> Silane SIGMA=12 STATWT=1 IA=IB=IC=0.9784 Nu=2189(3),2187,972(2),913(3)  
 HF298=34.31+/-2. kJ HF0=43.92 kJ REF=JANAF 1976 {HF298=34.27 kJ REF=Ho& Melius  
 JPC 94, (1990), 5120}

SiH<sub>4</sub> J 6/76SI 1.H 4. 0. 0.G 300.000 5000.000 B 32.11726 1  
 4.20920380E+00 9.08226280E-03-3.79053960E-06 7.13698880E-10-5.00462860E-14 2  
 2.13446270E+03-2.72768704E+00 1.59226390E+00 1.28410930E-02-1.94562780E-06 3  
 -4.31063720E-09 1.98748800E-12 3.10559420E+03 1.18336025E+01 4.12630413E+03 4

7631-86-9

SiO<sub>2</sub> Quarz REF=JANAF HF298(S)=-910.857 +/- 1.7 kJ

SiO<sub>2</sub>(Lqz) J 6/67SI 1.O 2. 0. 0.S 200.000 847.000 B 60.08430 1  
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2  
 0.00000000E+00 0.00000000E+00-7.58511380E-01 3.05773989E-02-4.00861855E-05 3  
 2.16194849E-08-6.17249042E-13-1.10371483E+05 1.78384529E+00-1.09550292E+05 4  
 SiO<sub>2</sub>(hqz) J 6/67SI 1.O 2. 0. 0.S 847.000 1696.000 B 60.08430 1  
 7.23537106E+00 7.61842227E-04 4.89502294E-07-2.35754591E-10 4.20839131E-14 2  
 -1.11823834E+05-3.69642796E+01 7.11787621E+00 1.13819527E-03 3.69734234E-08 3  
 0.00000000E+00 0.00000000E+00-1.11794194E+05-3.63708064E+01-1.09550292E+05 4  
 SiO<sub>2</sub>(L) J 6/67SI 1.O 2. 0. 0.L 1696.000 6000.000 B 60.08430 1  
 1.03160657E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2  
 -1.14600563E+05-5.76266603E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 3  
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00-1.09550292E+05 4

13759-10-9

SiS<sub>2</sub> Silicon Disulfide Data from Barin Database 1989 HF298(S)=-213.384 kJ.

SiS<sub>2</sub> Solid B /89SI 1.S 2. 0. 0.S 298.150 1363.000 C 92.21750 1  
 8.40271418E+00 3.13408157E-03-2.30381538E-06 1.32114291E-09-2.82789755E-13 2  
 -2.82649031E+04-3.89938340E+01 8.91436638E+00 1.35634414E-03 2.22767520E-09 3  
 -3.02264623E-12 1.41797358E-15-2.83821677E+04-4.15331497E+01-2.56640500E+04 4  
 SiS<sub>2</sub> Liquid B /89SI 1.S 2. 0. 0.L 1363.000 1500.000 C 92.21750 1  
 1.20789350E+01-2.42499074E-06 8.45243131E-10 0.00000000E+00 0.00000000E+00 2  
 -3.04270857E+04-6.17829516E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 3  
 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00-2.56640500E+04 4

12033-76-0

Si<sub>2</sub>N<sub>2</sub>O Silicon Oxynitride REF=Fegley Comm. Am. Ceram. Soc. 1981 C124-C126  
 HF298(S)=-947.71 kJ

Si<sub>2</sub>N<sub>2</sub>O(s) L 1/84SI 2.N 2.O 1. 0.S 298.150 2500.000 B 100.18388 1  
 1.18490230E+01 2.42446810E-03 3.65292350E-07-4.25788290E-10 8.62759300E-14 2  
 -1.18214940E+05-6.42500920E+01-4.12268540E+00 5.41728140E-02-4.23929300E-05 3  
 -1.07245950E-08 1.73668580E-11-1.14746000E+05 1.48221580E+01-1.13982840E+05 4

12033-89-5

Si<sub>3</sub>N<sub>4</sub> Silicon Nitride REF=JANAF HF298(S)=-744.752 +/- 29.3 kJ

Si<sub>3</sub>N<sub>4</sub>(a) J 3/67SI 3.N 4. 0. 0.S 300.000 3000.000 B 140.28346 1  
 2.79817450E+00 2.79750180E-02-1.50205780E-05 3.58722880E-09-3.17769690E-13 2  
 -9.10172410E+04-8.92688190E+00 7.16356800E+00 1.90071110E-02-1.14693330E-05 3  
 7.06659150E-09-2.74586400E-12-9.24666510E+04-3.24424310E+01-8.95746895E+04 4

Table 4 (continued)

7646-78-8

SnCl<sub>4</sub> Tetrachlorostanum SIGMA=12 STATWT=1 IA=IB=IC=82.3568 Nu=104(2),134(3),  
366,403(3) REF(Vib)=Shimanouchi. HF298=-114.4+/-1 kcal REF=Allendorf & Melius  
JPC 109,(2005),4939. {HF298=114.36 kcal REF=Gurvich 91} Max Lst Sq Error Cp @  
400 K 0.31%.

SnCl <sub>4</sub>	A 6/05SN 1.CL 4.	0.	0.G	200.000	6000.000	B 260.52080	1
	1.25468107E+01	4.79645391E-04	-1.91534394E-07	3.31148945E-11	-2.07745631E-15		2
	-6.14347051E+04	-2.80448484E+01	6.07625961E+00	3.67563794E-02	-7.83942220E-05		3
	7.48718751E-08	-2.64443330E-11	-6.04561975E+04	1.14105530E+00	-5.75679866E+04		4

13765-46-3

SnH<sub>3</sub> Trihydrostanum Radical SIGMA=3 STATWT=2 IA=IB=0.82007 IC=1.318462  
Nu=628.2,688.2(2),1758,1770.2(2) HF298=61.7+/-1 kcal/mol REF=Allendorf & Melius  
JPC A 109,(2005),4939 Max Lst Sq Error Cp @ 1300 K 0.57%.

SnH <sub>3</sub>	A 6/03SN 1.H 3.	0.	0.G	200.000	6000.000	B 121.73382	1
	5.74268626E+00	4.17438755E-03	-1.59271756E-06	2.67398805E-10	-1.64420757E-14		2
	2.88099739E+04	-5.79999417E+00	2.51665233E+00	1.19692102E-02	-8.98742665E-06		3
	4.28077808E-09	-1.20390097E-12	2.98376466E+04	1.13462623E+01	3.10484683E+04		4

2406-52-2

SnH<sub>4</sub> Tetrahydrostanum SIGMA=12 STATWT=1 IA=IB=IC=1.30953 Nu=677.4(3),  
730(2),1797(3),1811 HF298=38.9+/-1 kcal REF=Allendorf & Melius JPC A 109,  
(2005),4939 {HF298=39.0 +/-0.5 kcal REF=Wagman (CODATA) max Lst Sq Error Cp  
@ 1300 K 0.62%.

SnH <sub>4</sub>	A 6/05SN 1.H 4.	0.	0.G	200.000	6000.000	B 122.74176	1
	6.87731163E+00	6.00435553E-03	-2.29126546E-06	3.84721086E-10	-2.36582342E-14		2
	1.67360992E+04	-1.45555411E+01	1.45448972E+00	1.97331667E-02	-1.50202098E-05		3
	5.71807525E-09	-9.34057366E-13	1.83862382E+04	1.39894617E+01	1.95751283E+04		4

7440-63-3

Xe HF298=0.0 REF=C.E. Moore "Atomic Energy Levels" NSRDS-NBS 34 and NSRDS-  
NBS 35 1970. Max Lst Sq Error Cp = 0.00% @ 1000 K

Xe REF ELEMENT	G 8/02XE 1.	0.	0.	0.G	200.000	6000.000	B 131.29300	1
	2.50024132E+00	-4.69629643E-07	2.96003016E-10	-7.40582264E-14	6.36893090E-18		2	
	-7.45462928E+02	6.16312017E+00	2.50000000E+00	0.00000000E+00	0.00000000E+00		3	
	0.00000000E+00	0.00000000E+00	-7.45375000E+02	6.16444240E+00	0.00000000E+00		4	

24203-25-6

Xe+ HF298=1176.552 kJ HF298=1170.355 kJ REF=Moore NSRDS-NBS 35 1971; Gordon  
NASA/TP 1999-208523 {HF298=1176.543+/-5.9E-3 kJ REF=ATcT A} Max Lst Sq Error  
Cp @ 1300 K 0.17%.

Xe+	g 3/97XE 1.E -1.	0.	0.G	298.150	6000.000	A 131.28945	1
	2.59103639E+00	-1.66257715E-04	8.73848934E-08	-1.27035729E-11	5.69694480E-16		2
	1.40726554E+05	7.04851028E+00	2.50007882E+00	-6.54502970E-07	1.93487417E-09		3
	-2.42814950E-12	1.09865650E-15	1.40760519E+05	7.55038739E+00	1.41505901E+05		4

7440-66-6

Zn REFERENCE ELEMENT From Original Values REF=Cox et al CODATA 1989 p.221  
Max Lst sq Error Cp @ 200 K 0.07 %

Zn(cr) REF ELEMENT	coda89ZN 1.	0.	0.	0.S	200.000	692.730	B 65.39000	1
	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2	
	0.00000000E+00	0.00000000E+00	1.85068929E+00	9.17791410E-03	-2.61047009E-05		3	
	3.38568767E-08	-1.39430709E-11	-7.89403133E+02	-7.38526333E+00	0.00000000E+00		4	
Zn(L)	coda89ZN 1.	0.	0.	0.L	692.730	6000.000	B 65.39000	1
	3.77653043E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2	
	-4.31695298E+02	-1.56708437E+01	3.77653043E+00	0.00000000E+00	0.00000000E+00		3	
	0.00000000E+00	0.00000000E+00	-4.31695298E+02	-1.56708437E+01	0.00000000E+00		4	

Table 4 (continued)

7646-85-7

ZnCl<sub>2</sub>(G) Zinc Chloride Calculated by Ichsan Barin to 2000 K and extrapolated using Wilhoit's polynomials to 5000 K HF298=-256.684 kJ Max Lst Sq Error Cp @ 900 K 0.65% @ 1900 K 0.37%.

ZnCl <sub>2</sub>	T 2/03ZN 1.CL 2.	0.	0.G	298.150	5000.000	C 136.29540	1
	7.61145422E+00-3.15964547E-04	2.06215336E-07-5.29364361E-11	4.50903014E-15				2
	-3.43210793E+04-1.02719919E+01	3.85545098E+00 1.83777322E-02-3.71779377E-05					3
	3.42343110E-08-1.18362789E-11-3.36541943E+04	7.20305359E+00-3.19542583E+04					4

7733-02-0

ZnSO<sub>4</sub> Zinc Sulfate (S) From Original Values REF=JANAF 1979

HF298(S)=-234.26+/-0.25 kcal Max Lst Sq Error Cp @ 700 K 0.008%

ZnSO <sub>4</sub> (a)	j 3/79ZN 1.S 1.O 4.	0.S	200.000	540.000	B 161.45360	1
	0.00000000E+00 0.00000000E+00 0.00000000E+00	0.00000000E+00 0.00000000E+00				2
	0.00000000E+00 0.00000000E+00-1.38344657E+00	8.73784284E-02-2.28793506E-04				3
	3.46079600E-07-2.01391250E-10-1.19922252E+05	2.63494711E+00-1.17883536E+05				4
ZnSO <sub>4</sub> (a')	j 3/79ZN 1.S 1.O 4.	0.S	540.000	1013.000	B 161.45360	1
	1.59277011E+01 1.15160104E-03 0.00000000E+00	0.00000000E+00 0.00000000E+00				2
	-1.22619432E+05-7.81072009E+01 1.60863189E+01-1.48907178E-04	2.09558771E-06				3
	-1.11418108E-09 1.60483859E-13-1.22579876E+05-7.86189063E+01-1.17883536E+05					4
ZnSO <sub>4</sub> (b)	j 3/79ZN 1.S 1.O 4.	0.S	1013.000	6000.000	B 161.45360	1
	1.74616183E+01 0.00000000E+00 0.00000000E+00	0.00000000E+00 0.00000000E+00				2
	-1.21136788E+05-8.51421182E+01 0.00000000E+00	0.00000000E+00 0.00000000E+00				3
	0.00000000E+00 0.00000000E+00 0.00000000E+00	0.00000000E+00-1.17883536E+05				4

Throughout this table kJ/mol and kcal/mol were abbreviated to kJ and kcal.

##!## - This CAS number was assigned to the species first described in the A. Burcat paper cited as REF.



Table 5  
Third Millennium Thermodynamic Database of New NASA Polynomials  
with Active Thermochemical Tables updates.

DEDICATED TO THE MEMORY OF THE LATE Sanford Gordon, (1920-2001) OF NASA LEWIS  
IN CLEVELAND WHO INVESTIGATED AND DESIGNED THE NASA POLYNOMIALS;

AND THE MEMORY OF THE LATE Bonnie J. McBride, (1934-2005) OF NASA LEWIS WHO  
WROTE THE CEA AND PAC PROGRAMS, COMPILED AND MAINTAINED THE NASA  
THERMOCHEMICAL DATABASES FOR 45 YEARS

MAY THEY REST IN PEACE

Database Authors: Alexander Burcat and Branko Ruscic  
The Database was last updated on September 2005  
Discard Previous Versions

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For quotation write

Alexander Burcat and Branko Ruscic New NASA Thermodynamic Polynomials Database  
With Active Thermochemical Tables updates.

<ftp://ftp.technion.ac.il/pub/supported/aetdd/thermodynamics>; quote date.

mirrored at <http://garfield.chem.elte.hu/Burcat/burcat.html>; quote date.

FOR REFERENCIAL DATA SEE THE SAME SPECIES IN burcat.thr

FOR 9 CONSTANTS SPECIES NOT INCLUDED IN THIS FILE SEE <http://cea.grc.nasa.gov>

BRO M.W. Chase JPCRD 25 (1996), 1069

3	T02/97	BR	1.000	1.00	0.00	0.00	0.00	0	95.9034000	125800.000		
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	9066.782
	4.633842750D+02	-2.634323255D+01	4.022662780D+00	-3.646021530D-03	-6.531661370D-06							
	1.587195208D-07	-2.974521500D-10	0.000000000D+00	1.413037377D+04	5.576977070D+00							
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	9066.782
	1.514797345D+04	1.230798729D+02	-3.567102410D-01	2.143457427D-02	-3.550985620D-05							
	2.679236004D-08	-7.721723310D-12	0.000000000D+00	1.389787168D+04	2.551031642D+01							
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	9066.782
	-6.244739830D+05	1.819399377D+03	3.000756041D+00	7.197302760D-04	-1.566679356D-07							
	1.878706691D-11	-6.584413950D-16	0.000000000D+00	1.905229606D+03	1.372677748D+01							

BrO2 STRUCTURE Br-O-O M.W. Chase JPCRD 25 (1996), 1069

3	T02/97	BR	1.000	2.00	0.00	0.00	0.00	0	111.9028000	108000.000		
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12849.253
	-1.321414048D+02	6.609510540D+01	1.111094156D-01	7.858035570D-02	-4.947965810D-04							
	1.555835161D-06	-1.964058247D-09	0.000000000D+00	1.129988787D+04	2.298831550D+01							
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12849.253
	-4.352773790D+04	4.842708910D+02	3.313164720D+00	5.719916590D-03	-3.049501665D-06							
	-3.214232410D-10	5.748813360D-13	0.000000000D+00	8.869480150D+03	1.567228812D+01							
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12849.253
	5.362110860D+04	-7.778244760D+02	7.599701530D+00	-2.477967004D-04	5.640259650D-08							
	-6.637784160D-12	3.146145431D-16	0.000000000D+00	1.538311033D+04	-1.069810575D+01							



Table 5 (continued)

BrO2 STRUCTURE O-Br-O M.W. Chase JPCRD 25 (1996), 1069

3 T02/97 BR	1.000	2.00	0.00	0.00	0.00	0	111.9028000	152000.000			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11394.568
-2.997498539D+03	2.144995496D+02	-1.808281442D+00	7.227223910D-02	-4.136108320D-04							
1.286636434D-06	-1.571948369D-09	0.000000000D+00	1.622733076D+04	3.218087080D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11394.568
3.398767870D+04	-3.265786040D+02	3.843829580D+00	1.243528716D-02	-1.946925783D-05							
1.436838979D-08	-4.122060830D-12	0.000000000D+00	1.870289939D+04	6.841259930D+00							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11394.568
-2.304245111D+05	2.278722887D+01	6.945013450D+00	3.510091040D-05	-1.021421206D-08							
1.408646436D-12	-7.454995170D-17	0.000000000D+00	1.540506294D+04	-7.934637980D+00							

BrO3 M.W.Chase JPCRD 25 (1996), 1069

3 T02/97 BR	1.000	3.00	0.00	0.00	0.00	0	127.9022000	221000.000			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13100.348
-4.275526930D+03	2.505983139D+02	-1.005505479D+00	3.334634160D-02	4.127800660D-05							
-5.120719770D-07	9.969880310D-10	0.000000000D+00	2.414635876D+04	3.159039682D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13100.348
8.666261670D+04	-1.212634951D+03	8.066583160D+00	1.273294099D-02	-2.214256298D-05							
1.709728393D-08	-5.028899350D-12	0.000000000D+00	3.097315688D+04	-1.827506724D+01							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13100.348
-3.764729240D+05	-3.678481210D+00	9.953478630D+00	3.561372650D-05	-1.105848863D-08							
1.575994834D-12	-8.505518360D-17	0.000000000D+00	2.251161003D+04	-2.425894994D+01							

Br2O STRUCTURE BR-BR-O M.W. Chase JPCRD 25 (1996), 1069

3 T06/02 BR	2.000	1.00	0.00	0.00	0.00	0	175.8074000	168000.000			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13137.428
8.549739260D+02	4.496435650D-01	1.648062286D+00	6.467022000D-02	-4.396327850D-04							
1.490118944D-06	-1.961152508D-09	0.000000000D+00	1.869718495D+04	1.916775156D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13137.428
1.579902471D+04	-2.394635668D+02	5.867823070D+00	5.119785690D-03	-8.327646160D-06							
6.262559970D-09	-1.817272950D-12	0.000000000D+00	1.970809612D+04	2.254554647D+00							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13137.428
-1.167332837D+05	1.271057413D+01	6.972971070D+00	1.686798765D-05	-4.863491470D-09							
6.674481610D-13	-3.521782090D-17	0.000000000D+00	1.770768211D+04	-2.619114847D+00							

Br2O STRUCTURE BR-O-BR M.W. Chase JPCRD 25 (1996), 1069

3 T02/97 BR	2.000	1.00	0.00	0.00	0.00	0	175.8074000	107600.000			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12398.990
4.136131520D+03	-2.500342959D+02	9.345589120D+00	-5.131304290D-02	3.296542530D-04							
-8.827512500D-07	8.650058040D-10	0.000000000D+00	1.229682143D+04	-1.235262628D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12398.990
6.359162320D+04	-1.055317204D+03	9.863534040D+00	-4.341250740D-03	3.716540700D-06							
-1.654146481D-09	2.905227712D-13	0.000000000D+00	1.638978865D+04	-2.325939411D+01							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12398.990
-1.026317943D+05	-2.547315372D+01	7.016083710D+00	-5.417181360D-06	1.006352911D-09							
-9.701924380D-14	3.781809000D-18	0.000000000D+00	1.067229099D+04	-5.599958190D+00							

Table 5 (continued)

CBr	BROMOMETHYLYDENE		B97-1/Aug-VTZ calc JPC A 108, (2004), 7752 HF298=500.1 kJ									
3 T	2/04 C	1.00BR	1.00	0.00	0.00	0.00	0.00	0	91.9147000	495845.840		
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	8946.465
	4.347889670D+02-2.547093992D+01 4.034095090D+00-4.359293230D-03 2.491791199D-06											
	1.194808500D-07-2.821847711D-10 0.000000000D+00 5.864701480D+04 5.386521830D+00											
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	8946.465
	3.056720785D+04-3.586134890D+02 4.346264730D+00 2.469993992D-03-4.765184200D-06											
	3.859460890D-09-1.168948267D-12 0.000000000D+00 6.041136760D+04 1.418689926D+00											
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	8946.465
	-8.871648850D+04 1.690794392D+01 4.473953200D+00 1.505862284D-05-4.198525410D-09											
	5.656250160D-13-2.950203197D-17 0.000000000D+00 5.794179780D+04 1.921040081D+00											
CBr2	DIBROMOMETHYLENE RADICAL		B97-1/Aug-VTZ calc HF298=343.51 kJ									
3 T	4/04 C	1.00BR	2.00	0.00	0.00	0.00	0.00	0	171.8187000	343506.400		
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12191.800
	3.182805250D+03-1.715430383D+02 6.976543830D+00-1.832245948D-02 8.647908060D-05											
	-2.486036712D-08-2.942550800D-10 0.000000000D+00 4.045403760D+04-3.186165620D+00											
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12191.800
	6.857262130D+04-1.067675506D+03 9.460587480D+00-2.841505537D-03 1.370065573D-06											
	8.601247200D-11-2.100374464D-13 0.000000000D+00 4.492071300D+04-2.158885903D+01											
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12191.800
	-4.915090490D+05-2.723249278D+02 9.522335700D+00-3.099056032D-03 1.436382031D-06											
	-2.438909298D-10 1.408286668D-14 0.000000000D+00 3.894911750D+04-2.122176089D+01											
CBr3	TRIBROMOMETHYL Radical		B97-1/Aug-VTZ calc. HF298=266.437 kJ									
3 T	2/04 C	1.00BR	3.00	0.00	0.00	0.00	0.00	0	251.7227000	266437.120		
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16015.178
	3.381709630D+01 8.133039810D+01-1.545511174D+00 1.193597022D-01-7.326036610D-04											
	2.356671855D-06-3.008528505D-09 0.000000000D+00 2.996160839D+04 3.170070640D+01											
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16015.178
	4.764847560D+04-7.905280320D+02 9.365091300D+00 6.305296510D-03-1.161028004D-05											
	9.199415800D-09-2.748114485D-12 0.000000000D+00 3.372200200D+04-1.662260922D+01											
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16015.178
	-2.257262619D+05 1.504934369D+01 9.959713080D+00 2.615086182D-05-7.661751240D-09											
	1.060502164D-12-5.625188270D-17 0.000000000D+00 2.831128466D+04-1.720428058D+01											
CBr4	TetraBromoMethane		B97-1/Aug-VTZ calc HF298=28.49 kcal									
3 T	04/04 C	1.00BR	4.00	0.00	0.00	0.00	0.00	0	331.6267000	83889.200		
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	20395.755
	7.506281060D+03-3.761266410D+02 7.525902890D+00 6.701660900D-02-5.435701700D-04											
	2.199344498D-06-3.310092710D-09 0.000000000D+00 9.032557190D+03-9.802489130D+00											
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	20395.755
	9.247859210D+04-1.588238146D+03 1.568045623D+01-8.064876960D-04-3.182747550D-06											
	3.961340000D-09-1.415136523D-12 0.000000000D+00 1.483048622D+04-5.071854940D+01											
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	20395.755
	-2.491232744D+05 2.231809131D+00 1.297557062D+01 1.764384919D-05-5.376689080D-09											
	7.593499390D-13-4.076752490D-17 0.000000000D+00 5.443129350D+03-3.206058990D+01											

Table 5 (continued)

CCl2 IUPAC Task Force on Selected Radicals Ruscic et al JPCRD										
3 IU8/03 C	1.00CL	2.00	0.00	0.00	0.00	0	82.91670	231700.000		
50.000	200.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11727.903
-0.132366683D+04	0.906853688D+02	0.177702719D+01	0.222300745D-01	-0.753693684D-04						
0.173395692D-06	0.206899663D-10	0.000000000D+00	0.261616231D+05	0.174009676D+02						
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11727.903
0.926804851D+05	-0.404584520D+03	-0.257003990D+01	0.538280876D-01	-0.101752145D-03						
0.838081973D-07	-0.257343087D-10	0.000000000D+00	0.296023543D+05	0.335973337D+02						
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11727.903
-0.728179353D+06	0.248061757D+04	0.466992385D+01	0.107875078D-02	-0.264362652D-06						
0.327478007D-10	-0.161103758D-14	0.000000000D+00	0.995399111D+04	0.955762899D+01						
CCL3O* Radical Bozzelli JPC 105 (2001), 4504 B3LYP/6-31G*scaled 0.9806										
3 T12/01 C	1.00CL	3.000	1.00	0.00	0.00	0	134.3682000	-18409.600		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	17238.610
-4.722898970D+03	3.500236510D+02	-5.685548220D+00	1.096158271D-01	-2.945210631D-04						
2.574649780D-07	1.879665595D-10	0.000000000D+00	-5.390439370D+03	5.014333940D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	17238.610
5.675672480D+04	-1.323027623D+03	1.296496077D+01	4.876164000D-03	-8.549518890D-06						
6.259179350D-09	-1.737174641D-12	0.000000000D+00	1.496039407D+03	-4.029547200D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	17238.610
-2.799289609D+05	-3.444252060D+02	1.325122349D+01	-9.871572160D-05	2.151472732D-08						
-2.440807560D-12	1.121847114D-16	0.000000000D+00	-5.038478690D+03	-3.912039730D+01						
CDO Formyl-D Radical IUPAC Task Group on Selected Radicals Marenich and Boggs										
3 IU 5/0 C	1.00D	1.000	1.00	0.00	0.00	0	30.0242020	40944.897		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	10103.000
2.479400276D+02	-1.170047395D+01	4.164187000D+00	3.430980230D-05	-1.672666367D-05						
1.152192845D-07	-1.752807890D-10	0.000000000D+00	3.751876490D+03	3.793935660D+00						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	10103.000
2.701955619D+03	-9.925857940D+00	3.820557530D+00	1.026289982D-05	7.714893230D-06						
-7.748620050D-09	2.404425215D-12	0.000000000D+00	3.796588740D+03	5.426960500D+00						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	10103.000
3.563059180D+06	-1.254008702D+04	2.037267476D+01	-7.087715660D-03	2.173464451D-06						
-3.022253038D-10	1.512452601D-14	0.000000000D+00	8.137250930D+04	-1.116771107D+02						
CD3NO2 NitroMethane D3 Burcat JPCRD 28 (1999), 63-130										
3 T04/98 C	1.00D	3.00N	1.000	2.00	0.00	0	64.0585460	-61789.385		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	13556.087
1.340599725D+03	-1.062123895D+02	8.323368860D+00	-6.066330650D-02	4.472476130D-04						
-1.286000757D-06	1.576565319D-09	0.000000000D+00	-8.748976280D+03	-7.293157620D+00						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	13556.087
-1.343462738D+04	9.067797170D+02	-7.358242850D+00	5.580753390D-02	-6.153687760D-05						
3.655466090D-08	-9.184647970D-12	0.000000000D+00	-1.245387608D+04	6.466227550D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	13556.087
7.707229420D+05	-7.771435040D+03	2.378336714D+01	-1.980271626D-03	4.174658380D-07						
-4.614662240D-11	2.068797453D-15	0.000000000D+00	3.269096880D+04	-1.220282575D+02						

Table 5 (continued)

CD3OD Deuterated methyl alcohol Shimanouchi + Chem3D .

3 T06/02 C	1.00D	4.000	1.00	0.00	0.00	0	36.0665080	-217669.670			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11932.087
9.261040250D+02	-4.646807970D+01	4.732702160D+00	9.563725170D-03	-1.348459777D-04							
6.298973990D-07	-7.531531860D-10	0.000000000D+00	-2.743736410D+04	1.958698558D+00							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11932.087
-3.650161190D+04	1.437381347D+03	-1.010143481D+01	5.475784990D-02	-6.400584420D-05							
4.127647520D-08	-1.120328572D-11	0.000000000D+00	-3.342440640D+04	7.832331300D+01							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11932.087
1.355697006D+06	-8.682196460D+03	2.108843045D+01	-2.002655361D-03	4.072409220D-07							
-4.380798540D-11	1.931549936D-15	0.000000000D+00	2.167974558D+04	-1.110260358D+02							

CF3O Methane Trifluoro Oxyl Radical Burcat G3B3 calc HF298=-150.74 kcal

3 T07/04 C	1.00F	3.000	1.00	0.00	0.00	0	85.0053096	-630712.896			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13620.748
1.119833630D+03	-6.530599200D+01	5.651142040D+00	-2.832491252D-02	3.144027135D-04							
-9.808183090D-07	1.126003736D-09	0.000000000D+00	-7.727565560D+04	2.633298794D+00							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13620.748
-1.931432878D+04	4.890061770D+02	-2.294915524D+00	4.229118590D-02	-5.423536410D-05							
3.461268250D-08	-8.867349980D-12	0.000000000D+00	-7.948836450D+04	3.824584170D+01							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13620.748
-4.546314620D+05	-1.126450653D+03	1.381215090D+01	-3.161690868D-04	6.838910280D-08							
-7.710769090D-12	3.525982860D-16	0.000000000D+00	-7.478758330D+04	-5.007226300D+01							

CH METHYLIDYNE IUPAC Task Group on Selected Radicals

2 IU3/03 C	1.00H	1.00	0.00	0.00	0.00	0	13.01864	595800.000			
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	8625.000
0.223590108D+05	-0.342452257D+03	0.554012095D+01	-0.581298373D-02	0.798678629D-05							
-0.447225508D-08	0.959824993D-12	0.000000000D+00	0.722287398D+05	-0.915816739D+01							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	8625.000
0.205925350D+07	-0.539216675D+04	0.785217657D+01	-0.794574549D-03	0.175907549D-06							
-0.196956391D-10	0.499532673D-15	0.000000000D+00	0.106008917D+06	-0.315178740D+02							

CHBr Bromomethylene B97-1/Aug-VTZ calc.

3 T 2/04 C	1.00H	1.00BR	1.00	0.00	0.00	0	92.9226400	377857.000			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10415.748
7.514312050D+02	-4.565677760D+01	5.029514100D+00	-1.020666817D-02	3.639146840D-05							
2.521223246D-08	-1.093096214D-10	0.000000000D+00	4.434616700D+04	3.041016857D+00							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10415.748
1.306380528D+04	2.487765755D+02	-1.293417060D+00	2.736069244D-02	-4.344382290D-05							
3.316615100D-08	-9.770108760D-12	0.000000000D+00	4.356430850D+04	3.219019170D+01							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10415.748
5.062968000D+05	-2.225593644D+03	8.587600540D+00	-7.925228960D-04	2.350710520D-07							
-3.102429277D-11	1.507552267D-15	0.000000000D+00	5.713081480D+04	-2.335662412D+01							

CHFCLBr Gurvich,1991 NASA Tables have an error in S value.

3 A 6/05 C	1.00H	1.00F	1.00CL	1.00BR	1.00	0	147.3737432	-230000.000			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13787.186
-3.078141310D+03	2.335868452D+02	-2.609023984D+00	8.011133420D-02	-3.474533760D-04							
9.031280430D-07	-9.515966360D-10	0.000000000D+00	-3.005204611D+04	3.776710750D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13787.186
-3.643364060D+04	7.352736380D+02	-2.640712617D+00	4.005560770D-02	-5.230273010D-05							
3.497384280D-08	-9.412128680D-12	0.000000000D+00	-3.256957370D+04	4.407283060D+01							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13787.186
4.720091240D+05	-3.555772190D+03	1.497194298D+01	-6.154912170D-04	1.101433324D-07							
-1.052927096D-11	4.163481030D-16	0.000000000D+00	-1.030411643D+04	-5.785492520D+01							

Table 5 (continued)

CHBr2 DIBROMOMETHYL RADICAL B97-1/Aug-VTZ calc

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3 T 2/04 C 1.00H 1.00BR 2.00 0.00 0.00 0 172.8266400 198488.960
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12850.817
2.385803135D+03-1.377087092D+02 6.676395640D+00-2.297118169D-02 1.902177549D-04
-5.343221160D-07 5.746529710D-10 0.000000000D+00 2.280253106D+04-5.870632070D-01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12850.817
3.914953500D+04-4.763585730D+02 4.891198670D+00 1.503148083D-02-2.296902751D-05
1.742048468D-08-5.127670110D-12 0.000000000D+00 2.476251733D+04 3.061576009D+00
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12850.817
6.511939100D+05-2.875836539D+03 1.131363791D+01-3.169768440D-04 3.924538460D-08
-2.015282986D-12 8.975187430D-18 0.000000000D+00 3.886202280D+04-3.502661690D+01

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CHBr3 TRIBROMOETHANE BROMOFORM HF298 B97-1/Aug-VTZ calc.

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3 T 2/04 C 1.00H 1.00BR 3.00 0.00 0.00 0 252.7306400 54266.480
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15915.253
6.580801720D+03-3.615139940D+02 9.782555940D+00-1.517859712D-02 3.513908160D-05
2.450155340D-07-6.938709800D-10 0.000000000D+00 5.892247080D+03-1.497342947D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15915.253
2.521132334D+04-2.323352456D+02 4.101757770D+00 2.512008588D-02-3.569968390D-05
2.555904520D-08-7.241411570D-12 0.000000000D+00 5.863897330D+03 9.671621560D+00
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15915.253
5.118487220D+05-3.086762529D+03 1.459907206D+01-4.601182370D-04 7.479364090D-08
-6.385093100D-12 2.208926097D-16 0.000000000D+00 2.137921286D+04-5.104799790D+01

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CCL2OH RADICAL BOZZELLI JPC 105 (2001), 4504 B3lyp/6-31G\* scaled 0.9806

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3 T12/01 C 1.00CL 2.00O 1.00H 1.00 0.00 0 99.9234400 -94976.800
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14829.685
-2.571803707D+03 1.691060286D+02 1.767302021D-01 2.522666883D-02 1.610446344D-04
-9.916612300D-07 1.568802253D-09 0.000000000D+00-1.376461822D+04 2.749793251D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14829.685
2.126915912D+04-6.346484710D+02 7.810886100D+00 1.213007652D-02-1.645084232D-05
1.115684907D-08-2.956854431D-12 0.000000000D+00-1.047897969D+04-1.254725863D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14829.685
6.546889530D+05-2.840016593D+03 1.331238521D+01-1.908665298D-05-3.846914070D-08
7.698130720D-12-4.643046410D-16 0.000000000D+00 2.686884526D+03-4.551866370D+01

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CCL3OH TriChloroMethanol Bozzelli JPC 105 (2001), 4504 B3LYP/6-31G\*scaled 0.9806

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3 T12/01 C 1.00CL 3.00O 1.00H 1.00 0.00 0 135.3761400 -275976.640
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17481.420
-6.993082140D+03 4.753930400D+02-7.867576780D+00 1.188917071D-01-2.498623030D-04
-1.144350197D-07 8.929688680D-10 0.000000000D+00-3.683778140D+04 6.024377830D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17481.420
2.382235792D+04-7.875438460D+02 9.256461720D+00 1.801009742D-02-2.548040111D-05
1.779508323D-08-4.865525640D-12 0.000000000D+00-3.199322160D+04-2.071909966D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17481.420
5.641007770D+05-3.012085120D+03 1.653325051D+01-1.241672602D-04-1.352505034D-08
4.745902860D-12-3.256057370D-16 0.000000000D+00-1.931042730D+04-6.282513880D+01

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Table 5 (continued)

CHD2NO2 Nitromethane D2 Burcat JPCRD 28 (1999),63-130

3 T04/98 C 1.00H 1.00D 2.00O 2.00N 1.00 0 63.0523840 -57716.356  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13290.308  
 1.609048734D+03-1.211643330D+02 8.431736150D+00-5.920478800D-02 4.203125740D-04  
 -1.165426995D-06 1.354292542D-09 0.000000000D+00-8.170857810D+03-7.032763790D+00  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13290.308  
 -7.528646850D+04 1.753843762D+03-1.132899910D+01 6.289527190D-02-6.916667780D-05  
 4.086301090D-08-1.013198071D-11 0.000000000D+00-1.606949232D+04 8.877829900D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13290.308  
 1.293957455D+06-9.111404110D+03 2.433592688D+01-2.091682784D-03 4.263218870D-07  
 -4.596403410D-11 2.027170359D-15 0.000000000D+00 4.218555190D+04-1.264736298D+02

CHF3 (Fluoroform) HFC-23 Zachariah et al JPC 100,(1996),8737-8747

3 T 9/99 C 1.00H 1.00F 3.00 0.00 0.00 0 70.0138496 -693288.800  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11573.154  
 2.781427219D+03-2.074532012D+02 1.009808924D+01-8.806661390D-02 6.270927690D-04  
 -1.923551051D-06 2.344530683D-09 0.000000000D+00-8.412581620D+04-1.624699281D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11573.154  
 -1.103628694D+05 2.073514977D+03-1.204129301D+01 5.980585600D-02-7.277909800D-05  
 4.562034710D-08-1.162038288D-11 0.000000000D+00-9.407695380D+04 9.115929790D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11573.154  
 4.790004360D+05-4.432805500D+03 1.563268669D+01-8.839799960D-04 1.704968517D-07  
 -1.756449915D-11 7.473254250D-16 0.000000000D+00-6.110386240D+04-6.969502710D+01

HOCN Cyanic Acid Trans Melius,Jacox Webbook,Schuurman et al JCP,120,2004

3 A 5/05 H 1.00N 1.00C 1.00O 1.00 0.00 0 43.0247800 -15455.889  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11267.966  
 1.961914662D+03-1.613686633D+02 9.227070990D+00-8.318478400D-02 6.545004010D-04  
 -2.235770036D-06 2.940614903D-09 0.000000000D+00-2.724934006D+03-1.438754951D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11267.966  
 -5.532393740D+03 1.264120910D+02 1.878065519D+00 1.541181271D-02-1.777986514D-05  
 1.165773522D-08-3.179761150D-12 0.000000000D+00-3.707111030D+03 1.480570184D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11267.966  
 1.205667490D+06-4.876842550D+03 1.229576830D+01-5.951316410D-04 8.542749480D-08  
 -6.189772820D-12 1.675264541D-16 0.000000000D+00 2.597601489D+04-5.138760340D+01

HCNO Fulminic acid Melius C17B; Shuurman et al JCP 120,2004,11586

3 A 5/05 H 1.00N 1.00C 1.00O 1.00 0.00 0 43.0247800 167702.591  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10623.326  
 5.954942020D+03-4.187405510D+02 1.506575432D+01-1.568997402D-01 1.056041329D-03  
 -3.120082020D-06 3.545056030D-09 0.000000000D+00 2.022790498D+04-3.971800670D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10623.326  
 1.164694391D+05-1.778297691D+03 1.122771253D+01-3.499457980D-03 3.867834190D-06  
 -1.057904079D-09-1.592961144D-13 0.000000000D+00 2.746852550D+04-4.133509580D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10623.326  
 1.171114304D+06-4.883024740D+03 1.307728743D+01-7.684185120D-04 1.317316806D-07  
 -1.208947616D-11 4.596084900D-16 0.000000000D+00 4.770673310D+04-5.794044320D+01

Table 5 (continued)

HONC Melius C27; Schuurman et al JCP 120,2004,11586 HF0=56.34+/-2 kcal										
3 A 5/05 H	1.00N	1.00C	1.00O	1.00	0.00	0	43.0247800	234164.357		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.214816480D+03	3.888663820D+02	-6.971917160D+00	1.400626138D-01	-7.718480190D-04						
2.188172439D-06	-2.495095853D-09	0.000000000D+00	2.544911695D+04	4.899032910D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.140280250D+04	5.401604210D+02	1.668130216D+00	1.293228262D-02	-1.189730838D-05						
6.491083230D-09	-1.551640891D-12	0.000000000D+00	2.396772082D+04	1.856418772D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.276922819D+06	-4.953104950D+03	1.235418185D+01	-6.222012990D-04	9.238899160D-08						
-7.097164570D-12	2.141612786D-16	0.000000000D+00	5.664097790D+04	-5.074881280D+01						
CHO Formyl Radical IUPAC Task Group on Selected Radicals Marenich and Boggs										
3 T05/03 C	1.00H	1.00O	1.00	0.00	0.00	0	29.0180400	42300.000		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.909054361D+02	-6.505083940D+00	4.007960170D+00	1.976299520D-03	-2.595595158D-05						
1.244398772D-07	-1.867688014D-10	0.000000000D+00	3.911446940D+03	3.943182620D+00						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.217964230D+02	2.491028603D+01	4.021945390D+00	-2.474162328D-03	1.235893571D-05						
-1.190013708D-08	3.838988660D-12	0.000000000D+00	3.765811090D+03	4.423377420D+00						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.077147739D+06	-8.433987270D+03	1.602453231D+01	-5.394244960D-03	1.859525520D-06						
-2.779868187D-10	1.457229515D-14	0.000000000D+00	5.509247840D+04	-8.065557680D+01						
COH Hydroxymethylidyne Marenich and Boggs J Phys Chem 107, (2003), 2343.										
3 IU5/03 C	1.00H	1.00O	1.00	0.00	0.00	0	29.0180400	218100.000		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.062880214D+02	-1.793030382D+01	4.404994500D+00	-4.527761360D-03	2.797354914D-05						
-9.696426910D-08	1.700598213D-10	0.000000000D+00	2.508761419D+04	2.539192538D+00						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-8.779943920D+04	1.503614051D+03	-5.681166170D+00	2.802324360D-02	-3.470435850D-05						
2.304561932D-08	-6.241249840D-12	0.000000000D+00	1.808209311D+04	5.697912420D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-8.260392390D+05	9.576632540D+02	4.745620470D+00	9.307377250D-04	8.317790510D-08						
-3.542987150D-11	2.172782669D-15	0.000000000D+00	1.716034642D+04	-1.300718689D-01						
CH2 SINGLET Methylene Radical IUPAC Task Group for Selected Radicals										
3 IU3/03 C	1.00H	2.00	0.00	0.00	0.00	0	14.0265800	428800.000		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.282865690D+01	-3.126873888D+00	4.092782870D+00	-1.439679385D-03	1.240790484D-05						
-5.664925770D-08	1.078450834D-10	0.000000000D+00	5.038708520D+04	-4.018844800D-01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.712482601D+04	2.867463030D+02	2.333364882D+00	3.643294630D-03	-1.845501486D-06						
1.667755316D-09	-7.494030720D-13	0.000000000D+00	4.903726330D+04	9.311239710D+00						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.946875268D+05	-1.777640184D+03	6.502126510D+00	3.590503910D-04	6.760941970D-08						
-2.891563718D-11	2.213737217D-15	0.000000000D+00	6.061885350D+04	-1.873868416D+01						

Table 5 (continued)

## CH2 TRIPLET Methylene Radical IUPAC Task Group

3 IU3/03 C	1.00H	2.00	0.00	0.00	0.00	0	14.0265800	391200.000			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10027.357
2.154321755D+01-3.510041410D-01 3.975221970D+00 8.244726280D-04-8.765027650D-06											
3.066006610D-08 9.455151350D-12 0.000000000D+00 4.584682040D+04 6.007177000D-01											
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10027.357
5.517152260D+03 1.055786940D+02 1.968502705D+00 9.674644480D-03-1.554343926D-05											
1.353385097D-08-4.424619200D-12 0.000000000D+00 4.556320430D+04 1.024805253D+01											
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10027.357
1.682560056D+06-5.304297130D+03 9.491269230D+00-6.290210460D-04 8.478081770D-08											
-5.356749730D-12 1.003464211D-16 0.000000000D+00 7.952986310D+04-4.039228720D+01											

## CH2 METHYLENE RADICAL Equilibrium Singlete &amp; Triplete IUPAC Task Group

3 IU3/03 C	1.00H	2.00	0.00	0.00	0.00	0	14.0265800	391200.000			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10032.012
-4.206719340D+01 3.914041740D+00 3.861515610D+00 2.364451236D-03-1.992476440D-05											
7.156606640D-08-4.954528020D-11 0.000000000D+00 4.583246630D+04 1.053464211D+00											
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10032.012
-2.212055969D+03 1.973115562D+02 1.700343754D+00 9.129725830D-03-1.208871611D-05											
1.006390918D-08-3.323770130D-12 0.000000000D+00 4.509461030D+04 1.207964259D+01											
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10032.012
2.031444870D+06-7.101259870D+03 1.236674235D+01-1.977809678D-03 3.973637300D-07											
-4.167461660D-11 1.785246047D-15 0.000000000D+00 9.013164000D+04-6.048133690D+01											

## CH2Br2 W2 Calc Martin et al JPC 2004

3 T09/04 C	1.00BR	2.00H	2.00	0.00	0.00	0	173.8345800	4937.120			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12649.626
4.063717490D+03-2.409344579D+02 8.815634200D+00-3.694192920D-02 1.760417355D-04											
-2.226865651D-07-4.443409050D-11 0.000000000D+00-1.034381519D+02-1.044633843D+01											
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12649.626
-2.459107743D+04 7.613112250D+02-3.841345210D+00 3.991420890D-02-5.228346560D-05											
3.589610500D-08-9.909132180D-12 0.000000000D+00-4.059430180D+03 4.975931150D+01											
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12649.626
1.471860550D+06-6.401765950D+03 1.620496153D+01-8.901556930D-04 1.391660318D-07											
-1.134554873D-11 3.701229900D-16 0.000000000D+00 3.679443280D+04-7.104569770D+01											

## CH2DNO2 Nitromethane D Burcat JPCRD 28 (1999),63-130

3 T04/98 C	1.00H	2.00D	1.00O	2.00N	1.00	0	62.0462220	-52531.859			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13098.365
2.055919084D+03-1.520919188D+02 9.124981010D+00-6.681810440D-02 4.613404520D-04											
-1.278995017D-06 1.444502145D-09 0.000000000D+00-7.421959330D+03-1.010433227D+01											
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13098.365
-1.247828956D+05 2.412619180D+03-1.430072036D+01 6.799837930D-02-7.483284230D-05											
4.417352160D-08-1.087099957D-11 0.000000000D+00-1.866232424D+04 1.060644074D+02											
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13098.365
1.831981822D+06-1.039734018D+04 2.479383231D+01-2.153940270D-03 4.230335640D-07											
-4.430458070D-11 1.912295466D-15 0.000000000D+00 5.155869420D+04-1.312773431D+02											



Table 5 (continued)

CH2NO2 NITRO-METHYL RADICAL Burcat JPCRD 28 (1999), 63-130.

3 T04/98 C	1.00H	2.00N	1.00O	2.00	0.00	0	60.0321200	152464.960			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13143.456
2.612877052D+03-1.936811061D+02 1.017272473D+01-8.037664320D-02 5.511076850D-04											
-1.539700933D-06 1.706312699D-09 0.000000000D+00 1.736203163D+04-1.421449553D+01											
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13143.456
-4.782199090D+04 1.177793875D+03-7.323986950D+00 5.285944290D-02-6.526826480D-05											
4.229512140D-08-1.114929784D-11 0.000000000D+00 1.179875654D+04 6.686420530D+01											
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13143.456
1.406432678D+06-7.297646440D+03 1.944838903D+01-1.207368885D-03 2.124186187D-07											
-2.002066309D-11 7.822721680D-16 0.000000000D+00 5.858218370D+04-9.317713180D+01											

CH3 METHYL RADICAL IUPAC Task Group on Selected Radicals

3 IU1/03 C	1.00H	3.00	0.00	0.00	0.00	0	15.03452	146700.000			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10366.288
0.118053714D+04-0.803021345D+02 0.612539341D+01-0.272411169D-01 0.168957527D-03											
-0.436387090D-06 0.428176848D-09 0.000000000D+00 0.166563130D+05-0.821195667D+01											
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10366.288
-0.318321530D+05 0.553269109D+03-0.456705168D-01 0.143269736D-01-0.153738893D-04											
0.109219654D-07-0.326622436D-11 0.000000000D+00 0.138774782D+05 0.215922594D+02											
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10366.288
0.268335802D+07-0.913670211D+04 0.146793592D+02-0.134271770D-02 0.219685901D-06											
-0.190704534D-10 0.678982878D-15 0.000000000D+00 0.735224540D+05-0.777538285D+02											

CH3+ Methyl Carbonium Ion from B. Ruscic's ACTIVE TABLES generator.

3 A12/04 C	1.00H	3.00E	-1.00	0.00	0.00	0	15.0339714	1101792.000			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	9983.120
-3.926261550D+01 2.980118871D+00 3.918309440D+00 9.804304660D-04-4.469209380D-06											
-3.164899970D-09 5.682763030D-11 0.000000000D+00 1.313042786D+05-2.364572060D-02											
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	9983.120
-1.096212283D+05 1.771929293D+03-6.494275280D+00 2.678749965D-02-2.733825873D-05											
1.666307139D-08-4.352146430D-12 0.000000000D+00 1.230072586D+05 5.788806850D+01											
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	9983.120
2.752075802D+06-9.813865190D+03 1.542358895D+01-1.726893292D-03 3.263184180D-07											
-3.466245960D-11 1.636427640D-15 0.000000000D+00 1.923222721D+05-8.451054990D+01											

CH3Br MethylBromide W2 Calc Martin et al JPC A 2004

3 T09/04 C	1.00BR	1.00H	3.00	0.00	0.00	0	94.9385200	-36442.640			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10607.104
7.124005790D+02-4.648667140D+01 5.146920890D+00-1.284841989D-02 5.740089260D-05											
-2.152286002D-08-8.103237320D-11 0.000000000D+00-5.506276260D+03 1.731821173D+00											
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10607.104
-9.402690700D+04 1.840000831D+03-9.864886040D+00 4.659450820D-02-5.552085960D-05											
3.623088000D-08-9.715710870D-12 0.000000000D+00-1.388822056D+04 7.970464750D+01											
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10607.104
2.527864778D+06-9.944079610D+03 1.816202878D+01-1.505576662D-03 2.511635912D-07											
-2.231185942D-11 8.165689540D-16 0.000000000D+00 5.468766070D+04-9.450221720D+01											

Table 5 (continued)

CH3OD Methyl Alcohol-D Shimanouchi + Chem3D

3	T06/02	C	1.00H	3.00O	1.00D	1.00	0.00	0	33.0480220	-205330.898		
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11543.358
	7.247064450D+02	-3.840928680D+01	4.703803270D+00	6.839658370D-03	-8.971789990D-05							
	3.878976990D-07	-4.561621750D-10	0.000000000D+00	-2.593885066D+04	1.695623538D+00							
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11543.358
	-1.740781520D+05	3.138588561D+03	-1.646310427D+01	6.081391930D-02	-6.676501900D-05							
	4.118857980D-08	-1.072761435D-11	0.000000000D+00	-4.044274340D+04	1.170370449D+02							
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11543.358
	3.089361369D+06	-1.317219944D+04	2.320585313D+01	-2.549578652D-03	4.851366390D-07							
	-4.938015130D-11	2.078974116D-15	0.000000000D+00	5.325125240D+04	-1.308634898D+02							

CH3Hg MethylMercury Lee &amp; Wright Chem Phys Letters 376 (2003), 418

3	T04/04	C	1.00H	3.00HG	1.00	0.00	0.00	0	215.6245200	188280.000		
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11164.812
	-1.014342331D+03	5.277425610D+01	3.178281980D+00	1.014480507D-03	6.022415200D-05							
	-2.456020304D-07	4.106090150D-10	0.000000000D+00	2.111287869D+04	1.180177802D+01							
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11164.812
	-6.860300460D+04	1.377033795D+03	-6.968484820D+00	4.161009330D-02	-5.168087500D-05							
	3.497842600D-08	-9.628150450D-12	0.000000000D+00	1.518910558D+04	6.487786650D+01							
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11164.812
	2.505710857D+06	-9.484348670D+03	1.771141174D+01	-1.299301724D-03	2.017791022D-07							
	-1.634064817D-11	5.291869310D-16	0.000000000D+00	7.909473020D+04	-8.895322450D+01							

CH3I Iodomethane Kudchadker,1975. HF298=14.3 kJ Cox &amp; Pilcher 1970

3	g	8/99	C	1.00H	3.00I	1.00	0.00	0.00	0	141.9389900	14300.000	
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10815.834
	1.071687474D+03	-7.629765540D+01	6.119933840D+00	-2.844827019D-02	1.814316492D-04							
	-4.549086430D-07	4.988246710D-10	0.000000000D+00	6.616538410D+02	-1.131022842D+00							
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10815.834
	-6.116595620D+04	1.318813654D+03	-6.973503070D+00	4.051161750D-02	-4.868310180D-05							
	3.244271650D-08	-8.910905000D-12	0.000000000D+00	-5.350593360D+03	6.415355540D+01							
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10815.834
	2.383399561D+06	-9.638349380D+03	1.825800252D+01	-1.619118104D-03	2.866429035D-07							
	-2.717331219D-11	1.067633129D-15	0.000000000D+00	5.862906480D+04	-9.363322410D+01							

CH2NH MethaneImine CH2=NH HF298=20.08 kcal REF=Bauer &amp; Wilcox

3	T12/04	C	1.00H	3.00N	1.00	0.00	0.00	0	29.0412600	84014.720		
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10175.830
	-6.603426560D+02	4.483846260D+01	2.793910990D+00	1.627698434D-02	-1.137912521D-04							
	3.708623480D-07	-3.660227130D-10	0.000000000D+00	8.736259380D+03	8.529917960D+00							
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10175.830
	-1.810424261D+05	3.186778550D+03	-1.684039008D+01	5.947849390D-02	-6.731650330D-05							
	4.165763400D-08	-1.071110819D-11	0.000000000D+00	-5.764807470D+03	1.171795584D+02							
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10175.830
	2.523494975D+06	-1.052678545D+04	1.878485273D+01	-1.801130430D-03	3.233309750D-07							
	-3.114560988D-11	1.245244861D-15	0.000000000D+00	7.241735620D+04	-1.025943173D+02							

Table 5 (continued)

CH3ONO Methyl Nitrite Melius D30G 1987 HF298=-65.44 kJ Webbook											
3 A 5/05 C	1.00H	3.00O	2.00N	1.00	0.00	0	61.0400600	-65440.000			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15345.406
-3.801988110D+03	2.672216436D+02	-3.708653760D+00	1.278109805D-01	-7.535889450D-04							
2.269145168D-06	-2.644279279D-09	0.000000000D+00	-1.056725008D+04	3.897530560D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15345.406
-1.854715404D+05	3.035414985D+03	-1.322914698D+01	5.861069940D-02	-6.055899770D-05							
3.446379420D-08	-8.295133910D-12	0.000000000D+00	-2.397717073D+04	1.058722114D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15345.406
2.463159163D+06	-1.152030048D+04	2.475345057D+01	-2.248440888D-03	4.387795920D-07							
-4.763527040D-11	2.145761137D-15	0.000000000D+00	5.830156190D+04	-1.299439359D+02							
CH3N Methyl-N RADICAL Triplet HF298=76.47 kcal Melius G2 calc											
3 T12/04 C	1.00H	3.00N	1.00	0.00	0.00	0	29.0412600	319950.480			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10330.064
-6.408861400D+02	4.713757210D+01	2.608260728D+00	2.091954397D-02	-1.657033043D-04							
6.275933730D-07	-7.708279530D-10	0.000000000D+00	3.709076420D+04	9.667243310D+00							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10330.064
-1.148157065D+05	2.260844893D+03	-1.249858865D+01	5.180700760D-02	-6.050384790D-05							
3.890569250D-08	-1.038186238D-11	0.000000000D+00	2.710086139D+04	9.233365060D+01							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10330.064
2.364286817D+06	-1.005456256D+04	1.867432590D+01	-1.810833645D-03	3.326085610D-07							
-3.272945490D-11	1.334767277D-15	0.000000000D+00	9.766693810D+04	-1.004937829D+02							
CH3NO2 NITRO-METHANE Burcat JPCRD 28 (1999) 63-130.											
3 T05/98 C	1.00H	3.00N	1.00O	2.00	0.00	0	61.0400600	-80751.200			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12867.652
2.290488249D+03	-1.657608910D+02	9.197720250D+00	-6.464094630D-02	4.266766850D-04							
-1.124264165D-06	1.182266851D-09	0.000000000D+00	-1.073560287D+04	-1.196579859D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12867.652
-1.595508134D+05	2.883595876D+03	-1.646692481D+01	7.153452360D-02	-7.910251810D-05							
4.700425000D-08	-1.159527814D-11	0.000000000D+00	-2.433520533D+04	1.174720561D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12867.652
2.379555215D+06	-1.174112180D+04	2.532446635D+01	-2.251056592D-03	4.280136970D-07							
-4.359774950D-11	1.838497622D-15	0.000000000D+00	5.726163170D+04	-1.377641604D+02							
CH3N3 MethylAzyde Burcat G3B3 calc HF298=71.054 kcal HF0=74.004 kcal											
3 T11/04 C	1.00H	3.00N	3.00	0.00	0.00	0	57.0547400	297289.936			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14117.863
1.516652957D+03	-4.039630460D+01	2.883357281D+00	4.072000060D-02	-2.392920728D-04							
9.009221320D-07	-1.310772981D-09	0.000000000D+00	3.426164720D+04	1.014788763D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14117.863
-1.253988841D+05	1.956105683D+03	-7.562149490D+00	4.404050130D-02	-4.146917750D-05							
2.214744522D-08	-5.106234540D-12	0.000000000D+00	2.481207919D+04	7.108813770D+01							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14117.863
3.084116055D+06	-1.326984576D+04	2.614117730D+01	-2.501041740D-03	4.725655370D-07							
-4.789065320D-11	2.011068066D-15	0.000000000D+00	1.133127891D+05	-1.436553344D+02							

Table 5 (continued)

CH3O METHOXY RADICAL IUPAC Task Group on Selected Radicals B. Ruscic  
 3 IU1/03 C 1.00H 3.00O 1.00 0.00 0.00 0 31.0339200 21000.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10718.970  
 1.910973764D+00-6.962182440D+00 4.553523240D+00-5.828177080D-03 8.757814120D-06  
 1.256226091D-07-2.238275504D-10 0.000000000D+00 1.247602290D+03 2.893765703D+00  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10718.970  
 -1.057519107D+05 2.138493348D+03-1.215543272D+01 5.340655230D-02-6.333812720D-05  
 4.083929500D-08-1.090121013D-11 0.000000000D+00-8.278832600D+03 9.056436340D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10718.970  
 1.845883070D+06-8.746400530D+03 1.824227899D+01-1.764629503D-03 3.401801800D-07  
 -3.497799390D-11 1.484461558D-15 0.000000000D+00 5.286279160D+04-9.509355440D+01

CH2OH HYDROXYMETHYL RADICAL IUPAC Task Group on Selected Radicals B. Ruscic  
 2 IU2/03 C 1.00H 3.00O 1.00 0.00 0.00 0 31.0339200 -17000.000  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11781.000  
 -1.560076238D+05 2.685446279D+03-1.342022420D+01 5.757139470D-02-7.284449990D-05  
 4.836648860D-08-1.293492601D-11 0.000000000D+00-1.587198632E+04 9.963033700D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11781.000  
 2.250349506D+06-8.173186060D+03 1.599639179D+01-8.704133720D-04 6.069183950D-08  
 4.408349460D-12-5.702309500D-16 0.000000000D+00 4.654935208D+04-7.835158450D+01

CH3S IUPAC Task Group for Selected Radicals  
 3 IU3/03 H 3.00C 1.00S 1.00 0.00 0.00 0 47.1005200 124599.520  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11119.943  
 3.013180860D+03-2.038552136D+02 9.356310980D+00-6.786619810D-02 4.114015490D-04  
 -1.000783116D-06 8.822558850D-10 0.000000000D+00 1.430751566D+04-1.583012683D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11119.943  
 2.174295247D+04-2.388165438D+02 3.413438230D+00 1.072269805D-02-5.540133410D-06  
 1.928049677D-09-4.729546510D-13 0.000000000D+00 1.497045203D+04 6.016664060D+00  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11119.943  
 2.193331748D+06-9.362393260D+03 1.849692358D+01-1.792091386D-03 3.287800450D-07  
 -3.185932750D-11 1.332903666D-15 0.000000000D+00 6.977820070D+04-9.609908000D+01

CH2NH2 Methylen-Amine RADICAL Janoschek Int J. Chem Kinet 36 2004, p.  
 3 A10/04 C 1.00H 4.00N 1.00 0.00 0.00 0 30.0492000 153490.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11196.811  
 1.498608181D+03-1.017323643D+02 6.654672420D+00-3.247290080D-02 1.738742235D-04  
 -2.436689117D-07 5.875231750D-12 0.000000000D+00 1.744279285D+04-4.747233490D+00  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11196.811  
 -9.596438180D+04 1.943018758D+03-1.177372471D+01 5.828534900D-02-7.110392370D-05  
 4.599809430D-08-1.202717529D-11 0.000000000D+00 8.530805960D+03 8.788035990D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11196.811  
 2.864133708D+06-1.072130967D+04 1.990125152D+01-8.926312200D-04 7.330326720D-08  
 1.309123032D-12-3.827699020D-16 0.000000000D+00 8.225509490D+04-1.061919734D+02

CH3OH Methyl alcohol Shimanouchi HF298=-201.0 kJ NIST 2003  
 3 T06/02 C 1.00H 4.00O 1.00 0.00 0.00 0 32.0418600 -201000.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11443.888  
 5.514179570D+02-2.884594544D+01 4.520937250D+00 8.059475040D-03-8.756141560D-05  
 3.395731330D-07-3.682772360D-10 0.000000000D+00-2.543928883D+04 2.304530450D+00  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11443.888  
 -2.309816277D+05 3.960879410D+03-2.067161305D+01 7.011014720D-02-7.783114080D-05  
 4.743710360D-08-1.203193583D-11 0.000000000D+00-4.387018130D+04 1.408689123D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11443.888  
 3.291267750D+06-1.320371551D+04 2.235944200D+01-2.015660348D-03 3.408297480D-07  
 -3.086243963D-11 1.157693293D-15 0.000000000D+00 5.465578730D+04-1.259283514D+02

Table 5 (continued)

CH4O2 PEROXYMETHANE Matthews et al. J Chem Phys 122, (2005), #221101

3	A	7/05	C	1.00H	4.00O	2.00	0.00	0.00	0.00	0	48.0412600	-126732.825		
		50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14160.182
-3.939764900D+03		3.098182533D+02		-5.062558900D+00		1.147387035D-01		-5.525221150D-04						
1.401229153D-06		-1.228942379D-09		0.000000000D+00		-1.790501689D+04		4.349345460D+01						
		200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14160.182
-9.736691770D+04		2.337235994D+03		-1.625907657D+01		8.980320610D-02		-1.299073123D-04						
9.569386090D-08		-2.775644010D-11		0.000000000D+00		-2.705767639D+04		1.113211644D+02						
		1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14160.182
2.705390817D+06		-1.065979284D+04		2.274146121D+01		-1.089528050D-03		1.208346793D-07						
-4.116439250D-12		-1.422616140D-16		0.000000000D+00		4.700172430D+04		-1.188417443D+02						

CH3-NH-NH2 Methyl-Hydrazin Burcat G3B3 calc HF298=26.150 kcal

3	A10/04	C	1.00H	6.00N	2.00	0.00	0.00	0	46.0718200	109411.600				
		50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14096.674
-5.202183790D+03		3.742586550D+02		-6.113676640D+00		1.210088925D-01		-5.874013570D-04						
1.553546694D-06		-1.463918516D-09		0.000000000D+00		1.027252125D+04		4.826497170D+01						
		200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14096.674
-2.135584394D+05		4.136686700D+03		-2.671497318D+01		1.145823712D-01		-1.472913038D-04						
1.012614835D-07		-2.813944157D-11		0.000000000D+00		-7.139610730D+03		1.694064181D+02						
		1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14096.674
5.198347430D+06		-2.031816040D+04		3.514801630D+01		-2.810314928D-03		4.377350080D-07						
-3.550932250D-11		1.150144154D-15		0.000000000D+00		1.344868648D+05		-2.094181853D+02						

CH6Sn Stanummethyltrihydride CH3SnH3 Allendorf &amp; Melius JPC 109, (2005), 4939.

3	A	6/05	SN	1.00C	1.00H	6.00	0.00	0.00	0	136.7683400	118407.200			
		50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15097.463
2.856556998D+03		-2.784172114D+02		1.333196425D+01		-1.234004883D-01		8.864842990D-04						
-2.571471901D-06		2.892142990D-09		0.000000000D+00		1.323837339D+04		-2.809809171D+01						
		200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15097.463
7.132798270D+04		-9.575499990D+02		6.484011040D+00		1.835507155D-02		-7.526324790D-06						
-5.837512300D-10		9.175467860D-13		0.000000000D+00		1.725418250D+04		-1.052534446D+01						
		1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15097.463
2.721748394D+06		-1.335397950D+04		2.975766073D+01		-2.883119728D-03		5.767543670D-07						
-6.142540810D-11		2.692464088D-15		0.000000000D+00		9.023291320D+04		-1.651239836D+02						

CI4 Kudchadker + Nist 69

3	T07/03	C	1.00I	4.00	0.00	0.00	0.00	0	519.6285800	260412.160				
		50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22326.735
1.278003222D+04		-9.138184310D+02		2.588588700D+01		-1.693455413D-01		1.018365358D-03						
-2.884011158D-06		3.186081690D-09		0.000000000D+00		3.158242879D+04		-7.898432070D+01						
		200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22326.735
8.808169280D+04		-1.638129733D+03		1.787931079D+01		-8.280982850D-03		8.150842530D-06						
-4.329153520D-09		9.592455100D-13		0.000000000D+00		3.592247270D+04		-5.765694910D+01						
		1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22326.735
-1.450056977D+05		-5.290098100D+01		1.304018528D+01		-1.630954827D-05		3.648351170D-09						
-4.227387580D-13		1.976895800D-17		0.000000000D+00		2.727119576D+04		-2.815494928D+01						

Table 5 (continued)

CN	Cyanogen Radical IUPAC Thask Group for Selected Radicals .										
3 IU8/03 C	1.00N	1.00	0.00	0.00	0.00	0	26.0174400	438683.443			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	8671.995
-5.790150270D+01	3.942837300D+00	3.393249170D+00	1.479921549D-03	-1.098293016D-05							
4.180265220D-08	-6.367663090D-11	0.000000000D+00	5.170458850D+04	4.852102110D+00							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	8671.995
1.188397045D+04	-2.537136969D+02	5.571185480D+00	-8.087860440D-03	1.519306600D-05							
-1.182631770D-08	3.415791490D-12	0.000000000D+00	5.283256730D+04	-6.320094830D+00							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	8671.995
-4.559106190D+05	3.465116520D+02	4.151624970D+00	-2.436652121D-04	2.777076426D-07							
-5.570709590D-11	3.473763450D-15	0.000000000D+00	4.842762280D+04	3.952363430D-01							
CNO (NCO)	Hf0=30.49+/-1 kcal Allen & Schaefer JCP 120, (2004), 11586.										
3 A 5/05 N	1.00C	1.000	1.00	0.00	0.00	0	42.0168400	128039.801			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10198.245
2.631314620D+03	-2.601020106D+02	1.252913905D+01	-1.257916319D-01	8.612844230D-04							
-2.692261945D-06	3.264470240D-09	0.000000000D+00	1.492530259D+04	-2.772441261D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10198.245
2.199033327D+04	-3.995578430D+02	5.546618750D+00	-1.482855191D-04	6.444715800D-06							
-7.275825420D-09	2.504016485D-12	0.000000000D+00	1.605896001D+04	-5.071147100D+00							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10198.245
1.857166444D+05	-1.930180291D+03	8.846028740D+00	-4.976360030D-04	9.953348480D-08							
-1.026687307D-11	4.768585520D-16	0.000000000D+00	2.447049594D+04	-2.758544949D+01							
CNN	Gurvich, 1991. Jacox, 1994. HF298=591.87+/-3.19 kJ ATcT A										
3 ATcT/A C	1.00N	2.00	0.00	0.00	0.00	0	40.0241800	591870.000			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10377.660
-2.235813077D+03	1.085781234D+02	2.196031603D+00	-1.057601364D-02	2.851175751D-04							
-1.339251239D-06	2.071253584D-09	0.000000000D+00	6.953608380D+04	1.404997014D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10377.660
-6.386497180D+04	8.222957390D+02	-8.936911940D-01	1.809247346D-02	-1.845348537D-05							
9.236470260D-09	-1.804533260D-12	0.000000000D+00	6.589381390D+04	3.078950550D+01							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10377.660
-1.348702500D+05	-7.916894090D+02	7.973831160D+00	-1.174256576D-04	3.373748620D-09							
2.636992370D-12	-1.919193785D-16	0.000000000D+00	7.300455390D+04	-2.050632799D+01							
NCN	Gurvich, 1991. Jacox, 1998. HF298=465.89+/-1.78 ATcT A										
3 ATcT/A N	2.00C	1.00	0.00	0.00	0.00	0	40.0241800	465890.000			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10180.177
1.303186606D+02	-4.919201960D+01	6.194282930D+00	-5.795780180D-02	5.504625810D-04							
-2.061041844D-06	2.847398383D-09	0.000000000D+00	5.492186470D+04	-2.858552473D+00							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10180.177
-4.703840330D+04	5.955107910D+02	-6.666804130D-03	1.620476680D-02	-1.627518262D-05							
7.942912160D-09	-1.493796005D-12	0.000000000D+00	5.189315550D+04	2.475445798D+01							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10180.177
-1.136706125D+05	-9.057756660D+02	8.126913300D+00	-2.278063673D-04	4.570532710D-08							
-5.163206090D-12	3.031473359D-16	0.000000000D+00	5.852765220D+04	-2.241696262D+01							

Table 5 (continued)

## C2Br Bromoacetynyl Radical Martin &amp; Burcat 2004

3	T04/04	C	2.00BR	1.00	0.00	0.00	0.00	0.00	0	103.9254000	623667.040		
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11648.447
-3.211778690D+02	5.873478400D+01	1.419157139D+00	4.240299080D-02	-2.555970096D-04									
8.849069890D-07	-1.254856848D-09	0.000000000D+00	7.345804000D+04	2.093761580D+01									
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11648.447	
1.514026023D+04	-3.778530500D+02	6.884118430D+00	-3.075976933D-03	8.306036130D-06									
-7.668905600D-09	2.468648848D-12	0.000000000D+00	7.523793520D+04	-4.312149890D+00									
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11648.447	
1.139457021D+05	-1.144273137D+03	7.861841160D+00	-3.503720130D-04	7.883244040D-08									
-9.199327970D-12	4.332720750D-16	0.000000000D+00	7.961157570D+04	-1.233122120D+01									

## C2Br2 Dibromo Acetylene Martin &amp; Burcat 2004

3	T04/04	C	2.00BR	2.00	0.00	0.00	0.00	0	183.8294000	335305.760			
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15426.825
-4.306826650D+03	3.067248509D+02	-5.796885840D+00	1.390648873D-01	-6.622947490D-04									
1.622945557D-06	-1.591895355D-09	0.000000000D+00	3.750957640D+04	4.623364330D+01									
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15426.825	
4.148738800D+04	-9.844799790D+02	1.216815261D+01	-6.096449750D-03	9.241427230D-06									
-6.117713080D-09	1.515183100D-12	0.000000000D+00	4.264886340D+04	-3.552608000D+01									
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15426.825	
3.439923950D+05	-2.018699687D+03	1.184793028D+01	-4.990177090D-04	1.043906509D-07									
-1.150639193D-11	5.180037960D-16	0.000000000D+00	4.943907150D+04	-3.688267940D+01									

## C2Br3 TribromoVinyl Radical Martin &amp; Burcat 2004

3	T11/03	C	2.00BR	3.00	0.00	0.00	0.00	0	263.7334000	385388.240			
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18601.259
3.885432610D+03	-2.443871906D+02	8.580201780D+00	-7.523037240D-03	1.414169540D-04									
-4.369266450D-07	4.331742530D-10	0.000000000D+00	4.494139020D+04	-6.240640730D+00									
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18601.259	
7.202040180D+04	-1.390342172D+03	1.432255365D+01	-2.673164455D-03	5.025093560D-06									
-4.347335710D-09	1.370621865D-12	0.000000000D+00	5.032654570D+04	-4.076649190D+01									
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18601.259	
-6.804669690D+04	-1.114137452D+03	1.382876306D+01	-3.332022340D-04	7.426742590D-08									
-8.599373060D-12	4.024265490D-16	0.000000000D+00	4.844196870D+04	-3.811757590D+01									

## C2Br4 Tetrabromo ethylene Martin &amp; Burcat 2004

3	T11/03	C	2.00BR	4.00	0.00	0.00	0.00	0	343.6374000	190079.120			
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22410.400
2.101304395D+03	-3.462216920D+01	3.715748470D-01	1.423561470D-01	-8.775754670D-04									
2.936010977D-06	-3.923812740D-09	0.000000000D+00	2.041068558D+04	2.268203441D+01									
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22410.400	
4.885229650D+04	-9.730584260D+02	1.277599063D+01	1.101750607D-02	-1.439498035D-05									
9.153621240D-09	-2.338825507D-12	0.000000000D+00	2.438041730D+04	-3.190780920D+01									
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22410.400	
-2.365220575D+05	-9.407368180D+02	1.668195835D+01	-2.676734982D-04	5.841723520D-08									
-6.643480690D-12	3.062098376D-16	0.000000000D+00	2.261283590D+04	-5.247252450D+01									

Table 5 (continued)

## C2Br5 Pentabromo ethyl Radical Martin &amp; Burcat 2004

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3 T11/03 C 2.00BR 5.00 0.00 0.00 0.00 0 423.5414000 283256.800
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 27749.138
7.728444300D+03-4.435094340D+02 1.086151918D+01 5.590447920D-02-3.510804460D-04
1.326468799D-06-1.944016274D-09 0.000000000D+00 3.228369480D+04-1.882598996D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 27749.138
2.801982421D+04-6.305875260D+02 1.229238847D+01 2.451340729D-02-3.633473800D-05
2.466988944D-08-6.507521890D-12 0.000000000D+00 3.327539550D+04-2.440917730D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 27749.138
-1.093807248D+06 1.988994196D+03 1.679659342D+01 4.120295470D-04-8.111214190D-08
8.530126680D-12-3.702723310D-16 0.000000000D+00 1.438399047D+04-4.089622460D+01

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## C2Br6 Hexabromoethane Martin &amp; Burcat 2004

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3 T11/03 C 2.00BR 6.00 0.00 0.00 0.00 0 503.4454000 165480.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 31667.416
1.431090036D+04-8.066783020D+02 1.574974065D+01 7.277698700D-02-6.923402160D-04
3.020079292D-06-4.670066460D-09 0.000000000D+00 1.894011546D+04-4.561825480D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 31667.416
1.303940186D+05-2.141593204D+03 2.167046892D+01 1.068120699D-02-2.170648324D-05
1.784675670D-08-5.419425850D-12 0.000000000D+00 2.576510279D+04-7.706511180D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 31667.416
-1.095051166D+05-6.072345040D+02 2.123829525D+01 8.540044810D-04-3.680571200D-07
5.693458710D-11-3.113220513D-15 0.000000000D+00 1.652338845D+04-6.893150070D+01

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## C2Cl2F2 1,2-transDiflorodichloroEthylene Burcat G3B3 calc HF298=-81.617 kcal

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3 A 4/05 C 2.00CL 2.00F 2.00 0.00 0.00 0 132.9236064 -341485.528
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17924.568
3.776843230D+02-3.794918760D+01 4.854829140D+00-1.108564052D-02 4.072760280D-04
-1.769807420D-06 2.569216892D-09 0.000000000D+00-4.310832490D+04 7.373566670D+00
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17924.568
1.397328452D+04-5.167109180D+02 7.583803810D+00 2.082254556D-02-2.267220427D-05
1.222085315D-08-2.651944898D-12 0.000000000D+00-4.108935700D+04-1.081527132D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17924.568
-1.827862596D+05-2.037968313D+03 1.750189805D+01-5.987983870D-04 1.325119054D-07
-1.525142281D-11 7.101575910D-16 0.000000000D+00-3.505814200D+04-6.751215270D+01

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## C2Cl2F2 1,2-cisDiflorodichloroEthylene Burcat G3B3 calc HF298=-81.154 kcal

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3 A 4/05 C 2.00CL 2.00F 2.00 0.00 0.00 0 132.9236064 -339548.336
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17934.005
7.740302210D+02-8.200758840D+01 6.562926180D+00-4.238417340D-02 6.717445210D-04
-2.780653455D-06 4.011021480D-09 0.000000000D+00-4.275264110D+04 1.184028636D+00
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17934.005
-3.234980510D+03-3.130693210D+02 6.741323650D+00 2.265397607D-02-2.478047887D-05
1.345215777D-08-2.939986740D-12 0.000000000D+00-4.188823890D+04-5.889092710D+00
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17934.005
-1.872251158D+05-2.011206331D+03 1.748521620D+01-5.930630720D-04 1.313975078D-07
-1.513694788D-11 7.053313740D-16 0.000000000D+00-3.498756070D+04-6.735037910D+01

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Table 5 (continued)

C2Cl6 HexaChloroEthane Burcat G3B3 calc HF298=-162.11 kJ

3 A 4/05 C	2.00CL	6.00	0.00	0.00	0.00	0.00	0	236.7376000	-162110.000		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	27235.144
-7.419377350D+03 5.565139830D+02-1.355599120D+01 2.899827521D-01-1.457610021D-03											
4.043642730D-06-4.575996600D-09 0.000000000D+00-2.449833630D+04 7.972754020D+01											
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	27235.144
1.298158081D+05-2.179787831D+03 1.808668441D+01 2.376179685D-02-4.173207090D-05											
3.249070910D-08-9.594698150D-12 0.000000000D+00-1.278194441D+04-6.609499010D+01											
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	27235.144
7.177121300D+05-3.972720870D+03 2.547985588D+01-1.470743130D-03 2.230801200D-07											
-1.503137506D-11 2.965148294D-16 0.000000000D+00-2.363421067D+03-1.059727316D+02											

C2F4 TetraFluoroEthylene ATcT A HF298=-675.34+/-2.0 kJ

3 ATcT/A C	2.00F	4.00	0.00	0.00	0.00	0.00	0	100.0150128	-675340.000		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16330.554
3.042265559D+03-1.826446485D+02 8.116504010D+00-5.492560920D-02 6.086383760D-04											
-2.146109658D-06 2.731143836D-09 0.000000000D+00-8.257060370D+04-7.834082090D+00											
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16330.554
1.751041403D+03-3.011854699D+02 5.477017130D+00 2.318849075D-02-2.225600031D-05											
1.014359582D-08-1.730778244D-12 0.000000000D+00-8.198858990D+04-2.119878618D+00											
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16330.554
-8.998271610D+04-2.790747823D+03 1.806900467D+01-8.295337540D-04 1.844746365D-07											
-2.132053658D-11 9.962253940D-16 0.000000000D+00-7.075129560D+04-7.588452740D+01											

C2F6 HexaFluoroEthane ATcT A HF298=-1347.38+/-4.1 kJ

3 ATcT/A C	2.00F	6.00	0.00	0.00	0.00	0.00	0	138.0118192	-1347380.000		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	20228.830
-1.365220122D+03 8.578653510D+01 2.208310277D+00 2.077997890D-02 2.281344636D-04											
-1.044789672D-06 1.494981284D-09 0.000000000D+00-1.647757422D+05 1.868200649D+01											
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	20228.830
-9.065244700D+04 1.647141402D+03-9.887055230D+00 8.997991150D-02-1.185851382D-04											
7.688089070D-08-1.989065654D-11 0.000000000D+00-1.718867883D+05 8.016700840D+01											
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	20228.830
-1.329540385D+06-3.920553560D+02 2.231617200D+01-6.896708310D-04 1.688819928D-07											
-2.031100287D-11 9.647900690D-16 0.000000000D+00-1.702455374D+05-9.299024440D+01											

C2HBr Bromoacetylene Martin &amp; Burcat 2004 W2

3 T04/04 C	2.00BR	1.00H	1.00	0.00	0.00	0.00	0	104.9333400	282420.000		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11945.834
-2.612218331D+03 1.820549559D+02-1.020103874D+00 4.457495510D-02-1.296594299D-04											
3.494913640D-07-5.210337330D-10 0.000000000D+00 3.194122880D+04 2.720350577D+01											
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11945.834
1.344253374D+05-2.232772242D+03 1.555132314D+01-1.425710194D-02 1.732202807D-05											
-9.635269690D-09 2.051419825D-12 0.000000000D+00 4.300151590D+04-6.138312110D+01											
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11945.834
1.163876374D+06-4.455335660D+03 1.278527274D+01-6.594494590D-04 1.089247980D-07											
-9.583628010D-12 3.473467180D-16 0.000000000D+00 5.909260930D+04-5.167065450D+01											

Table 5 (continued)

## C2HBr2 Dibromovinyl Radical Martin &amp; Burcat

```

3 T02/04 C 2.00H 1.00BR 2.00 0.00 0.00 0 184.8373400 333590.320
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15542.231
4.932906980D+03-2.319617340D+02 5.869416680D+00 4.125564070D-02-3.826477050D-04
1.697982502D-06-2.644336719D-09 0.000000000D+00 3.913197440D+04-2.833572049D-02
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15542.231
3.316444490D+04-3.811541480D+02 5.414663380D+00 1.789734583D-02-2.250229795D-05
1.502933166D-08-4.089860230D-12 0.000000000D+00 4.016553510D+04 2.888550955D+00
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15542.231
7.264280130D+05-3.899353100D+03 1.512229255D+01-6.534439480D-04 1.158441224D-07
-1.100855835D-11 4.338842380D-16 0.000000000D+00 6.013206730D+04-5.610835090D+01

```

## C2HBr3 Tribromoethylene Burcat (unpublished)

```

3 T02/04 C 2.00H 1.00BR 3.00 0.00 0.00 0 264.7413400 144180.640
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18417.881
5.355600630D+03-3.055752322D+02 8.816451360D+00-6.414376370D-04 3.257253200D-05
8.828365860D-08-3.480851910D-10 0.000000000D+00 1.619830364D+04-9.292591860D+00
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18417.881
3.736211170D+04-5.349894140D+02 6.754593250D+00 2.422651129D-02-3.190252180D-05
2.161810605D-08-5.895798080D-12 0.000000000D+00 1.766555756D+04-2.758392412D+00
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18417.881
5.640849850D+05-3.819887260D+03 1.811064320D+01-6.590022760D-04 1.183550270D-07
-1.138408336D-11 4.538041140D-16 0.000000000D+00 3.552475430D+04-6.961390060D+01

```

## C2HBr4 1,1-2,2-TetraBromoethyl Radical CHBr2CBr2\* Martin &amp; Burcat JPC A 2004

```

3 A04/05 C 2.00H 1.00BR 4.00 0.00 0.00 0 344.6453400 218823.200
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 23519.212
4.632646880D+03-3.384527330D+02 1.193509870D+01-2.015992223D-02 2.361455988D-04
-7.497643940D-07 9.041293350D-10 0.000000000D+00 2.457272574D+04-1.762217756D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 23519.212
-1.189711587D+04 2.332235709D+02 4.042879660D+00 4.135554240D-02-5.635837370D-05
3.870471780D-08-1.062399744D-11 0.000000000D+00 2.233245612D+04 1.865536667D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 23519.212
1.330971401D+06-6.830465270D+03 2.535267889D+01-3.118008383D-03 6.786536230D-07
-7.507901200D-11 3.343927560D-15 0.000000000D+00 6.195367320D+04-1.087149653D+02

```

## C2HBr4 1,1-1,2-TetraBromoethyl Radical CBr3CHBr\* Martin &amp; Burcat JPC A 2004

```

3 A04/05 C 2.00H 1.00BR 4.00 0.00 0.00 0 344.6453400 243634.320
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 24421.988
5.737426990D+03-3.440862500D+02 9.699230040D+00 2.238863812D-02-2.266975291D-05
5.353457060D-08-1.319194608D-10 0.000000000D+00 2.755059885D+04-1.210401909D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 24421.988
3.696626600D+04-7.717982630D+02 1.138937576D+01 2.302568451D-02-3.325497660D-05
2.398127842D-08-6.844851700D-12 0.000000000D+00 2.965417076D+04-2.269407297D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 24421.988
1.471919429D+06-6.860060640D+03 2.553452199D+01-3.211326490D-03 7.008436240D-07
-7.768510170D-11 3.465572580D-15 0.000000000D+00 6.544518040D+04-1.102093912D+02

```

Table 5 (continued)

C2HBr5 Pentabromo ethane Burcat (unpublished)

```

3 T02/04 C 2.00H 1.00BR 5.00 0.00 0.00 0 424.5493400 113093.520
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 27231.045
1.237217807D+04-7.212719980D+02 1.635119491D+01 4.532096890D-03-1.504367730D-04
1.045114796D-06-1.910940474D-09 0.000000000D+00 1.282769702D+04-4.286252660D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 27231.045
3.332471520D+04-4.507915790D+02 9.040141720D+00 3.738996840D-02-5.349282180D-05
3.828360990D-08-1.084372267D-11 0.000000000D+00 1.232703089D+04-9.097546570D+00
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 27231.045
1.510353076D+06-7.337810290D+03 2.816638871D+01-2.941899237D-03 6.281907920D-07
-6.853272860D-11 3.018391363D-15 0.000000000D+00 5.179593590D+04-1.240217611D+02

```

C2HCLF 1,1-ChloroFluoroVinyl Radical Burcat G3B3 calc HF298=101.872 kJ

```

3 A12/04 C 2.00H 1.00CL 1.00F 1.00 0.00 0 79.4804432 101872.032
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13316.602
1.111959021D+03-1.218311975D+02 8.947790870D+00-9.436211250D-02 8.402462080D-04
-2.850874332D-06 3.628864470D-09 0.000000000D+00 1.098936070D+04-7.718220540D+00
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13316.602
9.136532340D+04-1.440645502D+03 9.649494260D+00 8.968292090D-03-1.215303879D-05
8.627407730D-09-2.442366068D-12 0.000000000D+00 1.758284308D+04-2.669288347D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13316.602
7.401564100D+05-3.939993780D+03 1.497277572D+01-5.537119320D-04 8.850900000D-08
-7.484725390D-12 2.583427800D-16 0.000000000D+00 3.252392330D+04-5.997089030D+01

```

C2HCl4 TetraChloroethyl Radical CHCl2-CHCl2\* Burcat G3B3 calc HF298=21.824 kJ

```

3 A04/05 C 2.00H 1.00CL 4.00 0.00 0.00 0 166.8401400 21823.744
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20418.543
-7.574701770D+03 5.562291840D+02-1.175320597D+01 2.229994778D-01-1.133144167D-03
3.232364760D-06-3.758286910D-09 0.000000000D+00-1.587716295D+03 7.663080720D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20418.543
2.023767980D+04-2.524016026D+02 4.321677220D+00 4.157897000D-02-5.494109750D-05
3.625348390D-08-9.643041670D-12 0.000000000D+00 1.412484788D+03 9.509021280D+00
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20418.543
-2.006188962D+05-2.701072086D+03 2.130127793D+01-1.298434336D-03 2.630025954D-07
-2.750065822D-11 1.173496289D-15 0.000000000D+00 1.130558253D+04-8.538304190D+01

```

C2HCl5 Pentachloro ethane Burcat G3B3 calc HF298=-160.45 kJ

```

3 A04/05 C 2.00H 1.00CL 5.00 0.00 0.00 0 202.2928400 -160410.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22715.892
-5.427726820D+03 4.949246680D+02-1.333264176D+01 2.887244836D-01-1.671896357D-03
5.184801070D-06-6.352973530D-09 0.000000000D+00-2.348105730D+04 7.821051330D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22715.892
4.101008270D+03 3.282240600D+02-4.889904870D-01 6.547438580D-02-9.100870770D-05
6.352159710D-08-1.773430748D-11 0.000000000D+00-2.322655312D+04 3.360129500D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22715.892
5.075054840D+05-6.159777270D+03 2.839131044D+01-3.314839910D-03 7.548897080D-07
-8.677940830D-11 3.993269560D-15 0.000000000D+00 9.375256910D+03-1.324574113D+02

```

Table 5 (continued)

C2HF2(E) DiFluoroEthylen Radical CHF=CF Zachariah et al. JPC 100 (1996),8737  
 3 T 6/02 C 2.00H 1.00F 2.00 0.00 0.00 0 63.0261464 -42500.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13183.490  
 -4.335605430D+03 3.012909580D+02-3.717306950D+00 8.500098310D-02-3.612609530D-04  
 9.051590700D-07-9.369338820D-10 0.000000000D+00-7.669035800D+03 4.033150810D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13183.490  
 -7.011290910D+04 1.161857792D+03-4.412859400D+00 4.004923890D-02-4.762624620D-05  
 2.953352052D-08-7.486486470D-12 0.000000000D+00-1.206492678D+04 5.217826080D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13183.490  
 6.240426590D+05-4.311879500D+03 1.553523114D+01-8.444472000D-04 1.618557993D-07  
 -1.659409750D-11 7.034267530D-16 0.000000000D+00 1.689994231D+04-6.576705060D+01

C2HF5 PentaFluoroEthane Burcat G3B3 calc HF298=-1120.0 kJ  
 3 A 4/05 C 2.00H 1.00F 5.00 0.00 0.00 0 120.0213560 -1120000.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18775.693  
 -2.533785305D+02 9.423281620D+00 4.090121910D+00 1.059735928D-03 2.897289838D-04  
 -1.215357536D-06 1.763995389D-09 0.000000000D+00-1.370056101D+05 1.106710459D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18775.693  
 -1.514737603D+05 2.698607531D+03-1.591958525D+01 9.847467120D-02-1.268450925D-04  
 8.226417550D-08-2.144350570D-11 0.000000000D+00-1.492501373D+05 1.147428955D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18775.693  
 3.775628960D+03-4.663766320D+03 2.501348153D+01-1.570852442D-03 3.293283320D-07  
 -3.574596240D-11 1.576263773D-15 0.000000000D+00-1.152532257D+05-1.167671119D+02

NCCHO HF298=10.545 kcal Burcat G3B3 calc (unpublished)  
 3 T06/04 C 2.00H 1.00N 1.00O 1.00 0.00 0 55.0354800 44120.280  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12984.389  
 -2.871303929D+03 2.388436734D+02-3.444771780D+00 1.027265465D-01-5.803570490D-04  
 1.788226593D-06-2.193997988D-09 0.000000000D+00 3.018929605D+03 3.667728430D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12984.389  
 -6.216839880D+03 1.457541882D+02 2.453363662D+00 1.629360013D-02-1.326140511D-05  
 6.436631530D-09-1.476985145D-12 0.000000000D+00 3.104590991D+03 1.473893214D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12984.389  
 1.371546533D+06-6.787620760D+03 1.720583365D+01-1.468679208D-03 2.935042212D-07  
 -3.120732516D-11 1.365286424D-15 0.000000000D+00 4.330806790D+04-8.064083020D+01

C2H(NO2) NitroAcetylene HCC-NO2 G3B3 calcc HF298=66.6 kcal Politzer JPC A 108  
 3 A 1/05 C 2.00H 1.00N 1.00O 2.00 0.00 0 71.0348800 278654.400  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14413.741  
 1.528136898D+03-2.885288256D+01 2.523027774D+00 4.333544530D-02-3.108153406D-04  
 1.494919919D-06-2.492062273D-09 0.000000000D+00 3.195550620D+04 1.291766048D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14413.741  
 1.037378870D+05-1.352212912D+03 7.992676400D+00 1.759715625D-02-2.052445455D-05  
 1.320941877D-08-3.553434690D-12 0.000000000D+00 3.855828300D+04-1.910378754D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14413.741  
 1.046685413D+06-5.923041610D+03 1.915075450D+01-9.531218150D-04 1.666660502D-07  
 -1.566759229D-11 6.121907720D-16 0.000000000D+00 6.489087950D+04-8.855584720D+01

Table 5 (continued)

C2H2Br2 DIBROMOETHYLENE trans PM3 calc. HF298 THERGAS + NIST 94

```

3 T03/04 C 2.00H 2.00BR 2.00 0.00 0.00 0 185.8452800 101900.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15447.032
2.967854586D+03-8.865428350D+01 1.929176440D+00 9.128592980D-02-7.044212190D-04
2.651433013D-06-3.630004270D-09 0.000000000D+00 1.082353176D+04 1.442777145D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15447.032
1.523817383D+03 5.460057510D+02-2.832463991D+00 4.632886450D-02-6.217220730D-05
4.362874990D-08-1.229933986D-11 0.000000000D+00 8.404075240D+03 4.446519890D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15447.032
1.450497280D+06-6.988541540D+03 1.963495452D+01-1.055076741D-03 1.739077548D-07
-1.514730411D-11 5.388727350D-16 0.000000000D+00 5.079336980D+04-8.986041070D+01

```

C2H2Br4 1,1,2,2,Tetrabromoethane B3LYP calc. HF298=53.35 kJ/mol from MOPAC PM3

```

3 T02/04 C 2.00H 2.00BR 4.00 0.00 0.00 0 345.6532800 53350.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 23074.822
6.849675250D+03-3.462292920D+02 7.853622530D+00 6.594531200D-02-4.863002480D-04
1.955985905D-06-2.874611401D-09 0.000000000D+00 4.910971610D+03-7.614927760D+00
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 23074.822
-6.149145930D+04 1.213390485D+03-3.136010859D+00 6.307671190D-02-8.417300680D-05
5.783769170D-08-1.593706203D-11 0.000000000D+00-1.934831114D+03 5.400490640D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 23074.822
2.317170101D+06-1.043908081D+04 2.968769291D+01-3.373188290D-03 6.991887770D-07
-7.480768480D-11 3.247937950D-15 0.000000000D+00 6.433682780D+04-1.438634557D+02

```

CHCL=CH\* Burcat G3B3 calc. HF298=65.671 kcal

```

3 A 8/05 C 2.00H 2.00CL 1.00 0.00 0.00 0 61.4899800 274767.464
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11996.018
-5.482272030D+02 3.351023420D+01 3.360466020D+00 2.639980437D-03 1.892222120D-05
1.278392709D-07-3.732426500D-10 0.000000000D+00 3.148964680D+04 1.143013004D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11996.018
4.925550270D+04-4.186316010D+02 2.206310563D+00 2.531034179D-02-3.414513470D-05
2.437903256D-08-6.945611260D-12 0.000000000D+00 3.407113430D+04 1.256369941D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11996.018
1.591893593D+06-6.572857800D+03 1.611616762D+01-8.058388360D-04 1.139675003D-07
-7.967271830D-12 1.980388369D-16 0.000000000D+00 7.056178150D+04-7.352591910D+01

```

CH2=CCL2 1,1 dichloro-Ethylene IR + Shimanouchi Webbook 2000

```

3 T05/01 C 2.00H 2.00CL 2.00 0.00 0.00 0 96.9426800 2200.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13871.984
-1.700333669D+03 8.973620630D+01 2.829202394D+00-1.083482484D-02 2.982438346D-04
-1.124765802D-06 1.503801169D-09 0.000000000D+00-1.727445740D+03 1.581503170D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13871.984
4.696010490D+04-5.891236420D+02 3.823588040D+00 2.794428434D-02-3.542717070D-05
2.413455286D-08-6.687475950D-12 0.000000000D+00 1.665112543D+03 4.218476650D+00
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13871.984
1.458403524D+06-7.074914290D+03 1.986082870D+01-1.190707074D-03 2.113034119D-07
-2.009128059D-11 7.920767130D-16 0.000000000D+00 3.923058160D+04-9.464769070D+01

```

Table 5 (continued)

CH2-CCL3 1,1,1-TrichloroEthane RADICAL LIU et al JPC 107 (2003),6231											
3	T08/03	C	2.00H	2.00CL	3.00	0.00	0.00	0	132.3953800	82810.000	
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0 18248.417
-9.676530780D+03 6.814456400D+02-1.372776086D+01 1.959314398D-01-7.640292140D-04											
	1.682678242D-06	-1.524618815D-09	0.000000000D+00	5.577160760D+03	8.380219200D+01	200.000	1000.000	7	-2.0	-1.0	0.0 1.0 2.0 3.0 4.0 0.0 18248.417
3.999027650D+04-7.148351060D+02 5.818737300D+00 3.953649430D-02-6.004233320D-05											
4.439578900D-08-1.273826918D-11 0.000000000D+00 1.112328688D+04-5.158674820D+00											
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0 18248.417
9.594143540D+05-4.727178380D+03 2.039255891D+01-3.486572490D-04 1.680487523D-08											
2.931915287D-12-3.010580344D-16 0.000000000D+00 3.365865850D+04-8.791498970D+01											
C2H2F4 CF3-CF2 1,1,1,2 TetraFluoroEthane HFC-134a Zachariah 1996											
3	T 5/03	C	2.00H	2.00F	4.00	0.00	0.00	0	102.0308928	-913300.000	
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0 16937.323
1.126052808D+03-8.128232020D+01 5.848936590D+00-1.694763396D-02 3.011967478D-04											
-1.047574273D-06 1.415941580D-09 0.000000000D+00-1.116171330D+05 2.541986397D+00											
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0 16937.323
-1.283973875D+05 2.529316853D+03-1.630989335D+01 9.601052750D-02-1.231423322D-04											
8.059691160D-08-2.125747297D-11 0.000000000D+00-1.231516473D+05 1.148420252D+02											
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0 16937.323
5.168435080D+05-6.103534560D+03 2.457199159D+01-7.746286500D-04 9.435001330D-08											
-6.570150990D-12 2.083024595D-16 0.000000000D+00-8.054164820D+04-1.191500403D+02											
C2H2F4 CHF2-CHF2 1,1,2,2 TetraFluoroEthane HFC-134 Zachariah 1996											
3	T 5/03	C	2.00H	2.00F	4.00	0.00	0.00	0	102.0308928	-883300.000	
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0 17130.423
2.969174082D+02 1.003033845D+01 2.339912220D+00 4.496831970D-02-1.456859413D-04											
3.873582560D-07-3.762588070D-10 0.000000000D+00-1.082891978D+05 1.475527029D+01											
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0 17130.423
-2.375905832D+05 4.175886520D+03-2.432149737D+01 1.115957395D-01-1.386857006D-04											
8.839484900D-08-2.280263654D-11 0.000000000D+00-1.274726331D+05 1.610619314D+02											
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0 17130.423
7.933510980D+05-7.141667700D+03 2.542974515D+01-1.090808727D-03 1.362200159D-07											
-7.925687190D-12 1.357819787D-16 0.000000000D+00-7.040459930D+04-1.263670737D+02											
CH2CN Methyl-Cyanid Radical MELIUS A66S											
3	T01/03	C	2.00H	2.00N	1.00	0.00	0.00	0	40.0440200	257776.240	
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0 12356.289
-2.100455061D+03 1.025029481D+02 2.814725636D+00-1.245952654D-02 3.025178153D-04											
-1.324826167D-06 2.008709315D-09 0.000000000D+00 2.913826790D+04 1.311707214D+01											
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0 12356.289
-3.693721460D+03 7.902406330D+01 2.022406508D+00 1.957375619D-02-2.106660784D-05											
1.343219698D-08-3.666510380D-12 0.000000000D+00 2.922887882D+04 1.447901336D+01											
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0 12356.289
1.745376887D+06-7.458452000D+03 1.720148106D+01-1.341338527D-03 2.468771780D-07											
-2.437053814D-11 9.977513240D-16 0.000000000D+00 7.384960760D+04-8.321026210D+01											

Table 5 (continued)

CH2NC Methylene Isocyanate radical Janoshchek & Rossi Int J Chem Kin 36,2004,661  
 3 A12/04 C 2.00H 2.00N 1.00 0.00 0.00 0 40.0440200 358230.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12550.171  
 -3.343233910D+03 2.092116186D+02-6.000070670D-01 3.711717460D-02-1.986677730D-05  
 -3.205013350D-07 7.437433370D-10 0.000000000D+00 4.087517110D+04 2.617671553D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12550.171  
 -4.857828990D+04 6.475317090D+02 8.128495810D-02 2.128747218D-02-2.092883102D-05  
 1.215971750D-08-3.057823672D-12 0.000000000D+00 3.842453550D+04 2.679198230D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12550.171  
 2.039433927D+06-8.117870280D+03 1.731240468D+01-1.298527013D-03 2.255518692D-07  
 -2.103452124D-11 8.147068920D-16 0.000000000D+00 9.050567890D+04-8.465337300D+01

NCCH2OO NC-CH2-OO\* Radical Burcat G3B3 calc. HF298=42.54 kcal  
 3 T06/04 C 2.00H 2.00N 1.00O 2.00 0.00 0 72.0428200 177987.360  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16206.829  
 3.502747330D+02-5.453753890D+01 6.347631150D+00-2.330136812D-02 3.455363250D-04  
 -1.407136019D-06 2.137051847D-09 0.000000000D+00 1.959747647D+04 1.094181709D+00  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16206.829  
 -1.211140493D+05 2.166460633D+03-1.063329700D+01 6.474487520D-02-7.715240020D-05  
 4.921527740D-08-1.292604736D-11 0.000000000D+00 9.540090430D+03 8.847212860D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16206.829  
 1.889424824D+06-9.590161270D+03 2.445803095D+01-1.758813163D-03 3.263868120D-07  
 -3.245025900D-11 1.336754104D-15 0.000000000D+00 7.482320530D+04-1.237331717D+02

C2H2(NO2)2 DI-NITRO-ETHYLENE trans HF298=9.788 kcal Burcat G3B3  
 3 A 5/05 C 2.00H 2.00N 2.00O 4.00 0.00 0 118.0483600 40952.992  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 21427.506  
 3.165527440D+03-2.163988341D+02 7.947824130D+00 2.202744917D-02-1.676425853D-04  
 1.037985775D-06-1.755598815D-09 0.000000000D+00 3.066587512D+03-7.437870060D+00  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 21427.506  
 -2.384723639D+05 4.519835370D+03-2.795201421D+01 1.364147679D-01-1.649464277D-04  
 1.011738275D-07-2.509873402D-11 0.000000000D+00-1.808666957D+04 1.823061425D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 21427.506  
 7.672256000D+05-9.234021290D+03 3.475932560D+01-2.968088795D-03 6.108455640D-07  
 -6.535420630D-11 2.850072874D-15 0.000000000D+00 5.001111370D+04-1.800642358D+02

C2H2O2 Oxyranone CH2(-O-)-C=O Burcat G3B3 calc HF=-42.523 kcal  
 3 A 3/05 C 2.00H 2.00O 2.00 0.00 0.00 0 58.0360800 -177916.232  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11713.127  
 2.421349112D+03-1.789012046D+02 9.201509510D+00-7.403914030D-02 5.151077290D-04  
 -1.513314534D-06 1.848746823D-09 0.000000000D+00-2.224546835D+04-1.233133110D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11713.127  
 -6.532311920D+04 1.627658379D+03-1.131276654D+01 6.269898200D-02-7.750192520D-05  
 5.061494020D-08-1.349333178D-11 0.000000000D+00-2.971391996D+04 8.562479210D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11713.127  
 1.615504550D+06-8.453546810D+03 2.058694921D+01-1.406035669D-03 2.478390926D-07  
 -2.339124419D-11 9.148129730D-16 0.000000000D+00 2.580234458D+04-1.052354114D+02

Table 5 (continued)

C2H2O4 HO-CO-CO-OH OXALIC Acid Dorofeeva et al JPCRD 30 (2001),475.

```

3 T 5/03 C 2.00H 2.00O 4.00 0.00 0.00 0 90.0348800 -731800.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17191.065
1.820990731D+03-1.533267529D+02 9.663677350D+00-7.732872810D-02 6.831782370D-04
-2.050493739D-06 2.271184078D-09 0.000000000D+00-8.963328310D+04-1.067498287D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17191.065
3.111073208D+04-4.011746360D+02 3.229060890D+00 3.727998910D-02-3.991470870D-05
2.276230039D-08-5.354407840D-12 0.000000000D+00-8.793426480D+04 9.466587740D+00
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17191.065
2.002528183D+06-9.733382340D+03 2.662275940D+01-1.434440102D-03 1.853910697D-07
-1.085296800D-11 1.667062846D-16 0.000000000D+00-3.427905070D+04-1.355610688D+02

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C2H2O4 HO-CO-CO-OH OXALIC Acid Dorofeeva et al JPCRD 30 (2001),475

```

3 T 5/03 C 2.00H 2.00O 4.00 0.00 0.00 0 90.0348800 -731800.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17191.065
1.820990731D+03-1.533267529D+02 9.663677350D+00-7.732872810D-02 6.831782370D-04
-2.050493739D-06 2.271184078D-09 0.000000000D+00-8.963328310D+04-1.067498287D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17191.065
3.111073208D+04-4.011746360D+02 3.229060890D+00 3.727998910D-02-3.991470870D-05
2.276230039D-08-5.354407840D-12 0.000000000D+00-8.793426480D+04 9.466587740D+00
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17191.065
2.002528183D+06-9.733382340D+03 2.662275940D+01-1.434440102D-03 1.853910697D-07
-1.085296800D-11 1.667062846D-16 0.000000000D+00-3.427905070D+04-1.355610688D+02

```

C2H3 Vinyl Radical. HF298=296.58+/-0.9 kJ from ATcT A

```

3 ATcT/A C 2.00H 3.00 0.00 0.00 0.00 0 27.0452200 296580.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10521.791
-2.922284245D+02 2.781567642D+01 2.970573713D+00 1.891567683D-02-1.794959839D-04
8.011000790D-07-1.142919872D-09 0.000000000D+00 3.432417660D+04 8.782026700D+00
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10521.791
-5.270888700D+04 1.344532354D+03-7.986780480D+00 4.379583700D-02-5.421840800D-05
3.667092730D-08-1.011648829D-11 0.000000000D+00 2.867877682D+04 6.686971470D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10521.791
2.553048273D+06-9.892565200D+03 1.795973155D+01-1.384212823D-03 2.183717030D-07
-1.806549427D-11 6.030168790D-16 0.000000000D+00 9.455440350D+04-9.463460830D+01

```

NCCH2OH Cyanometanol Radical Burcat G3B3 calc HF298=41.974 kcal

```

3 T06/04 C 2.00H 2.00N 1.00O 1.00 0.00 0 56.0434200 175619.216
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13443.657
-1.094898324D+03 1.051460934D+02 5.062404610D-01 4.609226230D-02-1.879320872D-04
5.527306810D-07-6.561938250D-10 0.000000000D+00 1.919651923D+04 2.228315842D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13443.657
-4.477372260D+04 9.198134740D+02-3.977420890D+00 4.139075280D-02-4.852325350D-05
3.147384853D-08-8.507409550D-12 0.000000000D+00 1.544781515D+04 4.884943970D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13443.657
1.867413796D+06-8.951713600D+03 2.126257158D+01-1.747533743D-03 3.333789210D-07
-3.399257430D-11 1.432755583D-15 0.000000000D+00 7.176889440D+04-1.073323114D+02

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Table 5 (continued)

CH<sub>2</sub>Br-COOH Bromoacetic acid Dorofeeva JPCRD 30 (2001), 475

```

3 T 6/03 C 2.00H 3.00O 2.00BR 1.00 0.00 0 138.9480200 -383500.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16862.437
1.261205546D+03-9.948938450D+01 6.855649360D+00-1.725697179D-02 2.173333077D-04
-6.379631350D-07 7.678927150D-10 0.000000000D+00-4.784672990D+04 7.685597190D-01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16862.437
-7.654774610D+04 1.625744210D+03-9.232480470D+00 6.851046540D-02-8.341205030D-05
5.389802050D-08-1.421772901D-11 0.000000000D+00-5.529903430D+04 8.099143430D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16862.437
2.219803717D+06-1.058070449D+04 2.653209586D+01-1.191187291D-03 1.189897631D-07
-3.431268920D-12-1.437345521D-16 0.000000000D+00 1.319089350D+04-1.347708927D+02

```

CH<sub>3</sub>CB<sub>3</sub> 1,1,1-TRIBROMOETHANE HF298 NIST94 est. Vib & Ir B3LYP-G3 calc

```

3 T11/03 C 2.00BR 3.00H 3.00 0.00 0.00 0 266.7572200 -26300.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20050.659
-3.428714170D+03 3.308290530D+02-8.233585840D+00 1.950406584D-01-9.870449990D-04
2.772753646D-06-3.221466560D-09 0.000000000D+00-6.526130320D+03 5.826438140D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20050.659
-1.411707321D+05 1.935911205D+03-5.584508980D+00 5.855879870D-02-6.750036860D-05
4.094682610D-08-1.015149587D-11 0.000000000D+00-1.508417368D+04 6.543813850D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20050.659
1.720058595D+06-8.585001840D+03 2.610704694D+01-1.402049310D-03 2.462568347D-07
-2.322944969D-11 9.100918860D-16 0.000000000D+00 4.337164060D+04-1.258635536D+02

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C<sub>2</sub>H<sub>3</sub><sup>+</sup> Vinylum FROM ORIGINAL ATcT A tables

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2 ATcT/A C 2.00H 3.00E -1.00 0.00 0.00 0 27.0446714 1122390.000
298.150 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11780.000
1.607381577D+05-2.041555104D+03 1.241283252D+01-7.721657400D-03 1.409085814D-05
-9.106449140D-09 2.126444466D-12 0.000000000D+00 1.436976135D+05-4.781122620D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11780.000
2.986773191D+06-1.088989861D+04 1.979215390D+01-2.357481771D-03 4.161033220D-07
-2.665180805D-11 2.134014753D-16 0.000000000D+00 2.002979794D+05-1.072429380D+02

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C<sub>2</sub>H<sub>3</sub>CL ChloroEthylene HF298 ATcT A 2005. Gurvich,1991

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3 ATcT/A C 2.00H 3.00CL 1.00 0.00 0.00 0 62.4979200 37872.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11819.647
3.722977050D+01-1.539552324D+01 4.880044060D+00-1.917109754D-02 1.696600637D-04
-4.338641110D-07 5.011620350D-10 0.000000000D+00 3.167895300D+03 4.938422210D+00
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11819.647
-4.345645830D+04 1.241756796D+03-8.699681730D+00 5.558577390D-02-7.029940020D-05
4.751804890D-08-1.305459661D-11 0.000000000D+00-2.009308473D+03 7.140002560D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11819.647
2.267340655D+06-1.000243919D+04 2.133189198D+01-1.598789596D-03 2.746727745D-07
-2.518626075D-11 9.542560860D-16 0.000000000D+00 6.228435850D+04-1.116581493D+02

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CH<sub>2</sub>Cl-COOH Chloroacetic acid Dorofeeva JPCRD 30 (2001), 475

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3 T 6/03 C 2.00H 3.00O 2.00CL 1.00 0.00 0 94.4967200 -427600.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16513.941
-3.392547970D+02 1.110122279D+01 4.080429330D+00 1.149532023D-02 6.303729890D-05
-2.452895771D-07 3.802809800D-10 0.000000000D+00-5.346709320D+04 1.118838521D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16513.941
-1.100242123D+05 2.138158840D+03-1.211980092D+01 7.474046480D-02-9.031926690D-05
5.783008220D-08-1.512992611D-11 0.000000000D+00-6.299719190D+04 9.605452030D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16513.941
2.123118360D+06-1.049379479D+04 2.647064535D+01-1.203394050D-03 1.411322273D-07
-8.179337050D-12 1.599402308D-16 0.000000000D+00 7.155960020D+03-1.358236627D+02

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Table 5 (continued)

C2H2F2 1,1 DiFluoroethylene Gurvich,1991 HF298=-336.4+/-4 kJ										
3 RUS 91 C	2.00H	2.00F	2.00	0.00	0.00	0	64.0340864	-336400.000		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.863475060D+03	-2.822023679D+02	1.213245342D+01	-1.150591172D-01	7.951722010D-04						
-2.272354093D-06	2.547853319D-09	0.000000000D+00	-4.107119010D+04	-2.402367947D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.629904640D+04	-1.525540113D+02	-6.511988010D-01	3.844715290D-02	-4.777957090D-05						
3.158840363D-08	-8.522908780D-12	0.000000000D+00	-4.061942280D+04	2.579833878D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.467562283D+06	-7.581205180D+03	2.016222600D+01	-1.292963501D-03	2.313040404D-07						
-2.218294569D-11	8.823901970D-16	0.000000000D+00	1.378041556D+03	-1.005481325D+02						
C2H2F2 cis-DiFluoroEthylene Gurvich,1991 HF287=-306.4+/-5. kJ										
3 RUS 91 C	2.00H	2.00F	2.00	0.00	0.00	0	64.0340864	-306500.000		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.115462509D+02	4.957358570D+01	1.692705616D+00	3.911588830D-02	-2.482906285D-04						
1.002570103D-06	-1.415555189D-09	0.000000000D+00	-3.851327880D+04	1.614044632D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.286254670D+04	1.545872687D+03	-1.013865480D+01	6.117946410D-02	-7.625229350D-05						
4.984717720D-08	-1.325846339D-11	0.000000000D+00	-4.499682740D+04	7.965130060D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.411303353D+06	-7.639075480D+03	2.016295184D+01	-1.280876337D-03	2.265435464D-07						
-2.144850085D-11	8.413236680D-16	0.000000000D+00	5.175626060D+03	-1.005836769D+02						
C2H2F2 trans-DiFluoroEthylene Gurvich,1991 HF298=-303.6+/-5 kJ										
3 RUS 91 C	2.00H	2.00F	2.00	0.00	0.00	0	64.0340864	-303600.000		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.335418010D+03	2.737050739D+02	-2.224273103D+00	5.792743840D-02	-1.736257851D-04						
2.759529626D-07	-4.400309040D-11	0.000000000D+00	-3.898441490D+04	3.389833080D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.039163020D+05	1.939584127D+03	-1.092994874D+01	6.134250840D-02	-7.469611260D-05						
4.785499530D-08	-1.251227641D-11	0.000000000D+00	-4.681043020D+04	8.504245490D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.452325436D+06	-7.675216720D+03	2.021430428D+01	-1.309218665D-03	2.342044291D-07						
-2.245813433D-11	8.931373570D-16	0.000000000D+00	5.834070480D+03	-1.009136760D+02						
CH3CCl3 1,1,1-Trichloroethane Ruscic & Burcat B3LYP-G3 + HF298 Manion										
3 T11/03 C	2.00H	3.00CL	3.00	0.00	0.00	0	133.4033200	-144600.000		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.123619596D+04	8.008208710D+02	-1.732195899D+01	2.482476384D-01	-1.129814532D-03						
2.856488509D-06	-2.995963104D-09	0.000000000D+00	-2.211723934D+04	9.671433900D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.190579028D+05	1.655871399D+03	-6.325616580D+00	6.305079060D-02	-7.580483860D-05						
4.758802030D-08	-1.212975508D-11	0.000000000D+00	-2.756010611D+04	6.363575200D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.741175660D+06	-8.764349080D+03	2.608017110D+01	-1.350284329D-03	2.286217604D-07						
-2.069587426D-11	7.749215400D-16	0.000000000D+00	3.020679652D+04	-1.304843183D+02						

Table 5 (continued)

CH3CD3 1,1,1-Deuterated Ethane Ruscic and Burcat G3B3LYP calc 2004

3	T11/03	C	2.00H	3.00D	3.00	0.00	0.00	0	33.0875260	-107570.000			
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12406.195
-1.492758368D+03	1.359748668D+02	-5.183780280D-01	6.671156190D-02	-4.366122950D-04									
1.585091826D-06	-2.064749269D-09	0.000000000D+00	-1.483291065D+04	2.208455557D+01									
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12406.195	
-9.843753110D+04	2.176762446D+03	-1.376197442D+01	6.616320990D-02	-7.114440400D-05									
4.372107940D-08	-1.150017836D-11	0.000000000D+00	-2.396012915D+04	9.733479550D+01									
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12406.195	
3.610269530D+06	-1.666504742D+04	3.131769964D+01	-3.272594620D-03	6.272993890D-07									
-6.429312170D-11	2.724038523D-15	0.000000000D+00	8.426327920D+04	-1.857826659D+02									

C2H3F FluoroEthylene Gurvich, 1991

3	tpis91	C	2.00H	3.00F	1.00	0.00	0.00	0	46.0436232	-140100.000			
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11335.928
1.004028717D+03	-7.258831720D+01	6.043282840D+00	-2.742800316D-02	1.669413336D-04									
-3.262491010D-07	3.018208182D-10	0.000000000D+00	-1.798372901D+04	-1.219667289D+00									
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11335.928	
-7.304811120D+04	1.808666383D+03	-1.245493578D+01	6.405175290D-02	-8.015881690D-05									
5.342751760D-08	-1.449763709D-11	0.000000000D+00	-2.592411808D+04	9.103049560D+01									
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11335.928	
2.283027588D+06	-1.027003730D+04	2.147608001D+01	-1.643219749D-03	2.826144842D-07									
-2.595090234D-11	9.848845110D-16	0.000000000D+00	4.243498960D+04	-1.145898994D+02									

CH3CF3 1,1,1-Trifluoroethane Ruscic and Burcat G3B3LYP calc

3	T11/03	C	2.00H	3.00F	3.00	0.00	0.00	0	84.0404296	-755655.000			
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15298.075
-1.377810077D+03	8.789794820D+01	2.235684801D+00	2.467147835D-03	2.527852566D-04									
-1.058469552D-06	1.525390914D-09	0.000000000D+00	-9.301849890D+04	1.654094195D+01									
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15298.075	
-9.792056230D+04	1.766761748D+03	-1.047025816D+01	7.179745020D-02	-8.696744790D-05									
5.567238490D-08	-1.454347429D-11	0.000000000D+00	-1.006828771D+05	8.162251700D+01									
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15298.075	
2.216380412D+06	-1.095245917D+04	2.740803889D+01	-1.802383154D-03	3.165532250D-07									
-2.979736606D-11	1.163108958D-15	0.000000000D+00	-2.966374005D+04	-1.467044923D+02									

C2H3I Ethylene Iodide Approximate value Burcat B3LYP/6-311G\* calc

3	A 8/05	C	2.00H	3.00I	1.00	0.00	0.00	0	153.9496900	128867.200			
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12368.495
-5.991528280D+02	2.950525086D+01	3.803887770D+00	-1.112358659D-02	1.994349836D-04									
-7.433428480D-07	1.066977974D-09	0.000000000D+00	1.390065267D+04	1.339991914D+01									
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12368.495	
-8.225250770D+04	1.628997545D+03	-9.280318310D+00	5.506618420D-02	-6.780336710D-05									
4.494515550D-08	-1.217557570D-11	0.000000000D+00	6.777200120D+03	8.013736290D+01									
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12368.495	
2.308153554D+06	-1.004374744D+04	2.142275865D+01	-1.651130787D-03	2.887608788D-07									
-2.701819548D-11	1.046938762D-15	0.000000000D+00	7.356599540D+04	-1.078117011D+02									

Table 5 (continued)

## CH3CN Methyl-Cyanid Melius R4A

3	T01/03	C	2.00H	3.00N	1.00	0.00	0.00	0	41.0519600	74040.064		
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12094.102
-4.649490110D+03	2.823131212D+02	-2.128992646D+00	5.352151060D-02	-1.309779216D-04								
-2.490517400D-08	5.441996350D-10	0.000000000D+00	6.497985560D+03	3.135921409D+01								
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12094.102
-1.122737345D+05	1.920539504D+03	-8.910690360D+00	4.578222820D-02	-4.921556410D-05								
3.034707254D-08	-7.977792750D-12	0.000000000D+00	-1.413648262D+03	7.412277070D+01								
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12094.102
2.832369559D+06	-1.211419144D+04	2.303101482D+01	-2.310227322D-03	4.369402830D-07								
-4.424067510D-11	1.854072785D-15	0.000000000D+00	8.003506850D+04	-1.276833918D+02								

## CH3NC Methyl-IsoCyanid Melius R4B

3	T01/03	C	2.00H	3.00N	1.00	0.00	0.00	0	41.0519600	163498.168		
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12659.906
-5.447117950D+03	4.202746310D+02	-8.290591220D+00	1.634587202D-01	-9.531688370D-04								
2.830854907D-06	-3.306187730D-09	0.000000000D+00	1.683460210D+04	5.339847850D+01								
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12659.906
-1.597999630D+05	2.579125965D+03	-1.119156698D+01	4.808594450D-02	-4.856221750D-05								
2.798425763D-08	-6.940372140D-12	0.000000000D+00	6.009921140D+03	8.877066040D+01								
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12659.906
2.873803913D+06	-1.231158225D+04	2.321682285D+01	-2.397183257D-03	4.584467950D-07								
-4.692324450D-11	1.986719257D-15	0.000000000D+00	9.201716940D+04	-1.287070495D+02								

## NCCH2OH Cyanomethanol Burcat G3B3 calc. HF298=-11.881 kcal

3	T06/04	C	2.00H	3.00N	1.00O	1.00	0.00	0	57.0513600	-49710.104		
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13745.295
-1.482599682D+03	1.015282252D+02	1.581761862D+00	1.753329672D-02	9.081842950D-05								
-5.700791090D-07	1.024615334D-09	0.000000000D+00	-7.962196630D+03	1.887537190D+01								
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13745.295
-1.168088823D+05	2.127892614D+03	-1.191989757D+01	6.677184670D-02	-8.234211990D-05								
5.421656300D-08	-1.454644274D-11	0.000000000D+00	-1.728103924D+04	9.146806920D+01								
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13745.295
2.528736341D+06	-1.092206338D+04	2.382181992D+01	-1.439524732D-03	2.187706837D-07								
-1.724320221D-11	5.376291270D-16	0.000000000D+00	5.700313520D+04	-1.257820354D+02								

## NC-CH2-O-OH Cyanomethylperoxide Burcat G3B3 calc HF298=7.045 kcal

3	A08/04	C	2.00H	3.00N	1.00O	2.00	0.00	0	73.0507600	29476.280		
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17659.292
-2.742428451D+03	1.946989087D+02	-1.634039342D+00	8.786167600D-02	-3.090722624D-04								
4.878297440D-07	-3.863978770D-11	0.000000000D+00	8.048735320D+02	3.215385790D+01								
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17659.292
-1.377324374D+05	2.367827621D+03	-1.104608082D+01	6.996194890D-02	-8.632459470D-05								
5.708122640D-08	-1.540541198D-11	0.000000000D+00	-9.566780640D+03	9.146447020D+01								
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17659.292
3.081209348D+06	-1.274970037D+04	2.803052981D+01	-2.180057766D-03	3.418050350D-07								
-2.747653892D-11	8.734623330D-16	0.000000000D+00	7.738185640D+04	-1.479817805D+02								

Table 5 (continued)

CH<sub>3</sub>CO ACETYL RADICAL IUPAC Task Force on Selected Radicals

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3 IU3/03 C 2.00H 3.000 1.00 0.00 0.00 0 43.04462 -10300.000
50.000 200.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12384.876
-0.289526090D+03-0.224742331D+02 0.605096002D+01-0.271517644D-01 0.215987228D-03
-0.680810164D-06 0.929713833D-09 0.000000000D+00-0.270326257D+04 0.312464303D+00
200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12384.876
-0.832517467D+05 0.166349507D+04-0.821828123D+01 0.440865769D-01-0.466819786D-04
0.281559250D-07-0.727271377D-11 0.000000000D+00-0.101449608D+05 0.727981860D+02
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12384.876
0.241707944D+07-0.110326222D+05 0.221114619D+02-0.223777883D-02 0.434799315D-06
-0.450988885D-10 0.193091426D-14 0.000000000D+00 0.627792109D+05-0.117810562D+03

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CH<sub>3</sub>CO<sup>+</sup> Acetylium Ion from B Ruscic ACTIVE TABLES generator. HF298=669.952 kJ.

```

3 A12/04 C 2.00H 3.000 1.00E -1.00 0.00 0 43.0440714 669952.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11977.000
-3.925439670D+03 2.171933733D+02-1.072511090D-01 2.674968268D-02 1.626223378D-05
-3.762764560D-07 8.463736500D-10 0.000000000D+00 7.837937190D+04 2.358037482D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11977.000
-9.502446620D+04 1.753104579D+03-9.037540410D+00 4.937113420D-02-5.705421630D-05
3.708566560D-08-1.007656173D-11 0.000000000D+00 7.120473910D+04 7.361901970D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11977.000
2.813803848D+06-1.196089831D+04 2.303011402D+01-2.341154304D-03 4.487660480D-07
-4.602119540D-11 1.951358410D-15 0.000000000D+00 1.507345913D+05-1.273376802D+02

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C<sub>2</sub>H<sub>3</sub>O Ethylene Oxide (Oxyran) radical Burcat G3B3 calc HF298=164.47 kJ

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3 A 1/05 C 2.00H 3.000 1.00 0.00 0.00 0 43.0446200 164473.040
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10722.521
-6.249174130D+02 5.035990420D+01 2.370345336D+00 2.679031770D-02-2.307943676D-04
9.384032040D-07-1.178438088D-09 0.000000000D+00 1.833856930D+04 1.335231790D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10722.521
-1.690943318D+05 3.598590680D+03-2.415994141D+01 9.496480590D-02-1.214286347D-04
8.100213950D-08-2.184447090D-11 0.000000000D+00 2.616433556D+03 1.555550362D+02
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10722.521
2.128234000D+06-1.005583145D+04 2.113582112D+01-1.460789489D-03 2.351904524D-07
-1.991372381D-11 6.838252120D-16 0.000000000D+00 7.748407760D+04-1.127030193D+02

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CH<sub>2</sub>BrCH<sub>2</sub>Br 1,2-DiBROMOETHANE HF298 CRC2001 -37.5 kJ/mol

```

3 T 1/04 C 2.00BR 2.00H 4.00 0.00 0.00 0 187.8611600 -37500.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16554.284
3.829389960D+03-1.944913702D+02 6.700448590D+00 2.331603554D-02-2.376239163D-04
1.162296415D-06-1.758120764D-09 0.000000000D+00-5.798061420D+03-2.435158601D+00
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16554.284
-1.302142474D+05 2.723434087D+03-1.616056140D+01 8.457534180D-02-1.042154012D-04
6.867293920D-08-1.858351839D-11 0.000000000D+00-1.861099589D+04 1.189042923D+02
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16554.284
2.266450017D+06-1.220165886D+04 2.932799026D+01-3.083496248D-03 6.392342330D-07
-6.959186290D-11 3.092347956D-15 0.000000000D+00 6.374219080D+04-1.555472067D+02

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Table 5 (continued)

CH<sub>3</sub>CHBr<sub>2</sub> 1,1-DiBROMOETHANE HF298 -41. kJ/mol Kudchadker JPCRD 8 1979 , 519  
 3 T 1/04 C 2.00BR 2.00H 4.00 0.00 0.00 0 187.8611600 -41000.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16288.081  
 -3.904390400D+03 3.242216150D+02-6.208383640D+00 1.402272254D-01-6.854993110D-04  
 1.880926725D-06-2.040976934D-09 0.000000000D+00-7.873541080D+03 5.187575800D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16288.081  
 -1.944627265D+05 3.348585260D+03-1.854615785D+01 9.223242460D-02-1.160103681D-04  
 7.676686740D-08-2.060462625D-11 0.000000000D+00-2.234919739D+04 1.321971657D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16288.081  
 2.545076215D+06-1.183192454D+04 2.793428482D+01-1.969912177D-03 3.459438260D-07  
 -3.246636280D-11 1.260562205D-15 0.000000000D+00 6.216753270D+04-1.462166108D+02

C<sub>2</sub>H<sub>4</sub>Cl<sub>2</sub> 1,2-DiChloroETHANE CH<sub>2</sub>ClCH<sub>2</sub>Cl HF298 --130.069+/-0.6 kJ REF=ATcT A  
 3 ATCT/A C 2.00H 4.00CL 2.00 0.00 0.00 0 98.9585600 -130069.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15531.491  
 -2.949009327D+03 2.323390693D+02-3.539793430D+00 1.296344781D-01-8.322109500D-04  
 2.824578699D-06-3.605014700D-09 0.000000000D+00-1.822335156D+04 3.790725250D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15531.491  
 -1.777837569D+05 3.405967820D+03-1.991139017D+01 8.972610710D-02-1.017902595D-04  
 6.158027770D-08-1.554243795D-11 0.000000000D+00-3.291224620D+04 1.376373445D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15531.491  
 1.406791008D+06-1.084562394D+04 2.945783904D+01-3.391164120D-03 7.430979470D-07  
 -8.432933940D-11 3.870603920D-15 0.000000000D+00 4.243734740D+04-1.583336292D+02

C<sub>2</sub>H<sub>4</sub>Cl<sub>2</sub>O<sub>2</sub> CHCl<sub>2</sub>CH<sub>2</sub>OOH ALFA-DI-Cl PEROXYETHANE BOZZELLI JPC 100 (1996) 8240  
 3 T01/97 C 2.00H 4.00O 2.00CL 2.00 0.00 0 130.9573600 -231375.200  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20696.633  
 -9.599873880D+03 6.352981640D+02-1.163993117D+01 1.775974664D-01-6.215491680D-04  
 1.222301973D-06-9.011155780D-10 0.000000000D+00-3.239864940D+04 7.760888970D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20696.633  
 -1.825655151D+05 2.918263056D+03-1.579435926D+01 1.025840982D-01-1.267628770D-04  
 8.060304750D-08-2.076678532D-11 0.000000000D+00-4.394729000D+04 1.166724609D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20696.633  
 1.201013850D+06-9.138632850D+03 3.215187150D+01-1.971407789D-03 3.970246860D-07  
 -4.293414910D-11 1.886387175D-15 0.000000000D+00 1.867502510D+04-1.632280929D+02

C<sub>2</sub>H<sub>4</sub>F<sub>2</sub> 1,2-DiFLUOROETHANE CH<sub>2</sub>FCH<sub>2</sub>F HF298=-450.36+/-4.9 kJ ATcT A  
 3 ATCT/A C 2.00H 4.00F 2.00 0.00 0.00 0 66.0499664 -450360.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14103.016  
 -1.221940252D+03 1.003090930D+02 3.771478120D-01 6.176142050D-02-3.158587842D-04  
 9.056509900D-07-9.351977530D-10 0.000000000D+00-5.615944420D+04 2.131153322D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14103.016  
 -3.261380340D+05 5.456764120D+03-3.003630522D+01 1.071120553D-01-1.182040185D-04  
 6.918097700D-08-1.674603321D-11 0.000000000D+00-8.123981770D+04 1.940124673D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14103.016  
 2.364561162D+06-1.291457274D+04 2.894847677D+01-2.313619810D-03 3.865969530D-07  
 -3.553040560D-11 1.389547961D-15 0.000000000D+00 1.850807338D+04-1.614502783D+02

Table 5 (continued)

C2H4F2 1,1-DiFluoroEthane CH3CHF2 HF298 -497.0+/-4.0 Webbook 2003											
3	ATCT/A	C	2.00H	4.00F	2.00	0.00	0.00	0	66.0499664	-501310.000	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13870.986
-9.269221200D+02	6.423989940D+01	2.504843731D+00	7.007955200D-03	1.534873066D-04							
-7.469972660D-07	1.227977249D-09	0.000000000D+00	-6.217030700D+04	1.517715678D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13870.986
-1.457268609D+05	2.559661486D+03	-1.421956548D+01	7.172560860D-02	-8.402525160D-05							
5.456955620D-08	-1.468723960D-11	0.000000000D+00	-7.367304280D+04	1.046217680D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13870.986
3.931066580D+06	-1.637040050D+04	3.061433639D+01	-2.869612573D-03	5.201481490D-07							
-5.053073730D-11	2.035403503D-15	0.000000000D+00	3.616706180D+04	-1.751146214D+02							
C2H4O3 Glycolic acid HO-CH2-COOH Dorofeeva JPCRD 30 (2001),475											
3	T	8/03	C	2.00H	4.00O	3.00	0.00	0.00	0	76.0513600	-583000.000
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17007.000
-3.819790040D+03	2.566028391D+02	-1.882845160D+00	7.349692530D-02	-2.962448408D-04							
9.738056180D-07	-1.282230066D-09	0.000000000D+00	-7.300850040D+04	3.504299440D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17007.000
-3.151149841D+05	5.706100580D+03	-3.690247080D+01	1.564348482D-01	-2.039991340D-04							
1.340128855D-07	-3.507644330D-11	0.000000000D+00	-9.808286750D+04	2.272524710D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17007.000
1.859541209D+06	-9.541099160D+03	2.813759069D+01	-6.189889660D-04	1.673639202D-08							
7.557318090D-12	-6.662798270D-16	0.000000000D+00	-1.861654321D+04	-1.452428283D+02							
C2H5Br Bromoethane. CH3CH2Br HF298=-61.60+/-1.01 kJ ATcT A											
3	ATcT/A	C	2.00H	5.00BR	1.00	0.00	0.00	0	108.9651000	-61600.000	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13584.044
-3.763733120D+03	3.020084708D+02	-5.074967980D+00	1.217492901D-01	-6.971155350D-04							
2.184006370D-06	-2.608001837D-09	0.000000000D+00	-9.971448920D+03	4.503299670D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13584.044
-1.905528693D+05	3.604454080D+03	-2.216622107D+01	9.579155080D-02	-1.185204121D-04							
7.874242930D-08	-2.137188883D-11	0.000000000D+00	-2.533175319D+04	1.479642742D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13584.044
3.557489400D+06	-1.551254932D+04	3.009009867D+01	-2.682562664D-03	4.812428880D-07							
-4.619637220D-11	1.836674424D-15	0.000000000D+00	8.320780020D+04	-1.703598468D+02							
C2H5Cl Chloroethane. CH3CH2Cl HF298=-106.8+/-0.41 kJ ATcT A											
3	ATcT/A	C	2.00H	5.00CL	1.00	0.00	0.00	0	64.5138000	-106827.000	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13294.268
-4.129470410D+03	3.104264164D+02	-4.836632550D+00	1.139144806D-01	-6.390715250D-04							
1.971676987D-06	-2.296219851D-09	0.000000000D+00	-1.542067009D+04	4.335611790D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13294.268
-1.917124663D+05	3.659952000D+03	-2.278810467D+01	9.699341620D-02	-1.196419280D-04							
7.928561020D-08	-2.148290369D-11	0.000000000D+00	-3.095049114D+04	1.500036580D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13294.268
3.562852590D+06	-1.564447991D+04	3.019772455D+01	-2.727827538D-03	4.915750400D-07							
-4.740905690D-11	1.893910977D-15	0.000000000D+00	7.852095230D+04	-1.727090003D+02							

Table 5 (continued)

C2H5ClO2 CH2CLCH2OOH ALFACHLORO PEROXYETHANE BOZZELLI JPC 100 (1996) 8240										
3 T01/97 C	2.00H	5.00O	2.00CL	1.00	0.00	0	96.5126000	-212965.600		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.707014110D+03	3.042855797D+02	-3.603902420D+00	9.150929360D-02	-2.841969481D-04						
5.354699530D-07	-2.913192175D-10	0.000000000D+00	-2.876097674D+04	4.317825530D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.293721412D+05	4.003997290D+03	-2.379719716D+01	1.146545900D-01	-1.385362517D-04						
8.886738530D-08	-2.338310691D-11	0.000000000D+00	-4.613773160D+04	1.594004765D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.897953710D+06	-1.877941453D+04	4.101366390D+01	-5.612267020D-03	1.184417742D-06						
-1.300898664D-10	5.780861780D-15	0.000000000D+00	8.169242970D+04	-2.347917145D+02						
C2H5F Fluoroethane. CH3CH2F HF298=-275.21/-4.91 kJ ATcT A										
3 ATcT/A C	2.00H	5.00F	1.00	0.00	0.00	0	48.0595032	-275210.000		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.211376628D+03	1.725300402D+02	-1.118570328D+00	6.730688130D-02	-3.491402260D-04						
1.017174919D-06	-1.030622210D-09	0.000000000D+00	-3.518384330D+04	2.800338085D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.201097812D+05	4.098913550D+03	-2.500993423D+01	9.950337180D-02	-1.200518509D-04						
7.825167390D-08	-2.096012916D-11	0.000000000D+00	-5.324216970D+04	1.625744615D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.719670290D+06	-1.634148045D+04	3.065082710D+01	-2.894382218D-03	5.265202260D-07						
-5.128997450D-11	2.070236770D-15	0.000000000D+00	6.262347630D+04	-1.774179538D+02						
C2H5I Iodoethane. HF298=-7.047+/-0.56 kJ ATcT A										
3 ATcT/A C	2.00H	5.00I	1.00	0.00	0.00	0	155.9655700	-7047.000		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.001900780D+02	8.113669910D+01	4.333181560D-01	5.476172740D-02	-2.509441227D-04						
8.101312100D-07	-9.537451290D-10	0.000000000D+00	-2.806016051D+03	2.324812581D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.761579660D+04	2.138907224D+03	-1.412255495D+01	8.052348300D-02	-1.015192715D-04						
6.924236340D-08	-1.925997293D-11	0.000000000D+00	-1.196079366D+04	1.029044800D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.573993280D+06	-1.553615464D+04	3.112732969D+01	-2.700368113D-03	4.853419500D-07						
-4.666120480D-11	1.857508464D-15	0.000000000D+00	8.963621050D+04	-1.750074785D+02						
C2H5N3 Ethyl Azyde Burcat G3B3 calc HF298=63.74 kcal HF0=68.310 kcal										
3 A12/04 C	2.00H	5.00N	3.00	0.00	0.00	0	71.0813200	266872.256		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
8.083205940D+02	-6.047740650D+01	5.367136530D+00	-1.194441553D-02	2.095767968D-04						
-6.156952500D-07	7.294761680D-10	0.000000000D+00	3.039712654D+04	3.916861010D+00						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.786588020D+05	3.146264965D+03	-1.824113698D+01	8.791973930D-02	-9.248120440D-05						
5.424712330D-08	-1.353019565D-11	0.000000000D+00	1.581888719D+04	1.273703780D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.986558680D+06	-2.552903564D+04	4.620231260D+01	-6.988961590D-03	1.339855730D-06						
-1.343224102D-10	5.524470500D-15	0.000000000D+00	1.826914953D+05	-2.806405034D+02						



Table 5 (continued)

CH<sub>3</sub>CH<sub>2</sub>O\* ETHOXY RADICAL IUPAC Task Group on Selected Radicals

3 IU2/03 C 2.00H 5.000 1.00 0.00 0.00 0 45.0605000 -13600.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14235.043  
 -2.349298547D+03 1.462346548D+02 6.734983650D-01 2.538756168D-02 1.258484790D-04  
 -1.004215068D-06 1.948715269D-09 0.000000000D+00 -3.834896340D+03 2.195419386D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14235.043  
 -2.278769249D+05 3.727431270D+03 -1.941223404D+01 8.142837940D-02 -9.290297980D-05  
 5.858782400D-08 -1.540244400D-11 0.000000000D+00 -2.075660097D+04 1.345800381D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14235.043  
 3.794599910D+06 -1.631514577D+04 3.082994592D+01 -3.020456626D-03 5.630596770D-07  
 -5.622948400D-11 2.326262713D-15 0.000000000D+00 9.412204410D+04 -1.770993428D+02

C<sub>2</sub>H<sub>5</sub>O CH<sub>3</sub>\*CHOH RADICAL Janoshck & Rossi IJCK 36, (2004), 661 HF298=-54.03+/-4. kJ

3 T10/04 C 2.00H 5.000 1.00 0.00 0.00 0 45.0605000 -54030.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14262.864  
 -1.312326708D+03 9.607753600D+01 1.619781235D+00 3.619952860D-02 -1.309508248D-04  
 3.338706340D-07 -2.729635404D-10 0.000000000D+00 -8.514220760D+03 1.846707377D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14262.864  
 -1.881087840D+05 3.346306630D+03 -1.867917916D+01 8.198885770D-02 -9.816423800D-05  
 6.371296120D-08 -1.692701242D-11 0.000000000D+00 -2.352069697D+04 1.307380062D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14262.864  
 4.059773200D+06 -1.588483659D+04 2.868944253D+01 -2.060687912D-03 3.090668441D-07  
 -2.389349796D-11 7.225541490D-16 0.000000000D+00 8.795159900D+04 -1.617534649D+02

C<sub>2</sub>H<sub>5</sub>O CH<sub>3</sub>-O-CH<sub>2</sub> HF298=0.96 kJ Janoschek Rossi Int. J. Chem. Kinet 36 (2004)

3 A10/04 C 2.00H 5.000 1.00 0.00 0.00 0 45.0605000 960.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14498.332  
 -4.630123320D+02 9.142368680D+01 -2.110014142D-01 6.861572930D-02 -3.248716140D-04  
 9.410121710D-07 -1.134628651D-09 0.000000000D+00 -1.856959007D+03 2.324219239D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14498.332  
 -1.892901419D+05 2.883291176D+03 -1.264996760D+01 5.904187390D-02 -6.099742000D-05  
 3.588728090D-08 -8.935262190D-12 0.000000000D+00 -1.532768325D+04 9.934745750D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14498.332  
 4.476671470D+06 -1.740082978D+04 3.036357348D+01 -2.855771139D-03 5.024727550D-07  
 -4.747379550D-11 1.863051152D-15 0.000000000D+00 1.040876028D+05 -1.748390292D+02

C<sub>2</sub>H<sub>5</sub>OO PEROXYETHYL RADICAL MELIUS A40

3 T08/00 C 2.00H 5.000 2.00 0.00 0.00 0 61.0599000 -28702.240  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15705.412  
 -3.094946036D+03 2.198568356D+02 -2.398031688D+00 1.011962073D-01 -5.471169080D-04  
 1.640120444D-06 -1.843644015D-09 0.000000000D+00 -6.038575860D+03 3.375180010D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15705.412  
 -2.760086474D+05 4.815010020D+03 -2.723386795D+01 1.077648504D-01 -1.230812281D-04  
 7.629117030D-08 -1.964948653D-11 0.000000000D+00 -2.753589565D+04 1.785504587D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15705.412  
 3.718597000D+06 -1.755546743D+04 3.529361470D+01 -3.413717220D-03 6.510109410D-07  
 -6.639921650D-11 2.800634531D-15 0.000000000D+00 9.796515020D+04 -2.038953649D+02

Table 5 (continued)

CH3-N*-CH3 Dimethyl-azide Dimethyl-amidogen Radical BURCAT G3B3 HF298=159.85 kJ														
3	A09/04	C	2.00H	6.00N	1.00	0.00	0.00	0	44.0757800	159853.904				
			50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14120.151
-4.113738680D+03 3.290953510D+02-5.911061350D+00 1.319464701D-01-7.075671750D-04														
			2.019296485D-06-2.160972968D-09	0.000000000D+00				1.651570630D+04	4.585156870D+01					
			200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14120.151
-2.526290988D+05 4.531416730D+03-2.685048423D+01 1.074025915D-01-1.300758290D-04														
			8.543323850D-08-2.301806719D-11	0.000000000D+00				-3.216601430D+03	1.723611770D+02					
			1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14120.151
4.638495910D+06-1.921923744D+04 3.443507650D+01-3.195357460D-03 5.621107640D-07														
			-5.291421270D-11	2.063180703D-15				0.000000000D+00				1.329731762D+05	-2.042702396D+02	
CH2*-NH-CH3 Methyliden-Methyl-Amine Janoschek & Rossi Int. J. Chem Kin.36,2004														
3	A09/04	C	2.00H	6.00N	1.00	0.00	0.00	0	44.0757800	156580.000				
			50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14356.235
-5.302012320D+03 3.821657690D+02-6.330796960D+00 1.236903111D-01-6.094910580D-04														
			1.737898983D-06-1.938625284D-09	0.000000000D+00				1.588953904D+04	4.963927970D+01					
			200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14356.235
-1.887484855D+05 3.408009060D+03-2.044344907D+01 9.383562670D-02-1.154624922D-04														
			7.675145840D-08-2.076783531D-11	0.000000000D+00				1.584359350D+03	1.370016743D+02					
			1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14356.235
4.854251650D+06-1.879138253D+04 3.322503330D+01-2.508824851D-03 3.828156060D-07														
			-3.027070798D-11	9.465721370D-16				0.000000000D+00				1.309056406D+05	-1.945814478D+02	
C2H6O2 Dimethyl Peroxide CH3-O-O-CH3 Dorofeeva et al JPCRD 30, (2001),475.														
3	T 8/03	C	2.00H	6.00O	2.00	0.00	0.00	0	62.0678400	-125000.000				
			50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17153.000
-2.368824916D+03 1.837315921D+02-7.523348540D-01 7.495185420D-02-2.995716928D-04														
			7.236750290D-07-6.325910000D-10	0.000000000D+00				-1.768037052D+04	2.780801357D+01					
			200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17153.000
-2.277642419D+05 3.804880100D+03-1.966401071D+01 8.807745900D-02-9.586884500D-05														
			5.862982290D-08-1.512504759D-11	0.000000000D+00				-3.479022590D+04	1.381236636D+02					
			1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17153.000
5.449236630D+06-2.254364983D+04 4.064923390D+01-4.748962180D-03 9.109938640D-07														
			-9.439638440D-11	4.038640590D-15				0.000000000D+00				1.183912289D+05	-2.417865296D+02	
CH3-NH-CH3 Dimethylamine BURCAT G3B3 calc HF298=-15.26 kJ														
3	A09/04	C	2.00H	7.00N	1.00	0.00	0.00	0	45.0837200	-15259.048				
			50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14319.927
-5.588118260D+03 4.293989070D+02-8.535246660D+00 1.648299594D-01-9.124310580D-04														
			2.676326816D-06-3.014230730D-09	0.000000000D+00				-4.893665130D+03	5.587382340D+01					
			200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14319.927
-3.233592170D+05 5.549915840D+03-3.207133830D+01 1.189527460D-01-1.380009645D-04														
			8.757487600D-08-2.295641765D-11	0.000000000D+00				-2.920896952D+04	2.015996220D+02					
			1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14319.927
5.752013300D+06-2.320550057D+04 3.926616700D+01-3.659052910D-03 6.271602450D-07														
			-5.751243140D-11	2.183643165D-15				0.000000000D+00				1.365771786D+05	-2.401312545D+02	

Table 5 (continued)

C2H7N2 Unsym. Dimethyl Hydrazin Radical (CH3)2N-NH* BURCAT G3B3 calc										
3 A10/04 C	2.00H	7.00N	2.00	0.00	0.00	0	59.0904600	207685.392		
50.000	200.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	15824.351	
8.939595140D+02	-1.081976516D+01	2.837327538D+00	2.421009658D-02	-1.696838999D-05						
8.128706420D-08	-1.209753330D-10	0.000000000D+00	2.316536907D+04	1.230393126D+01						
200.000	1000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	15824.351	
-2.119819246D+05	3.687625570D+03	-2.171062036D+01	9.950562530D-02	-1.106303913D-04						
6.880491550D-08	-1.794419341D-11	0.000000000D+00	6.157295710D+03	1.450042356D+02						
1000.000	6000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	15824.351	
6.225636970D+06	-2.607947730D+04	4.612464880D+01	-5.798589980D-03	1.142921464D-06						
-1.192762086D-10	5.115717850D-15	0.000000000D+00	1.794190302D+05	-2.822285342D+02						
CCN Radical Hf298:ATcT A. Gurvich,1991 Jacox,1998 p173.										
3 ATcT/A C	2.00N	1.00	0.00	0.00	0.00	0	38.0281400	679070.000		
50.000	200.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	11038.524	
-6.610172040D+03	4.487957620D+02	-7.035244560D+00	1.120723914D-01	-5.043051440D-04						
1.149993672D-06	-1.023352713D-09	0.000000000D+00	7.887729000D+04	5.094386670D+01						
200.000	1000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	11038.524	
-1.336745420D+04	4.574460320D+01	4.110483850D+00	4.508394290D-03	-1.226232947D-06						
-1.309532494D-09	7.273203050D-13	0.000000000D+00	7.995456720D+04	3.902269530D+00						
1000.000	6000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	11038.524	
1.132252251D+05	-1.430843601D+03	8.394405430D+00	-2.629551704D-04	2.796021903D-08						
1.215596917D-12	-1.975586638D-16	0.000000000D+00	8.778257510D+04	-2.321408794D+01						
CNC CNC radical Amidogen Methanetetraylbis- HF298 ATcT A; Gurvich 91										
3 tps91 C	2.00N	1.00	0.00	0.00	0.00	0	38.0281400	675850.000		
50.000	200.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	11356.611	
-1.587673032D+03	1.385388030D+02	-6.334695170D-01	5.777449600D-02	-2.739212321D-04						
6.843504840D-07	-6.935359570D-10	0.000000000D+00	7.950470490D+04	2.245113675D+01						
200.000	1000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	11356.611	
-6.590287500D+04	9.358273770D+02	-1.169308764D+00	1.937791816D-02	-2.108853022D-05						
1.156558505D-08	-2.559011844D-12	0.000000000D+00	7.538461130D+04	3.261304980D+01						
1000.000	6000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	11356.611	
-6.947460300D+04	-8.849345240D+02	8.167799400D+00	-2.707572774D-04	6.066001380D-08						
-7.046578710D-12	3.304554290D-16	0.000000000D+00	8.377720610D+04	-2.141616755D+01						
C2NO Cyanooxomethyl Radical OC*CN Dorofeeva et al JPCRD 30 (2001),475										
3 T 6/03 C	2.00N	1.00	0.00	0.00	0.00	0	54.0275400	210000.000		
50.000	200.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	13593.968	
1.423928473D+03	-3.532554930D+01	2.761570439D+00	4.167346960D-02	-2.266959954D-04						
7.166739790D-07	-9.329264690D-10	0.000000000D+00	2.380906411D+04	1.075736550D+01						
200.000	1000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	13593.968	
2.366787848D+04	-5.442038650D+02	8.543483650D+00	-3.265268870D-03	1.105174239D-05						
-9.998116510D-09	3.070129094D-12	0.000000000D+00	2.595564589D+04	-1.634720133D+01						
1000.000	6000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	13593.968	
9.518807040D+05	-4.476625510D+03	1.372012549D+01	-1.660644068D-03	3.849633530D-07						
-3.979109290D-11	1.524866360D-15	0.000000000D+00	4.974884340D+04	-5.439801760D+01						

Table 5 (continued)

C2(NO2)2 DiNitroAcetylene NO2-CC-NO2 Burcat G3B3 calc HF298=83.424 kcal  
 3 A 1/05 C 2.00N 2.00O 4.00 0.00 0.00 0 116.0324800 349046.016  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20932.713  
 -6.671020810D+02 2.331416436D+01 2.456322313D+00 7.346413160D-02-3.956010320D-04  
 1.532060621D-06-2.289961957D-09 0.000000000D+00 3.938115390D+04 1.526129490D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20932.713  
 -1.434151991D+04 4.119560990D+02 2.425184081D-02 5.184912910D-02-5.822312020D-05  
 3.290509590D-08-7.556033840D-12 0.000000000D+00 3.772626140D+04 3.057968353D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20932.713  
 -2.551310174D+05-3.654334330D+03 2.403202058D+01-8.405522400D-04 1.245748850D-07  
 -9.984519890D-12 3.440324790D-16 0.000000000D+00 5.517974590D+04-1.068483601D+02

C2(NO2)4 TetraNitroEthylene Burcat B3LYP/6-31G(d) calc. \*\*\*HF298=N/A\*\*\*  
 3 A 1/05 C 2.00N 4.00O 8.00 0.00 0.00 0 208.0435600 0.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 35016.062  
 5.935418970D+03-3.795022110D+02 9.591297850D+00 8.536574360D-02-4.623937960D-04  
 2.053007164D-06-3.290188240D-09 0.000000000D+00-2.917659601D+03-1.613729071D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 35016.062  
 -2.052170616D+05 3.579047560D+03-1.840154209D+01 1.472571800D-01-1.754799408D-04  
 1.028032624D-07-2.413021912D-11 0.000000000D+00-2.078038551D+04 1.351085583D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 35016.062  
 -1.502965521D+06-4.638517890D+03 4.484764420D+01-4.122891890D-03 9.425947220D-07  
 -1.082722965D-10 4.979526570D-15 0.000000000D+00 9.220978900D+03-2.192289325D+02

C3F Radical CCCF HF298=135.028 kcal Burcat G3B3 calc.  
 3 A 7/05 C 3.00F 1.00 0.00 0.00 0.00 0 55.0305032 564957.152  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13478.555  
 1.791016475D+03-4.209279420D+01 2.454613962D+00 5.053634200D-02-3.146540773D-04  
 1.073267526D-06-1.461433668D-09 0.000000000D+00 6.655500980D+04 1.149544997D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13478.555  
 -2.122018208D+04 1.920507327D+02 4.050043500D+00 8.664274960D-03-3.666054160D-06  
 -1.217528850D-09 1.007406196D-12 0.000000000D+00 6.522463890D+04 8.360405590D+00  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13478.555  
 2.313018032D+05-2.423239023D+03 1.176057135D+01-6.962308990D-04 1.533531606D-07  
 -1.760254246D-11 8.183643810D-16 0.000000000D+00 7.914086780D+04-4.008858890D+01

C3F3 PerfluoroPropargyl Radical Burcat G3B3 calc HF298=-32.127 HF0=-32.39 kcal  
 3 A12/04 C 3.00F 3.00 0.00 0.00 0.00 0 93.0273096 -134419.368  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17210.298  
 3.420595310D+03-2.823783527D+02 1.214006552D+01-1.006262883D-01 8.986075100D-04  
 -3.116344991D-06 4.044526420D-09 0.000000000D+00-1.736767344D+04-2.117938547D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17210.298  
 2.535452051D+04-6.510535760D+02 8.273675050D+00 1.463026079D-02-1.067047848D-05  
 2.684483273D-09 1.466614677D-13 0.000000000D+00-1.540052854D+04-1.382863382D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17210.298  
 1.139644601D+05-3.324791120D+03 1.841926878D+01-9.573784870D-04 2.109250765D-07  
 -2.421117015D-11 1.125493399D-15 0.000000000D+00-2.115021780D+03-7.545512540D+01

Table 5 (continued)

C3F3 PerfluoroPropynyl Radical CF<sub>3</sub>-CC\* Burcat G3B3 calc HF298=-18.90 kcal  
 3 A 3/05 C 3.00F 3.00 0.00 0.00 0.00 0 93.0273096 -79077.600  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16929.197  
 6.359947200D+03-5.025849340D+02 1.818452790D+01-1.724638812D-01 1.297045579D-03  
 -4.223722370D-06 5.319730030D-09 0.000000000D+00-9.983816480D+03-4.692859120D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16929.197  
 2.965110170D+04-4.450020980D+02 5.045590590D+00 2.777723755D-02-3.329650480D-05  
 2.053947684D-08-5.201790450D-12 0.000000000D+00-9.358817970D+03 6.352811790D-01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16929.197  
 3.618252480D+04-3.032488095D+03 1.808259201D+01-7.869595910D-04 1.671113111D-07  
 -1.862489337D-11 8.454694760D-16 0.000000000D+00 2.710990197D+03-7.462092380D+01

C3F4 PerfluoroAllene Burcat G3B3 calc HF298=-132.33 kcal HF0=-131.99 kcal  
 3 A12/04 C 3.00F 4.00 0.00 0.00 0.00 0 112.0257128 -553685.456  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19020.702  
 8.784567960D+03-6.584794930D+02 2.173492394D+01-1.869150356D-01 1.244286987D-03  
 -3.542095340D-06 3.883343080D-09 0.000000000D+00-6.680449200D+04-6.143501040D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19020.702  
 7.279458570D+04-1.041403158D+03 8.174257310D+00 2.548292919D-02-2.658870493D-05  
 1.398502054D-08-3.015449987D-12 0.000000000D+00-6.377612010D+04-1.569120465D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19020.702  
 -1.629116600D+03-3.784001240D+03 2.170570185D+01-1.055594640D-03 2.299070736D-07  
 -2.614676722D-11 1.206389078D-15 0.000000000D+00-5.120760690D+04-9.489747920D+01

C3F6 PerfluoroPropene CF<sub>2</sub>=CF-CF<sub>3</sub> G3B3 calc HF298=-276.59 kcal HF0=-275.24 kcal  
 3 A11/04 C 3.00F 6.00 0.00 0.00 0.00 0 150.0225192 -1157252.560  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 23336.707  
 2.130204778D+03-1.372697511D+02 6.893360280D+00-6.986570580D-03 3.700981500D-04  
 -1.337771821D-06 1.633863699D-09 0.000000000D+00-1.415359596D+05-5.541333050D-01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 23336.707  
 -6.123536000D+04 9.030968630D+02-2.841526028D+00 7.302376640D-02-8.954627430D-05  
 5.425371170D-08-1.320025175D-11 0.000000000D+00-1.462438890D+05 4.557172600D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 23336.707  
 -1.193839526D+06-1.287970165D+03 2.563169243D+01-7.882402540D-04 1.918404085D-07  
 -2.331909351D-11 1.123712886D-15 0.000000000D+00-1.427920758D+05-1.101367192D+02

C3F7 CF<sub>3</sub>CF\*CF<sub>3</sub> Melius Molec 45 in MP2.97y HF298(G3MP2)=322.41 kcal  
 3 T12/99 C 3.00F 7.00 0.00 0.00 0.00 0 169.0209224 -1347122.480  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 26401.479  
 -3.209927390D+01 8.641792320D+00 4.393520870D+00 3.031109129D-02 1.869997971D-04  
 -8.565716690D-07 1.148864098D-09 0.000000000D+00-1.652265165D+05 1.303142302D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 26401.479  
 -9.268956920D+04 1.507751123D+03-6.431344130D+00 9.059490890D-02-1.117335566D-04  
 6.891773330D-08-1.712933959D-11 0.000000000D+00-1.721722141D+05 6.863865070D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 26401.479  
 -8.658710510D+05-3.007174452D+03 3.021153192D+01-8.767072530D-04 1.926929404D-07  
 -2.202793366D-11 1.019273863D-15 0.000000000D+00-1.561643439D+05-1.351770640D+02

Table 5 (continued)

C3H Radical CC-CH HF298=171.94 kcal Burcat G3B3 calc											
3 A 7/05 C	3.00H	1.00	0.00	0.00	0.00	0.00	0	37.0400400	719392.776		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12695.889
-3.759807260D+03	2.371933767D+02	-1.291060829D+00	4.379555470D-02	-2.775884627D-05							
-3.962948530D-07	9.081247010D-10	0.000000000D+00	8.420418960D+04	2.784182496D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12695.889
-7.996695870D+03	-1.576691670D+02	6.013789640D+00	3.627872400D-03	-2.349637630D-07							
-1.285382488D-09	5.558659370D-13	0.000000000D+00	8.544417940D+04	-6.096137210D+00							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12695.889
1.060461380D+06	-4.270459160D+03	1.229408959D+01	-6.623009490D-04	9.393153300D-08							
-4.148656840D-12	-5.784616800D-17	0.000000000D+00	1.104688155D+05	-4.921984460D+01							
CF3CHFCF3 MELIUS Molec 48 in MP2.97y HF298(CBS-4)=374.47 kcal											
3 T12/99 C	3.00H	1.00F	7.00	0.00	0.00	0	170.0288624	-1564816.000			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	25901.254
-1.128401047D+03	1.070136559D+02	6.141693160D-01	7.910789350D-02	-1.243096100D-04							
1.102068219D-07	-3.653663810D-13	0.000000000D+00	-1.916362533D+05	2.581048163D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	25901.254
-1.661680469D+05	2.765832248D+03	-1.473016441D+01	1.140529546D-01	-1.389340054D-04							
8.596830610D-08	-2.155059484D-11	0.000000000D+00	-2.041287011D+05	1.117173147D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	25901.254
-9.268076300D+04	-6.443414210D+03	3.517541420D+01	-1.511748262D-03	3.108954389D-07							
-3.381205300D-11	1.505926580D-15	0.000000000D+00	-1.617880777D+05	-1.729691122D+02							
C3HN Cyano-Acetylene HCC-CN Burcat G3B3 calc. HF298=88.053 kcal											
3 A 2/05 C	3.00H	1.00N	1.00	0.00	0.00	0	51.0467800	368413.752			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12918.213
2.937389551D+02	3.506911300D+01	1.262065637D+00	3.591227570D-02	-1.583680848D-04							
7.254716590D-07	-1.277955096D-09	0.000000000D+00	4.269771270D+04	1.517037217D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12918.213
1.790375913D+05	-2.774379850D+03	1.741345965D+01	-1.257670664D-02	1.519433093D-05							
-7.549862690D-09	1.248968939D-12	0.000000000D+00	5.596479150D+04	-7.454819530D+01							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12918.213
1.580169162D+06	-6.500524190D+03	1.690821764D+01	-1.010038617D-03	1.721322862D-07							
-1.570147037D-11	5.931071320D-16	0.000000000D+00	8.120065870D+04	-8.033854750D+01							
C3H2F3 CF3-CH=CH* Radical Burcat G3B3 calc HF298=-90.080 kcal											
3 A10/04 C	3.00H	2.00F	3.00	0.00	0.00	0	95.0431896	-376894.720			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17441.709
8.631818300D+02	-7.716526700D+01	6.332642530D+00	-2.817025687D-02	3.786899150D-04							
-1.174123246D-06	1.391322805D-09	0.000000000D+00	-4.719591440D+04	1.750004464D+00							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17441.709
4.676745000D+04	-2.247301983D+02	-9.803873070D-01	6.059522790D-02	-8.251558710D-05							
5.709019040D-08	-1.576255475D-11	0.000000000D+00	-4.566980150D+04	2.908334754D+01							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17441.709
9.372963500D+05	-6.535012900D+03	2.439446351D+01	-5.848392840D-04	3.577943500D-08							
1.445940747D-12	-2.066763842D-16	0.000000000D+00	-1.237160688D+04	-1.170715520D+02							

Table 5 (continued)

C3H2F3 CF3-C\*=CH2 Radical Burcat G3B3 calc HF298=-89.613 kcal

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3 A10/04 C 3.00H 2.00F 3.00 0.00 0.00 0 95.0431896 -374940.792
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17741.309
3.444278050D+03-2.446157322D+02 1.022044479D+01-7.116503570D-02 6.649855190D-04
-2.164426590D-06 2.722573373D-09 0.000000000D+00-4.644188010D+04-1.443770437D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17741.309
1.403222438D+04 1.547213720D+02-1.844956403D+00 5.978697000D-02-7.875093480D-05
5.338264490D-08-1.455153083D-11 0.000000000D+00-4.743936540D+04 3.548267510D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17741.309
1.067385727D+06-7.075479160D+03 2.500069068D+01-9.275585280D-04 1.379837084D-07
-1.259147011D-11 5.155049840D-16 0.000000000D+00-8.787845190D+03-1.212335392D+02

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C3H2N Cyano-Ethylene Radical CH=CHCN Burcat B3G3 calc. HF298=105.84 kcal

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3 A12/04 C 3.00H 2.00N 1.00 0.00 0.00 0 52.0547200 442855.480
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13333.128
2.432210974D+02-2.989158254D+01 5.816917720D+00-2.627580509D-02 2.283761596D-04
-6.000862780D-07 6.397664050D-10 0.000000000D+00 5.173957880D+04 1.217677277D+00
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13333.128
5.427763760D+04-4.316065810D+02 2.290433084D+00 2.732465128D-02-3.391924270D-05
2.372228741D-08-6.823899020D-12 0.000000000D+00 5.426276500D+04 1.168993068D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13333.128
2.021101796D+06-8.873126020D+03 2.030207069D+01-1.467790444D-03 2.579772252D-07
-2.427903679D-11 9.469285870D-16 0.000000000D+00 1.041053887D+05-1.022750190D+02

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C3H3Cl 1 Chloro 1 propyne ClCC-CH3 Burcat G3B3 calc HF298=184.7 kJ

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0 3 A01/05 C 3.00H 3.00CL 1.00 0.00 0.00 0 74.5086200 184711.048
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15611.036
-2.522680074D+03 2.315212639D+02-4.052868050D+00 1.192878316D-01-5.808186370D-04
1.527307757D-06-1.600329457D-09 0.000000000D+00 1.965954791D+04 3.789743180D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15611.036
-1.237491347D+05 1.851461016D+03-6.195397030D+00 4.511621050D-02-4.700706330D-05
2.809693650D-08-7.179815650D-12 0.000000000D+00 1.145662415D+04 6.335232680D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15611.036
3.039513930D+06-1.280380648D+04 2.627258125D+01-2.343769901D-03 4.357184570D-07
-4.345108910D-11 1.796758821D-15 0.000000000D+00 9.690141440D+04-1.426788419D+02

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C3H3F2 \*CF2-CH=CH2 Radical Burcat G3B3 calc HF298=-53.642 kcal

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3 A10/04 C 3.00H 3.00F 2.00 0.00 0.00 0 77.0527264 -224438.128
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17179.821
1.925410735D+03-8.646246320D+01 5.004162320D+00-8.214558380D-03 2.768775171D-04
-9.632905950D-07 1.213838107D-09 0.000000000D+00-2.873126398D+04 5.581289200D+00
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17179.821
-3.259008440D+04 7.540605210D+02-4.664327310D+00 6.387793920D-02-7.924078400D-05
5.159258550D-08-1.370616294D-11 0.000000000D+00-3.224309260D+04 5.106771600D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17179.821
2.250784156D+06-1.164548128D+04 3.084744763D+01-3.495985350D-03 6.943648500D-07
-7.363210130D-11 3.222966050D-15 0.000000000D+00 3.739809690D+04-1.642957133D+02

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Table 5 (continued)

C3H3F3 CF3-CH=CH2 {HF298=-614.2+/-6.7 kJ EXPER Kolesov.} Burcat G3B3 calc.										
3 A10/04 C	3.00H	3.00F	3.00	0.00	0.00	0	96.0511296	-631131.296		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.567636381D+03	6.790541260D+01	3.471933670D+00	-5.473733880D-04	2.475878348D-04						
-9.180167030D-07	1.278837372D-09	0.000000000D+00	-7.827584360D+04	1.364188641D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-7.008599760D+04	1.694105709D+03	-1.238354628D+01	8.985694810D-02	-1.155167810D-04						
7.698613810D-08	-2.070318556D-11	0.000000000D+00	-8.521810270D+04	9.197147650D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.406997165D+06	-1.196352493D+04	3.118806492D+01	-2.061158676D-03	3.172996260D-07						
-2.484436303D-11	7.593320850D-16	0.000000000D+00	-9.509410770D+03	-1.669342321D+02						
C3H3I Propargyl Iodide HCC-CH2I R. Sivaramakrishnan private communication										
3 A08/05 C	3.00H	3.00I	1.00	0.00	0.00	0	165.9603900	269072.289		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.138595090D+02	-1.898985394D+01	4.012855840D+00	4.143701100D-03	1.100672651D-04						
-3.430498410D-07	4.032340790D-10	0.000000000D+00	3.061133020D+04	1.056606190D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.538506690D+04	-3.858912990D+02	2.193965662D+00	3.649756350D-02	-4.731658590D-05						
3.376345730D-08	-9.770675260D-12	0.000000000D+00	3.279224460D+04	1.476802317D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.503783666D+06	-1.075200500D+04	2.472051730D+01	-1.713282808D-03	2.941495893D-07						
-2.696540219D-11	1.021731924D-15	0.000000000D+00	9.405911250D+04	-1.267507687D+02						
C3H3I 1 Iodo 1 Allene CH2=C=CHI R. Sivaramakrishnan private communication										
3 A08/05 C	3.00H	3.00I	1.00	0.00	0.00	0	165.9603900	264117.250		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.016073920D+03	-2.782427986D+02	1.107171858D+01	-8.412710340D-02	6.198884140D-04						
-1.831721328D-06	2.183949168D-09	0.000000000D+00	3.092781552D+04	-1.776473489D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.727626360D+04	-8.235320530D+01	-9.350536230D-01	4.517742750D-02	-5.843381700D-05						
4.086404140D-08	-1.160108009D-11	0.000000000D+00	3.107183541D+04	3.083635268D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.319095707D+06	-1.058539920D+04	2.479135848D+01	-1.786135295D-03	3.163088630D-07						
-2.996258794D-11	1.175269816D-15	0.000000000D+00	9.198117020D+04	-1.279182719D+02						
C3H3N CyanoEthylene (Acrylonitrile) CH2=CHCN Burcat B3G3 calc. HF298=43.986 kcal										
3 A12/04 C	3.00H	3.00N	1.00	0.00	0.00	0	53.0626600	184037.424		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.836943450D+02	5.548697930D+01	3.514536420D+00	3.489844470D-03	4.345298030D-05						
-8.799418110D-08	1.332949430D-10	0.000000000D+00	2.034441247D+04	9.383768610D+00						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.141067990D+04	1.496759589D+03	-9.333045730D+00	5.746756960D-02	-6.836191360D-05						
4.469700270D-08	-1.207068306D-11	0.000000000D+00	1.415031975D+04	7.505041790D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.935627353D+06	-1.261355154D+04	2.521076683D+01	-2.015574396D-03	3.479209240D-07						
-3.213999960D-11	1.229663624D-15	0.000000000D+00	9.568031840D+04	-1.391616150D+02						



Table 5 (continued)

C3H3O CH2=CH*CO Acrolein Radical Janoschek Rossi Int. J. Chem Kin 36 (2004)										
3 A10/04 C	3.00H	3.00O	1.00	0.00	0.00	0	55.0553200	88530.000		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.342613784D+03	-1.377860523D+02	8.987736010D+00	-5.049258970D-02	3.354890900D-04						
-9.050116360D-07	1.044863708D-09	0.000000000D+00	9.338267740D+03	-9.410934400D+00						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
14131.563										
-1.008747515D+05	2.065883271D+03	-1.146269555D+01	6.096893110D-02	-6.954683320D-05						
4.327888530D-08	-1.118149982D-11	0.000000000D+00	-2.193361539D+02	9.238462950D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
14131.563										
2.697779680D+06	-1.202152415D+04	2.505341299D+01	-2.048200253D-03	3.769424030D-07						
-3.821349860D-11	1.599166904D-15	0.000000000D+00	8.016886810D+04	-1.328492905D+02						
C3H3O *CH2-CH=CO HF298=93.56 kJ Janoschek Rossi Int J Chem Kinet 36 (2004)										
3 A10/04 C	3.00H	3.00O	1.00	0.00	0.00	0	55.0553200	93560.000		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
14885.225										
1.314872711D+03	-8.493703540D+01	5.529673940D+00	-2.920240100D-03	9.144077910D-05						
-2.154494154D-07	1.919935735D-10	0.000000000D+00	9.750630100D+03	1.882733222D+00						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
14885.225										
-3.250706770D+04	7.610411060D+02	-3.034976057D+00	4.313574130D-02	-5.112022050D-05						
3.373197670D-08	-9.193696630D-12	0.000000000D+00	6.184436180D+03	4.412409840D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
14885.225										
2.820609579D+06	-1.161646796D+04	2.454040011D+01	-1.768220756D-03	2.965972714D-07						
-2.653955519D-11	9.801565570D-16	0.000000000D+00	7.887671570D+04	-1.291610799D+02						
C3H4Cl 3-Chloro-1-Propen-1yl *CH=CH-CH2Cl Burcat G3B3 calc HF298=59.812 kcal										
3 A 1/05 C	3.00H	4.00CL	1.00	0.00	0.00	0	75.5165600	250253.408		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
15260.630										
-2.618259956D+03	1.608453925D+02	-1.400325972D-01	6.210367090D-02	-2.997387683D-04						
9.585406900D-07	-1.093161501D-09	0.000000000D+00	2.772932081D+04	2.637181718D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
15260.630										
-9.975913360D+04	2.347190022D+03	-1.623648443D+01	9.045721440D-02	-1.191641839D-04						
8.187092790D-08	-2.258866062D-11	0.000000000D+00	1.811250724D+04	1.140007462D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
15260.630										
2.789950021D+06	-1.215356822D+04	2.709534089D+01	-1.252997358D-03	1.080285009D-07						
-1.424396522D-13	-3.671145210D-16	0.000000000D+00	9.988589100D+04	-1.446634136D+02						
ClC3H4 1-Chloro-1-Propen-5yl CHCl=CH-CH2* Burcat G3B3 calc HF298=32.850 kcal										
3 A 2/05 C	3.00H	4.00CL	1.00	0.00	0.00	0	75.5165600	137444.400		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
15012.045										
2.818206483D+03	-1.618912385D+02	6.686755800D+00	-4.599851140D-03	1.805400497D-05						
2.409706825D-07	-5.426235160D-10	0.000000000D+00	1.529115503D+04	-2.632337673D+00						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
15012.045										
-1.173764459D+05	2.452042641D+03	-1.553339030D+01	8.337851030D-02	-1.046163117D-04						
6.949944420D-08	-1.871520400D-11	0.000000000D+00	3.887371700D+03	1.117697119D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
15012.045										
3.140851844D+06	-1.338052456D+04	2.816948456D+01	-1.848165878D-03	2.889018936D-07						
-2.360764535D-11	7.744568940D-16	0.000000000D+00	9.409272560D+04	-1.530530803D+02						

Table 5 (continued)

C3H4N 2-Propionitrile Radical CH3-CH*-CN Burcat G3B3 calc HF298=222.71 kJ										
3 A01/05 C	3.00H	4.00N	1.00	0.00	0.00	0	54.0706000	222705.952		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
9.327479530D+02	-2.315163205D+00	2.303195371D+00	3.543540000D-02	-1.242870979D-04						
4.305329730D-07	-5.930675230D-10	0.000000000D+00	2.506406335D+04	1.401530101D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.877064710D+04	1.298944364D+03	-6.377328030D+00	5.319248820D-02	-6.004251140D-05						
3.843318170D-08	-1.031260549D-11	0.000000000D+00	1.915024804D+04	6.161866220D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.626307760D+06	-1.514022041D+04	2.979084491D+01	-2.570565202D-03	4.593026620D-07						
-4.402182290D-11	1.750795738D-15	0.000000000D+00	1.155055657D+05	-1.670545591D+02						
C3H4O CH2=CH-CHO PROPENAL Acrolein Burcat G3B3 calc HF298=-16.268 kcal										
3 A10/04 C	3.00H	4.00O	1.00	0.00	0.00	0	56.0632600	-68065.312		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.627859217D+03	-1.637674947D+02	9.916451360D+00	-6.479535740D-02	4.322218010D-04						
-1.215116459D-06	1.496344482D-09	0.000000000D+00	-9.437795700D+03	-1.339420287D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.411767029D+05	2.930863078D+03	-1.828904523D+01	8.376802810D-02	-9.799458820D-05						
6.223132550D-08	-1.637179346D-11	0.000000000D+00	-2.287853671D+04	1.278260418D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.040795754D+06	-1.444472405D+04	2.977434268D+01	-2.701101245D-03	5.161432710D-07						
-5.419698200D-11	2.353641614D-15	0.000000000D+00	7.496055690D+04	-1.660866130D+02						
C3H4O2 Acrylic Acid CH2=CH-C(O)-OH Burcat G3B3 calc HF298=-326.051 kJ										
3 A01/05 C	3.00H	4.00O	2.00	0.00	0.00	0	72.0626600	-326050.752		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.336761950D+03	-3.040849404D+02	1.194423940D+01	-9.957129370D-02	7.417088960D-04						
-2.158414616D-06	2.520619815D-09	0.000000000D+00	-4.006963630D+04	-2.048987021D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.496579280D+04	1.466672610D+03	-1.138054240D+01	7.897860630D-02	-9.437186760D-05						
5.964717580D-08	-1.543385710D-11	0.000000000D+00	-4.714959470D+04	8.731595740D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.182326154D+06	-1.164023993D+04	2.949704226D+01	-1.339778071D-03	1.614518970D-07						
-9.792861820D-12	2.123752855D-16	0.000000000D+00	2.522497078D+04	-1.579657969D+02						
C3H5 Allyl radical CH3-CH=CH* Burcat G3B3 calc HF298=63.464 kcal										
3 A12/04 C	3.00H	5.00	0.00	0.00	0.00	0	41.0718000	265533.376		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.111117158D+03	-5.358900310D+01	4.571211840D+00	1.723382511D-03	4.583143540D-05						
-5.336964460D-08	4.096103400D-12	0.000000000D+00	3.050384182D+04	4.322737240D+00						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.208717941D+05	2.217752429D+03	-1.220459386D+01	6.367106630D-02	-7.120871220D-05						
4.491153190D-08	-1.184698425D-11	0.000000000D+00	2.024966192D+04	9.273376100D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.326553430D+06	-1.734308805D+04	3.081507467D+01	-2.829729117D-03	4.949951080D-07						
-4.642376200D-11	1.806268495D-15	0.000000000D+00	1.350178104D+05	-1.790999799D+02						

Table 5 (continued)

## C3H5 Cyclopropyl radical Melius H4

3	T02/03	C	3.00H	5.00	0.00	0.00	0.00	0.00	0	41.0718000	279909.600		
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11523.950
	8.867169560D+02		-4.552900610D+01		4.680270990D+00		1.016449052D-03		-1.058963195D-04				
	7.753551560D-07		-1.159803040D-09		0.000000000D+00		3.244307270D+04		3.299513120D+00				
	200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11523.950
	-1.256800195D+05		3.367716180D+03		-2.686423241D+01		1.162656674D-01		-1.521784174D-04				
	1.046955302D-07		-2.907608176D-11		0.000000000D+00		1.804901532D+04		1.651283782D+02				
	1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11523.950
	3.347798250D+06		-1.550616473D+04		3.038354516D+01		-2.542141770D-03		4.405949150D-07				
	-4.067916870D-11		1.549538416D-15		0.000000000D+00		1.235502931D+05		-1.773214363D+02				

C3H5Cl 3 Chloro-1-Propene CH<sub>2</sub>=CH-CH<sub>2</sub>Cl Burcat G3B3 calc HF298=88.3 cal

3	A	1/05	C	3.00H	5.00CL	1.00	0.00	0.00	0	76.5245000	369.447		
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15238.767
	-1.747559967D+03		9.777780650D+01		1.629857546D+00		3.881063890D-02		-1.432726322D-04				
	4.188176980D-07		-3.417982410D-10		0.000000000D+00		-2.122498087D+03		1.986531210D+01				
	200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15238.767
	-1.957505622D+05		3.897445650D+03		-2.539724968D+01		1.137220326D-01		-1.439650175D-04				
	9.619620360D-08		-2.602843388D-11		0.000000000D+00		-1.920647996D+04		1.654023904D+02				
	1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15238.767
	3.787031940D+06		-1.616713919D+04		3.235776560D+01		-1.971217135D-03		2.345202413D-07				
	-1.180441306D-11		7.299049170D-17		0.000000000D+00		9.424894210D+04		-1.824726249D+02				

C3H5Cl 1Chloro-1-propen CHCl=CH-CH<sub>3</sub> Burcat G3B3 calc HF298=-1.936 kcal

3	A	1/05	C	3.00H	5.00CL	1.00	0.00	0.00	0	76.5245000	-8100.224		
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15884.494
	-3.220053450D+03		3.039079448D+02		-6.615933240D+00		1.602191055D-01		-9.133665690D-04				
	2.822028949D-06		-3.418451060D-09		0.000000000D+00		-3.771572200D+03		4.928840780D+01				
	200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15884.494
	-2.036163201D+05		3.452679730D+03		-1.831205442D+01		8.482921780D-02		-9.602402100D-05				
	5.973077600D-08		-1.543235912D-11		0.000000000D+00		-1.890217784D+04		1.292331229D+02				
	1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15884.494
	4.285664890D+06		-1.793202896D+04		3.416360640D+01		-2.947792154D-03		5.181063230D-07				
	-4.884454530D-11		1.910911356D-15		0.000000000D+00		1.043976238D+05		-1.968220491D+02				

C3H5N Propionitrile C<sub>2</sub>H<sub>5</sub>CN Burcat G3B3 calc HF298=12.7 kcal

3	A	1/05	C	3.00H	5.00N	1.00	0.00	0.00	0	55.0785400	53191.192		
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14883.190
	-1.260344871D+03		1.478078628D+02		-1.699600438D+00		8.738732180D-02		-4.588445720D-04				
	1.439819286D-06		-1.738258277D-09		0.000000000D+00		4.197796850D+03		2.951263861D+01				
	200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14883.190
	-1.513229096D+05		2.728076040D+03		-1.523491043D+01		7.639692860D-02		-8.616921000D-05				
	5.464305730D-08		-1.450376419D-11		0.000000000D+00		-7.846776570D+03		1.100014383D+02				
	1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14883.190
	4.663801140D+06		-1.931374390D+04		3.513315610D+01		-3.314800740D-03		5.955397670D-07				
	-5.739300930D-11		2.295000466D-15		0.000000000D+00		1.205679611D+05		-2.066267740D+02				

Table 5 (continued)

C3H5NO2 NitroCycloPropane Burcat G3B3 calc HF298=5.027 kcal

3 A 2/05 C	3.00H	5.00N	1.00O	2.00	0.00	0	87.0773400	21032.968			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16913.322
-4.233818540D+03	2.763051052D+02	-3.025189034D+00	1.010162257D-01	-5.675177370D-04							
1.998473297D-06	-2.472171729D-09	0.000000000D+00	-4.119233590D+02	3.792762980D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16913.322
-2.232346495D+05	5.036331130D+03	-3.801976170D+01	1.694124310D-01	-2.197970992D-04							
1.471590821D-07	-3.972768680D-11	0.000000000D+00	-2.143847141D+04	2.277328081D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16913.322
2.959612743D+06	-1.653412317D+04	4.021014620D+01	-3.357555180D-03	6.201841540D-07							
-6.064498320D-11	2.442166401D-15	0.000000000D+00	9.428935890D+04	-2.309372271D+02							

C3H5O CH3CH2\*CO PROPANAL Radical Janoschek Rossi HF298=-32.83kJ

3 A10/04 C	3.00H	5.00O	1.00	0.00	0.00	0	57.0712000	-32830.000			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15702.558
5.244969100D+03	-3.432976010D+02	1.080125586D+01	-1.043387371D-02	-1.704248259D-04							
1.234065610D-06	-2.094660683D-09	0.000000000D+00	-4.690811890D+03	-2.099197549D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15702.558
-2.143174758D+05	4.019422380D+03	-2.235114606D+01	8.963105260D-02	-9.835976600D-05							
5.970506970D-08	-1.518580298D-11	0.000000000D+00	-2.413003296D+04	1.545745924D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15702.558
4.437456650D+06	-1.897641825D+04	3.457311660D+01	-3.341883720D-03	6.094791350D-07							
-5.966194730D-11	2.423787278D-15	0.000000000D+00	1.078473753D+05	-1.997014027D+02							

C3H5O CH3-C(O)-CH2 Acetone Radical HF298=-33.34 kJ Janoschek Rossi Int JCK

3 A10/04 C	3.00H	5.00O	1.00	0.00	0.00	0	57.0712000	-33340.000			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15947.972
7.610186690D+03	-5.507162560D+02	1.774771769D+01	-1.266548629D-01	7.265940990D-04							
-1.880659631D-06	2.021473414D-09	0.000000000D+00	-4.161183020D+03	-4.783543910D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15947.972
-1.665010450D+05	3.143100924D+03	-1.777306814D+01	8.339585780D-02	-9.509163380D-05							
5.943416850D-08	-1.539190736D-11	0.000000000D+00	-2.015412832D+04	1.267223860D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15947.972
4.278527040D+06	-1.778853212D+04	3.345224480D+01	-2.839352290D-03	4.908502240D-07							
-4.546700540D-11	1.746139576D-15	0.000000000D+00	1.007041407D+05	-1.914165591D+02							

C3H5O \*CH2C2H3O Propylene Oxide Radical Burcat G3B3 calc HF298=24.873 kcal

3 A11/04 C	3.00H	5.00O	1.00	0.00	0.00	0	57.0712000	104068.632			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14666.951
1.728522773D+03	-1.348082738D+02	7.394172590D+00	-3.172724570D-02	2.776735166D-04							
-8.588695720D-07	1.212559030D-09	0.000000000D+00	1.117995973D+04	-4.955479830D+00							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14666.951
-2.198512429D+05	4.260849680D+03	-2.747124186D+01	1.167516735D-01	-1.454901909D-04							
9.595623800D-08	-2.570546474D-11	0.000000000D+00	-8.388270310D+03	1.756976877D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14666.951
3.877830460D+06	-1.677266101D+04	3.305150610D+01	-2.436626646D-03	3.945351370D-07							
-3.374914200D-11	1.177589668D-15	0.000000000D+00	1.103030843D+05	-1.895473749D+02							

Table 5 (continued)

C3H6O Acetone CH<sub>3</sub>-O-CH<sub>3</sub> HF298=-214.814+/-0.26 REF=ATcT A

3	ATcT/A	C	3.00H	6.00O	1.00	0.00	0.00	0	58.0791400	-214814.000		
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16193.193
	6.846369460D+03	-4.934367130D+02	1.608546982D+01	-1.011179859D-01	5.558778000D-04							
	-1.367580433D-06	1.461561687D-09	0.000000000D+00	-2.619792875D+04	-4.305814930D+01							
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16193.193
	-2.432896318D+05	4.438395120D+03	-2.540777969D+01	1.025793089D-01	-1.137113717D-04							
	6.977060670D-08	-1.794458680D-11	0.000000000D+00	-4.804899590D+04	1.677299052D+02							
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16193.193
	4.847278020D+06	-2.131889568D+04	3.927883560D+01	-4.006152660D-03	7.528424380D-07							
	-7.578398360D-11	3.159323889D-15	0.000000000D+00	9.929005910D+04	-2.341728617D+02							

C3H6O Propylene Oxide CH<sub>3</sub>-C<sub>2</sub>H<sub>3</sub>O Swalen & Hirshbach JPC 27 (1957),100.

3	A01/05	C	3.00H	6.00O	1.00	0.00	0.00	0	58.0791400	-92760.000		
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14415.419
	-2.089725179D+03	1.524866317D+02	-3.606096540D-01	5.479615760D-02	-2.146123502D-04							
	5.542111580D-07	-3.824035150D-10	0.000000000D+00	-1.336974417D+04	2.550326597D+01							
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14415.419
	-2.555306560D+05	4.857197370D+03	-3.145376615D+01	1.274651328D-01	-1.536368946D-04							
	9.964262800D-08	-2.655285808D-11	0.000000000D+00	-3.480229590D+04	1.959167574D+02							
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14415.419
	4.417490060D+06	-2.019427530D+04	3.885188720D+01	-3.606449410D-03	6.591634410D-07							
	-6.452421370D-11	2.617112080D-15	0.000000000D+00	1.063339788D+05	-2.319320510D+02							

C3H6O -CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>O- OXETANE HF298=-19.38 kcal Burcat G3B3; Dorofeeva Thermochim

3	A11/04	C	3.00H	6.00O	1.00	0.00	0.00	0	58.0791400	-81085.920		
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13309.349
	-1.395742898D+03	7.908513290D+01	2.211948788D+00	4.652492360D-02	-3.977534910D-04							
	1.598934050D-06	-2.018812622D-09	0.000000000D+00	-1.162780018D+04	1.436252519D+01							
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13309.349
	-3.790170370D+05	7.341061320D+03	-4.825138240D+01	1.685975174D-01	-2.040781689D-04							
	1.311221245D-07	-3.447114570D-11	0.000000000D+00	-4.439728740D+04	2.881552873D+02							
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13309.349
	4.549727370D+06	-2.132075645D+04	3.968394850D+01	-3.616932040D-03	6.439845030D-07							
	-6.140998240D-11	2.427255559D-15	0.000000000D+00	1.143526250D+05	-2.405150802D+02							

C3H6O Vinyl Methyl Ether C<sub>2</sub>H<sub>3</sub>-O-CH<sub>3</sub> Burcat G3B3 Calc. HF298=-100.378 kJ

3	A01/05	C	3.00H	6.00O	1.00	0.00	0.00	0	58.0791400	-100378.344		
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16350.635
	-4.163416370D+03	3.053435728D+02	-4.853165180D+00	1.425284218D-01	-8.595472150D-04							
	2.780722146D-06	-3.443149010D-09	0.000000000D+00	-1.500300611D+04	4.362672420D+01							
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16350.635
	-2.519057251D+05	4.424451320D+03	-2.465236290D+01	1.014459528D-01	-1.141994931D-04							
	7.070535890D-08	-1.818906446D-11	0.000000000D+00	-3.440735350D+04	1.651941840D+02							
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16350.635
	5.078048020D+06	-2.099455891D+04	3.785548010D+01	-3.126961789D-03	5.166725460D-07							
	-4.760418550D-11	1.861198571D-15	0.000000000D+00	1.121008504D+05	-2.230973103D+02							

Table 5 (continued)

C3H6O CyC3H5-OH CycloPropanol Burcat G3B3 Calc. HF298=-101.50 kJ										
3 A01/05 C	3.00H	6.000	1.00	0.00	0.00	0	58.0791400	-101503.840		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.093675530D+03	3.436232190D+01	4.475252910D+00	-2.862740736D-02	3.368637510D-04						
-1.154910203D-06	1.738609885D-09	0.000000000D+00	-1.396512591D+04	8.377432890D+00						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.064205429D+05	6.019041570D+03	-4.206514310D+01	1.643541834D-01	-2.094448535D-04						
1.384639961D-07	-3.688768700D-11	0.000000000D+00	-4.069893770D+04	2.506610868D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.915107820D+06	-1.759638951D+04	3.554407320D+01	-1.969089472D-03	2.539362778D-07						
-1.472039048D-11	1.992649116D-16	0.000000000D+00	8.954713470D+04	-2.085375749D+02						
C3H7,n-propyl Radical. Ruscic G3B3 2005 HF298=101.32 kJ										
3 A 5/05 C	3.00H	7.00	0.00	0.00	0.00	0	43.0876800	101320.000		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.586920540D+03	2.479114563D+02	-1.889388071D+00	7.085286330D-02	-2.844343374D-04						
6.870240090D-07	-5.293608360D-10	0.000000000D+00	9.585943470D+03	3.302346130D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.492144738D+05	4.485185910D+03	-2.688600280D+01	1.098565235D-01	-1.305396503D-04						
8.501019010D-08	-2.278438648D-11	0.000000000D+00	-1.007537058D+04	1.741036009D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.740463940D+06	-2.293272503D+04	3.914129460D+01	-3.621737310D-03	6.199079960D-07						
-5.670405870D-11	2.145446309D-15	0.000000000D+00	1.490119242D+05	-2.358624028D+02						
C3H7,i-propyl Radical. RUSCIC G3B3 2005 HF298=90.19 kJ										
3 A 5/05 C	3.00H	7.00	0.00	0.00	0.00	0	43.0876800	90190.000		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.987611250D+03	2.352648217D+02	8.011211550D-02	4.063094310D-02	-8.663405020D-05						
-3.394750710D-08	4.943780010D-10	0.000000000D+00	8.271827070D+03	2.629299135D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.180693560D+05	5.456019300D+03	-3.080326889D+01	1.106491182D-01	-1.221774455D-04						
7.500061360D-08	-1.926695749D-11	0.000000000D+00	-1.609940666D+04	1.987228584D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.950861390D+06	-2.436002317D+04	4.048681710D+01	-4.232211290D-03	7.659662210D-07						
-7.440018310D-11	2.999575509D-15	0.000000000D+00	1.562156525D+05	-2.467960478D+02						
C3H8O2 DiMethoxyMethane CH3-O-CH2-O-CH3 Burcat G3B3 calc										
3 A11/04 C	3.00H	8.000	2.00	0.00	0.00	0	76.0944200	-345966.592		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.711928417D+03	1.118495775D+02	4.563026350D-01	8.922162600D-02	-3.913799830D-04						
1.095184968D-06	-1.248219880D-09	0.000000000D+00	-4.448291980D+04	2.305748807D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.430769840D+05	5.309318200D+03	-2.537377653D+01	1.053146375D-01	-1.044537705D-04						
5.848388550D-08	-1.395718930D-11	0.000000000D+00	-6.931287670D+04	1.749474296D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.580531040D+06	-3.050692158D+04	5.266496820D+01	-5.622127880D-03	9.450600980D-07						
-8.462733220D-11	3.145351603D-15	0.000000000D+00	1.401673064D+05	-3.217094530D+02						

Table 5 (continued)

C3N2O	Oxopropanedinitrile	NC-CO-NC	Dorofeeva	JPCRD 30 (2001), 475
3 T 6/03 C	3.00N	2.00O	1.00	0.00 0.00 0 80.0449800 247500.000
50.000	200.000	7 -2.0 -1.0	0.0 1.0 2.0 3.0 4.0 0.0	17147.758
1.106828425D+03	-1.270765414D+00	1.295396539D+00	7.142037700D-02	-3.719963670D-04
1.316783755D-06	-1.925180791D-09	0.000000000D+00	2.779739761D+04	1.727475329D+01
200.000	1000.000	7 -2.0 -1.0	0.0 1.0 2.0 3.0 4.0 0.0	17147.758
1.114948240D+05	-1.954611762D+03	1.613087532D+01	-7.946973790D-03	1.828836751D-05
-1.491342666D-08	4.309553790D-12	0.000000000D+00	3.668744160D+04	-5.886800480D+01
1000.000	6000.000	7 -2.0 -1.0	0.0 1.0 2.0 3.0 4.0 0.0	17147.758
7.616487860D+05	-5.246839540D+03	1.962876136D+01	-1.382603243D-03	2.960423127D-07
-3.325036290D-11	1.519880587D-15	0.000000000D+00	5.643843250D+04	-8.744895460D+01
C4Cl2	Dichloro-Diacetylene	ClCC-CCCl	Burcat	G3B3 calc HF298=108.411 kcal
3 A04/05 C	4.00CL	2.00	0.00	0.00 0.00 0 118.9482000 453591.624
50.000	200.000	7 -2.0 -1.0	0.0 1.0 2.0 3.0 4.0 0.0	19778.542
-2.609261215D+03	1.853503944D+02	-2.157459901D+00	1.078035970D-01	-4.177249360D-04
9.716246920D-07	-1.013697840D-09	0.000000000D+00	5.158763450D+04	3.112717121D+01
200.000	1000.000	7 -2.0 -1.0	0.0 1.0 2.0 3.0 4.0 0.0	19778.542
1.017685461D+05	-2.025895649D+03	1.868035128D+01	-9.772494790D-03	1.631803051D-05
-1.139406519D-08	2.941914478D-12	0.000000000D+00	6.118006110D+04	-7.198058680D+01
1000.000	6000.000	7 -2.0 -1.0	0.0 1.0 2.0 3.0 4.0 0.0	19778.542
7.505794120D+05	-4.507191980D+03	1.951527964D+01	-1.118953160D-03	2.346493248D-07
-2.592351970D-11	1.169459977D-15	0.000000000D+00	7.691460120D+04	-8.357100380D+01
C4F2	Perfluoro-Diacetylene	FCC-CCF	Burcat	G3B3 calc HF298=51.46 kcal
3 A04/05 C	4.00F	2.00	0.00	0.00 0.00 0 86.0396064 215308.640
50.000	200.000	7 -2.0 -1.0	0.0 1.0 2.0 3.0 4.0 0.0	18157.101
-3.270726780D+03	1.765751474D+02	-3.898932430D-01	4.601703450D-02	1.315068181D-04
-1.117689095D-06	1.925592266D-09	0.000000000D+00	2.309996510D+04	2.478440838D+01
200.000	1000.000	7 -2.0 -1.0	0.0 1.0 2.0 3.0 4.0 0.0	18157.101
7.498069280D+04	-1.757904627D+03	1.692932173D+01	-7.670440810D-03	1.558835654D-05
-1.182804891D-08	3.244497750D-12	0.000000000D+00	3.134041823D+04	-6.479670460D+01
1000.000	6000.000	7 -2.0 -1.0	0.0 1.0 2.0 3.0 4.0 0.0	18157.101
9.777651230D+05	-5.403751610D+03	2.008029231D+01	-1.320259148D-03	2.757274868D-07
-3.037983780D-11	1.368058130D-15	0.000000000D+00	5.390517840D+04	-9.157293410D+01
C4H2	Butadiyne (Diacetylene)		Burcat	G3B3 calc. HF298=109.536 kcal
3 T07/04 C	4.00H	2.00	0.00	0.00 0.00 0 50.0586800 458298.624
50.000	200.000	7 -2.0 -1.0	0.0 1.0 2.0 3.0 4.0 0.0	14328.361
4.745192210D+03	-2.629048891D+02	8.853104680D+00	-5.812343220D-02	4.671401220D-04
-1.159156865D-06	9.076591520D-10	0.000000000D+00	5.430860660D+04	-1.627771996D+01
200.000	1000.000	7 -2.0 -1.0	0.0 1.0 2.0 3.0 4.0 0.0	14328.361
2.400396981D+05	-3.819897540D+03	2.318472484D+01	-2.042424691D-02	2.497410518D-05
-1.343873456D-08	2.683537762D-12	0.000000000D+00	7.148958790D+04	-1.084447487D+02
1000.000	6000.000	7 -2.0 -1.0	0.0 1.0 2.0 3.0 4.0 0.0	14328.361
2.244330623D+06	-8.703211320D+03	2.094052973D+01	-1.273299956D-03	2.087236749D-07
-1.819649813D-11	6.522154900D-16	0.000000000D+00	1.053319068D+05	-1.073946139D+02

Table 5 (continued)

C4H2N2 Fumaronitrile NC-CH=CH-CN Burcat G3B3 HF298=331.+/-3 kJ HF0=334.46 kJ

3	T05/04	C	4.00H	2.00N	2.00	0.00	0.00	0	78.0721600	330996.240				
			50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17548.644
			4.340575560D+03	-2.980952506D+02	1.085108876D+01	-6.087984600D-02	5.325465110D-04							
			-1.729666313D-06	2.211144541D-09	0.000000000D+00	3.867471070D+04	-2.020171633D+01							
			200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17548.644
			-9.558678590D+03	3.620883320D+02	-3.958081330D-01	4.440963800D-02	-5.007928530D-05							
			3.184600580D-08	-8.544938480D-12	0.000000000D+00	3.624206590D+04	2.930021875D+01							
			1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17548.644
			2.450846353D+06	-1.179298016D+04	2.875113946D+01	-2.191452299D-03	4.099881980D-07							
			-4.110769760D-11	1.707693852D-15	0.000000000D+00	1.062529984D+05	-1.531157985D+02							

C4H3 E,1-butene-3yne-1yl Radical Burcat G3B3 calc HF298=129.81 kcal

3	T06/04	C	4.00H	3.00	0.00	0.00	0.00	0	51.0666200	543104.120				
			50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14369.460
			1.255622383D+03	-5.634804110D+01	4.821556600D+00	-8.950489750D-03	1.342900905D-04							
			-1.589793358D-07	-1.517129681D-10	0.000000000D+00	6.380261370D+04	4.631415600D+00							
			200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14369.460
			1.156433024D+05	-1.454953016D+03	7.335993470D+00	2.387528316D-02	-3.170362770D-05							
			2.379663792D-08	-7.161490660D-12	0.000000000D+00	7.098569060D+04	-1.804455120D+01							
			1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14369.460
			2.754301124D+06	-1.117359229D+04	2.452419326D+01	-1.518164983D-03	2.351337444D-07							
			-1.899825951D-11	6.138890240D-16	0.000000000D+00	1.301420887D+05	-1.296036527D+02							

C4H3 i-1-butene-3yne-2-yl Burcat G3B3 calc HF298=119.94 kcal

3	T06/04	C	4.00H	3.00	0.00	0.00	0.00	0	51.0666200	501828.960				
			50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16739.097
			3.935550970D+03	-2.586739722D+02	9.344211360D+00	-2.885523408D-02	2.215530567D-04							
			-5.285279800D-07	4.740818230D-10	0.000000000D+00	5.920439580D+04	-1.486322992D+01							
			200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16739.097
			5.290631900D+04	-6.759510050D+02	6.608856810D+00	1.974156062D-02	-2.089290359D-05							
			1.410076481D-08	-4.093159670D-12	0.000000000D+00	6.169532500D+04	-7.970883690D+00							
			1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16739.097
			2.900499871D+06	-1.153996494D+04	2.494375975D+01	-1.724471893D-03	2.867552101D-07							
			-2.543447656D-11	9.307659690D-16	0.000000000D+00	1.276398270D+05	-1.295027098D+02							

C4H4 1-butene-3yne CH2=CH-CCH Burcat G3B3 calc HF298=68.80 kcal HF0=70.37 kcal

3	T06/04	C	4.00H	4.00	0.00	0.00	0.00	0	52.0745600	287859.200				
			50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14292.255
			2.343541723D+02	1.621359434D+01	2.810600802D+00	1.797450191D-02	-4.018087580D-05							
			3.422632830D-07	-6.643775120D-10	0.000000000D+00	3.288229680D+04	1.210279809D+01							
			200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14292.255
			6.782249670D+03	3.865120400D+02	-3.947149200D+00	5.350389380D-02	-6.584167990D-05							
			4.476703120D-08	-1.244989595D-11	0.000000000D+00	3.173974370D+04	4.378073320D+01							
			1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14292.255
			3.666653130D+06	-1.489937021D+04	2.942062642D+01	-2.060279355D-03	3.236552160D-07							
			-2.667851899D-11	8.875351060D-16	0.000000000D+00	1.220582183D+05	-1.658715955D+02							



Table 5 (continued)

C4H4N2 PYRAZINE Melius PJ11 HF298=47.0+/-0.3 kcal Pedley et al 1986

3 T 9/96 C	4.00H	4.00N	2.00	0.00	0.00	0	80.0880400	195811.200
50.000	200.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.498695530D+02	1.087747161D+01	4.648737280D+00	-2.341070720D-02	2.391308741D-04				
-6.092668480D-07	8.345947010D-10	0.000000000D+00	2.185363151D+04	7.407066150D+00				
200.000	1000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.091869958D+05	4.656358450D+03	-3.549182180D+01	1.501031157D-01	-1.866307766D-04				
1.211532557D-07	-3.201594570D-11	0.000000000D+00	1.653708132D+03	2.129152540D+02				
1000.000	6000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.500867764D+06	-1.532239227D+04	3.672066590D+01	-2.802805295D-03	5.177406920D-07				
-5.117191440D-11	2.093885536D-15	0.000000000D+00	1.081272163D+05	-2.128060341D+02				

C4H4N2 PYRIMIDINE MELIUS PI11 HF298=47.0+/-0.2 kcal Pedley et al 1986

3 T 9/96 C	4.00H	4.00N	2.00	0.00	0.00	0	80.0880400	196648.000
50.000	200.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.228047407D+03	5.660945200D+01	3.489031630D+00	-1.001539749D-02	1.702602593D-04				
-4.433314830D-07	6.655084420D-10	0.000000000D+00	2.180057554D+04	1.212972836D+01				
200.000	1000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.385860580D+05	5.039051920D+03	-3.704551470D+01	1.524165434D-01	-1.880049736D-04				
1.212022888D-07	-3.184454840D-11	0.000000000D+00	-1.523144828D+02	2.222922906D+02				
1000.000	6000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.538935309D+06	-1.548660927D+04	3.684898480D+01	-2.856791717D-03	5.302419300D-07				
-5.266512930D-11	2.165543086D-15	0.000000000D+00	1.092529432D+05	-2.138273620D+02				

C4H4N2 Succinonitrile NC-CH2-CH2-CN PM3 HF298 Webbook 2003

3 T12/03 C	4.00H	4.00N	2.00	0.00	0.00	0	80.0880400	209700.000
50.000	200.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.505268970D+02	-8.288287760D+01	7.446842740D+00	-3.578259560D-02	4.577077870D-04				
-1.725127083D-06	2.611842523D-09	0.000000000D+00	2.322560659D+04	-3.097776474D+00				
200.000	1000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.215833790D+04	2.336997580D+03	-1.673201461D+01	1.026691052D-01	-1.324190694D-04				
9.100734000D-08	-2.544785944D-11	0.000000000D+00	1.302400950D+04	1.162753628D+02				
1000.000	6000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.102877055D+06	-1.581993604D+04	3.680007960D+01	-3.344952850D-03	6.481278990D-07				
-6.667914250D-11	2.824566892D-15	0.000000000D+00	1.144402693D+05	-2.065948646D+02				

1,4-C4H4O Vinyl-Ketene H2C=CH-CH=C=O Burcat G3B3 calc HF298=22.72 kJ

3 A 1/05 C	4.00H	4.00O	1.00	0.00	0.00	0	68.0739600	22719.120
50.000	200.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.587128700D+03	-4.137263180D+02	1.308130208D+01	-8.775595430D-02	6.103438440D-04				
-1.684731548D-06	1.882080875D-09	0.000000000D+00	2.167434693D+03	-2.847362678D+01				
200.000	1000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.290158270D+04	1.444509160D+03	-9.153210070D+00	6.929900210D-02	-7.901783960D-05				
4.982065040D-08	-1.316223763D-11	0.000000000D+00	-5.453954370D+03	7.626331070D+01				
1000.000	6000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.148263975D+06	-1.546380196D+04	3.419081660D+01	-3.245769870D-03	5.955510510D-07				
-5.959028350D-11	2.503239617D-15	0.000000000D+00	9.078336100D+04	-1.923757084D+02				

Table 5 (continued)

C4H4O2 1,4-Dioxin Zhu & Bozzelli JPCRD 32 (2003), 1713 HF298=86+/-7 kJ										
3 T02/04 C	4.00H	4.00O	2.00	0.00	0.00	0	84.0733600	-86000.000		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.543271110D+03	-2.824082804D+02	1.222988692D+01	-9.427824360D-02	5.928510720D-04						
-1.391307890D-06	1.401769643D-09	0.000000000D+00	-1.131790214D+04	-2.504974536D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.027410841D+05	2.915190654D+03	-2.454632657D+01	1.245918015D-01	-1.571345922D-04						
1.034049328D-07	-2.757869154D-11	0.000000000D+00	-2.431982115D+04	1.522732882D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.921776524D+06	-1.528279615D+04	3.581283500D+01	-2.236328882D-03	3.644116350D-07						
-3.143324383D-11	1.108685051D-15	0.000000000D+00	7.531030300D+04	-2.056962897D+02						
C4H5 E n-1,3-Butadiene 1-yl Burcat G3B3 calc HF298=86.84 kcal										
3 T05/04 C	4.00H	5.00	0.00	0.00	0.00	0	53.0825000	363338.560		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.391259008D+03	6.245740360D+01	3.072516301D+00	1.870925652D-02	-1.845916599D-05						
7.909628650D-08	-2.485035744D-11	0.000000000D+00	4.161526530D+04	1.382190377D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.346273329D+05	2.765376947D+03	-1.759517455D+01	8.936295250D-02	-1.082166972D-04						
7.087238290D-08	-1.900769293D-11	0.000000000D+00	2.959089268D+04	1.228590407D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.107255700D+06	-1.725446996D+04	3.337023480D+01	-2.572019902D-03	4.348032990D-07						
-4.089464630D-11	1.611212430D-15	0.000000000D+00	1.448363474D+05	-1.906017847D+02						
C4H5 1,3-Butadiene-2-yl Burcat G3B3 calc HF298=75.34 kcal										
3 T05/04 C	4.00H	5.00	0.00	0.00	0.00	0	53.0825000	315222.560		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.326980970D+03	-8.885312870D+01	4.284178130D+00	1.589863169D-02	-5.869259240D-05						
4.432260860D-07	-7.750272480D-10	0.000000000D+00	3.644858490D+04	5.675832990D+00						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.819849320D+04	1.704746211D+03	-1.225013082D+01	7.944279440D-02	-9.793992640D-05						
6.562852330D-08	-1.797072927D-11	0.000000000D+00	2.883612454D+04	9.014649590D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.176927600D+06	-1.743541480D+04	3.403353400D+01	-2.627393910D-03	4.366104600D-07						
-3.858756370D-11	1.402997978D-15	0.000000000D+00	1.400784006D+05	-1.963094084D+02						
C4H5 1,2-butadiene-4-yl Burcat G3B3 calc HF298=75.34 kcal										
3 T05/04 C	4.00H	5.00	0.00	0.00	0.00	0	53.0825000	315222.560		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.683696440D+03	-5.227014660D+01	3.659761000D+00	1.776313750D-02	-4.054105710D-05						
3.564788880D-07	-6.773338940D-10	0.000000000D+00	3.630623140D+04	9.009881980D+00						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.702054810D+04	8.132206610D+02	-6.759226470D+00	6.545310900D-02	-8.128834040D-05						
5.548339710D-08	-1.545857809D-11	0.000000000D+00	3.294376090D+04	6.012149110D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.215514380D+06	-1.715979800D+04	3.333752020D+01	-2.551469326D-03	4.202151830D-07						
-3.673941080D-11	1.318446486D-15	0.000000000D+00	1.387869224D+05	-1.909217348D+02						

Table 5 (continued)

C4H5 1-butyne-3yl radical HCC-*CH-CH3 G3B3 calc Janoschek Rossi 2004											
3 A11/04 C	4.00H	5.00	0.00	0.00	0.00	0.00	0	53.0825000	316530.000		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15927.686
-2.973831260D+03	2.091850942D+02	-1.276162435D+00	4.919551080D-02	-2.381269227D-05							
-2.131699603D-07	4.538616130D-10	0.000000000D+00	3.548045080D+04	3.068078052D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15927.686
-9.463181870D+04	1.478236157D+03	-6.877477840D+00	5.804536310D-02	-6.057438140D-05							
3.534566040D-08	-8.712184060D-12	0.000000000D+00	2.926982129D+04	6.404544220D+01							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15927.686
3.660985880D+06	-1.600643777D+04	3.321474640D+01	-2.696445657D-03	4.822535460D-07							
-4.637083160D-11	1.853215145D-15	0.000000000D+00	1.308369564D+05	-1.886763706D+02							
C4H6 Dimethyl Acetylene Yost Osborne Garner JACS 63,(1942),492 HF298=34.97 kcal											
3 A 1/05 C	4.00H	6.00	0.00	0.00	0.00	0.00	0	54.0904400	146314.480		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16544.445
-4.435691500D+03	3.515986740D+02	-6.179710480D+00	1.438751109D-01	-7.301693630D-04							
1.976014431D-06	-2.019841853D-09	0.000000000D+00	1.452598807D+04	4.756308110D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16544.445
-2.598609538D+05	4.388118600D+03	-2.339526063D+01	9.644718960D-02	-1.054750955D-04							
6.497843010D-08	-1.691457360D-11	0.000000000D+00	-4.775857740D+03	1.570529373D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16544.445
5.198941590D+06	-2.237619275D+04	4.048199320D+01	-4.263666710D-03	8.060302360D-07							
-8.157539610D-11	3.417321050D-15	0.000000000D+00	1.494967934D+05	-2.432029460D+02							
C4H6 1,3-butadiene Burcat G3B3 calc HF298=26.49 kcal											
3 T05/04 C	4.00H	6.00	0.00	0.00	0.00	0.00	0	54.0904400	110834.160		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15334.917
-2.179339454D+03	1.107884956D+02	1.999241569D+00	2.964992773D-02	-6.306995300D-05							
9.640744240D-08	1.403338683D-10	0.000000000D+00	1.108698195D+04	1.711329742D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15334.917
-2.428643465D+05	4.555053620D+03	-2.830755323D+01	1.169784096D-01	-1.392211966D-04							
8.957588700D-08	-2.366602763D-11	0.000000000D+00	-9.132482260D+03	1.810422236D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15334.917
5.008466620D+06	-2.098021125D+04	3.828384500D+01	-3.115938116D-03	5.221897620D-07							
-4.853884770D-11	1.895124239D-15	0.000000000D+00	1.370573782D+05	-2.276839761D+02							
C4H6 1,2-butadiene Burcat G3B3 calc HF298=38.55 kcal											
3 T07/04 C	4.00H	6.00	0.00	0.00	0.00	0.00	0	54.0904400	161314.120		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15496.311
-1.810619113D+03	1.846873746D+02	-2.560478229D+00	9.537461590D-02	-4.880965980D-04							
1.527111385D-06	-1.791650472D-09	0.000000000D+00	1.700699283D+04	3.350293530D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15496.311
-1.563138124D+05	3.117272588D+03	-2.019598042D+01	9.991507040D-02	-1.213984445D-04							
8.056115070D-08	-2.193747779D-11	0.000000000D+00	3.620497760D+03	1.345805871D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15496.311
5.066874010D+06	-2.098209489D+04	3.862218910D+01	-3.320029200D-03	5.683385360D-07							
-5.196448190D-11	1.964188116D-15	0.000000000D+00	1.432253948D+05	-2.295708214D+02							

Table 5 (continued)

C4H6Cl2 3,4-DichloroButen-1 H2C=CH-CHCl-CH2CL HF298=-12.804 kcal Burcat G3B3											
3	A	1/05	C	4.00H	6.00CL	2.00	0.00	0.00	0	124.9958400	-53571.936
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	21348.826
-3.072395753D+03 2.315880334D+02-3.111046185D+00 1.347721988D-01-7.117508660D-04											
2.241261284D-06	-2.631371574D-09	0.000000000D+00	-9.734354530D+03	4.097069410D+01	200.000	1000.000	7	-2.0	-1.0	0.0	21348.826
-2.639162740D+05 5.230885330D+03-3.455709210D+01 1.629391899D-01-2.124239174D-04											
1.432776408D-07	-3.884071840D-11	0.000000000D+00	-3.245883530D+04	2.182554368D+02	1000.000	6000.000	7	-2.0	-1.0	0.0	21348.826
3.808489460D+06-1.760422764D+04 4.105596380D+01-2.135054287D-03 2.481489703D-07											
-1.121362327D-11-3.498690670D-17 0.000000000D+00 9.344039700D+04-2.280689679D+02											
C4H6Cl2 1,4-DichloroButen-1 ClHC=CH-CH2-CH2Cl HF298=-12.400 kcal Burcat G3B3											
3	A	1/05	C	4.00H	6.00CL	2.00	0.00	0.00	0	124.9958400	-51881.600
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	21504.645
-2.731458199D+03 1.826275761D+02-5.536635310D-01 9.713744320D-02-4.490578170D-04											
1.316324281D-06	-1.356204472D-09	0.000000000D+00	-9.428791960D+03	3.226132900D+01	200.000	1000.000	7	-2.0	-1.0	0.0	21504.645
-2.870432047D+05 5.584341480D+03-3.610437220D+01 1.643709574D-01-2.117232530D-04											
1.414324019D-07-3.809044500D-11 0.000000000D+00-3.395216850D+04 2.284873441D+02											
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	21504.645
3.576638810D+06-1.744809173D+04 4.144375560D+01-2.829258531D-03 4.813699160D-07											
-4.343787240D-11 1.610997119D-15 0.000000000D+00 9.208158020D+04-2.295632337D+02											
C4H6O4 DiacetylPeroxide CH3-CO-O-O-CO-CH3 Dorofeeva et al JPCRD 30 (2001),475											
3	T	8/03	C	4.00H	6.00O	4.00	0.00	0.00	0	118.0880400	-500000.000
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	23944.000
-3.754602740D+03 2.142602344D+02 1.471924079D+00 6.570651560D-02-2.809062424D-04											
1.228162685D-06	-1.904654658D-09	0.000000000D+00	-6.378617150D+04	2.506828343D+01	200.000	1000.000	7	-2.0	-1.0	0.0	23944.000
-1.429893314D+05 3.027493489D+03-1.969907952D+01 1.202175450D-01-1.350767077D-04											
8.275201860D-08	-2.115240107D-11	0.000000000D+00	-7.629502630D+04	1.380469426D+02	1000.000	6000.000	7	-2.0	-1.0	0.0	23944.000
1.408641675D+07-5.307578060D+04 8.777914910D+01-2.456797442D-02 6.513732840D-06											
-8.533371730D-10 4.367253140D-14 0.000000000D+00 2.598619094D+05-5.568151970D+02											
C4H7 tt-1-Buten-1-yl HF0=62.8 kcal Miller JPC-A, 108, (2004),2268-2277											
3	T05/04	C	4.00H	7.00	0.00	0.00	0.00	0	55.0983800	245870.817	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16967.972
-4.159693890D+03 2.713900407D+02-2.959868300D+00 1.006418556D-01-4.827218210D-04											
1.390482250D-06	-1.487252407D-09	0.000000000D+00	2.664060300D+04	3.729875590D+01	200.000	1000.000	7	-2.0	-1.0	0.0	16967.972
-2.164374137D+05 3.971318650D+03-2.361891050D+01 1.069382577D-01-1.239854972D-04											
7.945303180D-08	-2.110083393D-11	0.000000000D+00	9.455646580D+03	1.570786999D+02	1000.000	6000.000	7	-2.0	-1.0	0.0	16967.972
5.722301740D+06-2.362476549D+04 4.243757200D+01-3.655992500D-03 6.173018990D-07											
-5.777328340D-11 2.284507734D-15 0.000000000D+00 1.693848355D+05-2.543293578D+02											

Table 5 (continued)

C4H7 trans-1-Butene-2-yl HF0=59.4 kcal Miller JPC-A, 108, (2004), 2268-2277											
3	T05/04	C	4.00H	7.00	0.00	0.00	0.00	0	55.0983800	231161.760	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16484.515
-4.640219760D+03	3.988598950D+02	-8.891135970D+00	1.835564680D-01	-1.039308433D-03							
3.247339030D-06	-3.946073100D-09	0.000000000D+00	2.462155684D+04	5.866577520D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16484.515
-2.152325949D+05	3.850944120D+03	-2.269942761D+01	1.037887726D-01	-1.175846917D-04							
7.418749420D-08	-1.952209953D-11	0.000000000D+00	8.195400780D+03	1.508646843D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16484.515
5.914767100D+06	-2.456970310D+04	4.395584060D+01	-4.171936190D-03	7.453865170D-07							
-7.143634390D-11	2.840957986D-15	0.000000000D+00	1.731897477D+05	-2.662618325D+02							
C4H7 trans-2-Butene-2-yl hf0=57.3 kcal Miller JPC-A, 108, (2004), 2268-2277											
3	T05/04	C	4.00H	7.00	0.00	0.00	0.00	0	55.0983800	223852.516	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17961.671
-1.996966905D+03	2.236157526D+02	-5.823959130D+00	1.865770393D-01	-1.128403095D-03							
3.410522880D-06	-3.924975360D-09	0.000000000D+00	2.415668241D+04	4.370964880D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17961.671
-3.792568050D+05	6.210556130D+03	-3.205913810D+01	1.169214980D-01	-1.260938746D-04							
7.568730530D-08	-1.910218725D-11	0.000000000D+00	-4.399046570D+03	2.091463765D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17961.671
6.117593420D+06	-2.538708910D+04	4.422486780D+01	-4.521340100D-03	8.291372460D-07							
-8.159858470D-11	3.331888770D-15	0.000000000D+00	1.776174690D+05	-2.676928345D+02							
C4H7 trans-3-Butene-1yl HF0=52.8 kcal Miller JPC-A, 108, (2004), 2268-2277											
3	T05/04	C	4.00H	7.00	0.00	0.00	0.00	0	55.0983800	204595.355	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17532.510
-2.678132823D+03	1.438495482D+02	8.121836700D-01	6.151309840D-02	-2.545227022D-04							
6.524533450D-07	-4.800219640D-10	0.000000000D+00	2.199604000D+04	2.219371113D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17532.510
-2.815682811D+05	5.1644440450D+03	-3.109002935D+01	1.287183693D-01	-1.538512613D-04							
9.970568970D-08	-2.653343315D-11	0.000000000D+00	-1.039138897D+03	1.986767034D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17532.510
5.631976470D+06	-2.336332988D+04	4.245158040D+01	-3.387672820D-03	5.465623480D-07							
-4.874524030D-11	1.835946099D-15	0.000000000D+00	1.626142870D+05	-2.533769463D+02							
C4H7 trans-Methylallyl HF0=36.7 kcal Miller JPC-A, 108, (2004), 2268-2277											
3	T05/04	C	4.00H	7.00	0.00	0.00	0.00	0	55.0983800	136110.970	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16410.525
1.719042649D+03	-6.275502220D+01	3.219462900D+00	5.693784760D-02	-4.170501940D-04							
1.715570252D-06	-2.421869424D-09	0.000000000D+00	1.466857536D+04	9.418680090D+00							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16410.525
-2.745242157D+05	5.084147060D+03	-3.131023105D+01	1.276770712D-01	-1.501530631D-04							
9.593743840D-08	-2.524595240D-11	0.000000000D+00	-8.708663760D+03	1.985240110D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16410.525
5.798739880D+06	-2.418698784D+04	4.335219410D+01	-3.854422980D-03	6.642886650D-07							
-6.126593260D-11	2.340084781D-15	0.000000000D+00	1.593433259D+05	-2.616499400D+02							

Table 5 (continued)

C4H7 2-methylallyl CH <sub>2</sub> C*(CH <sub>3</sub> )CH <sub>2</sub> HF0=37.1 kcal Miller JPC-A, 108, (2004), 2268.											
3	T05/04	C	4.00H	7.00	0.00	0.00	0.00	0	55.0983800	137603.470	
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	4.533109600D+03	-3.514348650D+02	1.491501638D+01	-1.359577551D-01	9.626111720D-04						
-2.828272945D-06	3.353655440D-09	0.000000000D+00	1.567744126D+04	-3.380189570D+01							
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
											16229.425
-1.575936833D+05	3.179762700D+03	-2.136842272D+01	1.054630362D-01	-1.241573696D-04							
8.011736740D-08	-2.129329859D-11	0.000000000D+00	5.363639430D+02	1.411141673D+02							
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
											16229.425
5.908563320D+06	-2.396535672D+04	4.277901910D+01	-3.400391830D-03	4.982809440D-07							
-3.776332900D-11	1.130371722D-15	0.000000000D+00	1.586266484D+05	-2.581823309D+02							
C4H7 Cyclobutyl Radical HF0=59.6 kcal Miller JPC-A, 108, (2004), 2268-2277											
3	T05/04	C	4.00H	7.00	0.00	0.00	0.00	0	55.0983800	230305.602	
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
											14791.557
-1.768662897D+03	1.443721955D+02	-1.099333548D+00	1.023721950D-01	-7.558018730D-04							
2.788994074D-06	-3.547933170D-09	0.000000000D+00	2.548532720D+04	2.662710158D+01							
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
											14791.557
-3.393941210D+05	6.874409760D+03	-4.693309060D+01	1.758411025D-01	-2.190258844D-04							
1.446055372D-07	-3.887509010D-11	0.000000000D+00	-4.761528670D+03	2.791175404D+02							
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
											14791.557
5.162413220D+06	-2.337627881D+04	4.355964510D+01	-3.797968700D-03	6.584036850D-07							
-6.095795380D-11	2.333564577D-15	0.000000000D+00	1.641944753D+05	-2.651841811D+02							
C4H7O 2-Butanone radical CH <sub>3</sub> -CO-CH*CH <sub>3</sub> HF298=-18.163 kcal Burcat G3B3 calc											
3	A 8/05	C	4.00H	7.000	1.00	0.00	0.00	0	71.0977800	-75993.992	
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
											19867.916
1.329517848D+03	-8.570321340D+01	4.484550210D+00	4.334012930D-02	-1.376627476D-04							
3.001098374D-07	-1.265749458D-10	0.000000000D+00	-1.122464790D+04	6.427175720D+00							
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
											19867.916
-3.173814930D+05	5.349501280D+03	-2.907636915D+01	1.233980624D-01	-1.408630753D-04							
8.798763770D-08	-2.277729158D-11	0.000000000D+00	-3.641787610D+04	1.920122725D+02							
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
											19867.916
5.875903010D+06	-2.446826656D+04	4.553823200D+01	-3.795326000D-03	5.992498310D-07							
-5.046588330D-11	1.757575667D-15	0.000000000D+00	1.350309524D+05	-2.700147599D+02							
C4H7O 2-Methyl-Allyl Oxy radical H <sub>2</sub> C=C(CH <sub>3</sub> )CH <sub>2</sub> O* Burcat G3B3 HF298=13.324 kcal											
3	A 2/05	C	4.00H	7.000	1.00	0.00	0.00	0	71.0977800	55747.616	
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
											18562.431
-6.854646770D+02	4.313742450D+01	2.366490387D+00	3.993382850D-02	-7.249510750D-05							
1.500816124D-07	-2.216670009D-11	0.000000000D+00	4.336494040D+03	1.691435842D+01							
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
											18562.431
-1.992815239D+05	3.733988380D+03	-2.311728823D+01	1.148528717D-01	-1.344451006D-04							
8.630939950D-08	-2.292038420D-11	0.000000000D+00	-1.242265401D+04	1.543328612D+02							
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
											18562.431
5.617062240D+06	-2.404429378D+04	4.583745500D+01	-3.740679450D-03	5.932969060D-07							
-5.041525070D-11	1.779269725D-15	0.000000000D+00	1.476140192D+05	-2.727293243D+02							

Table 5 (continued)

C4H8CL2S MUSTARD S(CH2CH2Cl)2 REF=Melius BAC/MP4 P28L

3	S03/01	CL	2.00S	1.00C	4.00H	8.00	0.00	0	159.0777200	-124766.880		
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	27569.060
-2.087431777D+03	1.479563772D+02	-6.815295680D-01	1.716795640D-01	-1.123154864D-03								
3.964721580D-06	-5.107842070D-09	0.000000000D+00	-1.879673753D+04	2.871376192D+01								
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	27569.060
-3.228529730D+05	6.416241850D+03	-4.002018840D+01	1.843529903D-01	-2.253414201D-04								
1.471734326D-07	-3.938447080D-11	0.000000000D+00	-4.718919900D+04	2.521361105D+02								
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	27569.060
5.587570460D+06	-2.693340661D+04	5.831661920D+01	-4.919289000D-03	9.083338110D-07								
-8.976946520D-11	3.673985310D-15	0.000000000D+00	1.389133537D+05	-3.421568280D+02								

C4H8O Methyl Allyl alcohol H2C=C(CH3)CH2OH G3B3 calc. HF298=-38.51 kcal

3	T	7/04	C	4.00H	8.00O	1.00	0.00	0.00	0	72.1057200	-161142.576	
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18621.809
-5.354901050D+03	4.580335710D+02	-1.065740845D+01	2.032168220D-01	-1.054087412D-03								
3.088672057D-06	-3.523029550D-09	0.000000000D+00	-2.299927520D+04	6.616628730D+01								
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18621.809
-3.294396650D+05	5.770375280D+03	-3.526594690D+01	1.495458083D-01	-1.765518700D-04								
1.126955898D-07	-2.956592771D-11	0.000000000D+00	-4.814432930D+04	2.187828266D+02								
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18621.809
6.467841400D+06	-2.719688982D+04	5.043952190D+01	-4.018636020D-03	6.628481240D-07								
-5.819982540D-11	2.103256203D-15	0.000000000D+00	1.406627732D+05	-3.076685285D+02								

C4H8O Di-Methyl OXYRAN (t-Di-Methyl Ethylene Oxide) G3B3 calc. HF298=-32.90 kcal

3	T	7/04	C	4.00H	8.00O	1.00	0.00	0.00	0	72.1057200	-137657.784	
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17777.027
-7.163747680D+03	5.796481380D+02	-1.355613655D+01	2.338293125D-01	-1.252346539D-03								
3.669728290D-06	-4.146487910D-09	0.000000000D+00	-2.047184840D+04	7.737426860D+01								
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17777.027
-3.942600450D+05	7.001246590D+03	-4.387203550D+01	1.732653143D-01	-2.101202281D-04								
1.362933709D-07	-3.614999050D-11	0.000000000D+00	-5.078549460D+04	2.643134424D+02								
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17777.027
6.221596760D+06	-2.693332036D+04	5.038280970D+01	-4.329237370D-03	7.480292970D-07								
-6.910199440D-11	2.641616586D-15	0.000000000D+00	1.413551496D+05	-3.088261781D+02								

C4H8O Ethyl OXYRAN (Ethyl-Ethylene-Oxide) G3B3 calc. HF298=-27.71 kcal

3	T	7/04	C	4.00H	8.00O	1.00	0.00	0.00	0	72.1057200	-115959.560	
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17582.301
-3.166342920D+03	2.369803175D+02	-3.305089260D+00	1.178283116D-01	-6.311529600D-04								
1.919760999D-06	-2.066352190D-09	0.000000000D+00	-1.679902826D+04	3.772933390D+01								
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17582.301
-4.319163580D+05	7.892588200D+03	-5.017805560D+01	1.883152865D-01	-2.271750519D-04								
1.463563740D-07	-3.860031280D-11	0.000000000D+00	-5.203745350D+04	3.007368748D+02								
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17582.301
6.488711880D+06	-2.828118199D+04	5.192475230D+01	-4.650523600D-03	7.606182910D-07								
-6.580306160D-11	2.338114235D-15	0.000000000D+00	1.520492813D+05	-3.191230870D+02								

Table 5 (continued)

C4H9 n-butyl Radical Ruscic G3B3 calc. HF298=19.55 kcal

```

3 T 7/04 C 4.00H 9.00 0.00 0.00 0.00 0 57.1142600 81801.384
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18215.583
-4.455716920D+03 3.745702640D+02-8.335908210D+00 1.864087416D-01-1.037079055D-03
3.186200710D-06-3.762843230D-09 0.000000000D+00 6.520901920D+03 5.549346880D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18215.583
-3.649565630D+05 6.383377960D+03-3.837258020D+01 1.529180141D-01-1.795907724D-04
1.151968516D-07-3.046839407D-11 0.000000000D+00-2.173812939D+04 2.364198411D+02
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18215.583
7.383354750D+06-3.027061163D+04 5.271781520D+01-4.905879500D-03 8.532567760D-07
-7.946197170D-11 3.066617980D-15 0.000000000D+00 1.896053000D+05-3.271807010D+02

```

C4H9 s-BUTYL RADICAL Burcat G3B3 calc

```

3 T 6/04 C 4.00H 9.00 0.00 0.00 0.00 0 57.1142600 70224.256
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17600.211
-6.028755900D+03 4.320850560D+02-6.674478950D+00 1.397307858D-01-6.718785550D-04
1.801480689D-06-1.763894467D-09 0.000000000D+00 4.953175840D+03 5.390758270D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17600.211
-4.041345580D+05 7.016207240D+03-4.168382680D+01 1.548745242D-01-1.781318990D-04
1.124319437D-07-2.942069729D-11 0.000000000D+00-2.597517186D+04 2.582491665D+02
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17600.211
7.370704700D+06-3.063117675D+04 5.232016700D+01-5.227141420D-03 9.358410820D-07
-8.985661620D-11 3.579715860D-15 0.000000000D+00 1.904617698D+05-3.241483890D+02

```

C4H9 ISOBUTYL RADICAL Burcat G3B3 calc. HF298=17.635 kcal

```

3 T 6/04 C 4.00H 9.00 0.00 0.00 0.00 0 57.1142600 73784.840
50.000 200.000 5 0.0 1.0 2.0 3.0 4.0 0.0 0.0 0.0 18183.870
4.547183040D+00-4.305351910D-02 8.782994330D-04-4.064451920D-06 6.430690800D-09
0.000000000D+00 0.000000000D+00 0.000000000D+00 6.684518690D+03 7.777354550D+00
200.000 1000.000 5 0.0 1.0 2.0 3.0 4.0 0.0 0.0 0.0 18183.870
3.246800720D+00 2.375211555D-02 3.198663650D-05-5.959778650D-08 2.627466183D-11
0.000000000D+00 0.000000000D+00 0.000000000D+00 6.673257560D+03 1.011447720D+01
1000.000 6000.000 5 0.0 1.0 2.0 3.0 4.0 0.0 0.0 0.0 18183.870
9.886194540D+00 2.250541045D-02-7.914261140D-06 1.259810617D-09-7.472635650D-14
0.000000000D+00 0.000000000D+00 0.000000000D+00 4.012993870D+03-2.825019524D+01

```

t-C4H9 t-Butyl Radical G3B3 calc. HF298=13.155 kcal HF0=18.55 kcal

```

3 T 6/04 C 4.00H 9.00 0.00 0.00 0.00 0 57.1142600 55040.520
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17641.745
-6.865720960D+03 4.629502680D+02-6.278457250D+00 1.354169050D-01-6.724110780D-04
1.832048087D-06-1.829593582D-09 0.000000000D+00 2.994827929D+03 5.299941870D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17641.745
-4.243657510D+05 7.221822590D+03-4.124530810D+01 1.455634211D-01-1.577111287D-04
9.502666610D-08-2.405598332D-11 0.000000000D+00-2.890616201D+04 2.584270429D+02
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17641.745
7.630370770D+06-3.198102280D+04 5.352771820D+01-5.764264440D-03 1.063228612D-06
-1.052268528D-10 4.320117830D-15 0.000000000D+00 1.968891799D+05-3.337812450D+02

```



Table 5 (continued)

C4H9O n-butoxy radical												CH3CH2CH2CH2O*	HF298=-56.350 kJ	Burcat	G3B3	calc
3	A08/04	C	4.00H	9.000	1.00	0.00	0.00	0	73.1136600		-56350.112					
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	19313.821			
-3.488666030D+03												2.207382122D+02	-2.290907752D+00	1.006801619D-01	-4.282421310D-04	
1.157912285D-06												-1.119053307D-09	0.000000000D+00	-9.817513250D+03	3.536633030D+01	
	200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	19313.821			
-4.885832290D+05												8.234037770D+03	-4.833000860D+01	1.771343538D-01	-1.924581720D-04	
1.117148715D-07												-2.695974435D-11	0.000000000D+00	-4.730142620D+04	2.956454184D+02	
	1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	19313.821			
5.225066510D+06												-2.681459942D+04	5.527070870D+01	-5.799319530D-03	1.065530987D-06	
-1.049344697D-10												4.301889960D-15	0.000000000D+00	1.464399928D+05	-3.354907170D+02	
C4H9O i-butoxy radical												(CH3)2CHCH2O*	HF298=-65.07 kJ	Burcat	G3B3	calc
3	A08/04	C	4.00H	9.000	1.00	0.00	0.00	0	73.1136600		-65069.568					
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18294.072			
-1.208637219D+04												8.210091200D+02	-1.674303696D+01	2.279426044D-01	-9.669911880D-04	
2.282413914D-06												-2.035957078D-09	0.000000000D+00	-1.269012113D+04	9.532912940D+01	
	200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18294.072			
-4.548010730D+05												7.443052380D+03	-4.372427990D+01	1.665804070D-01	-1.820808753D-04	
1.073586337D-07												-2.635496440D-11	0.000000000D+00	-4.471757550D+04	2.674311398D+02	
	1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18294.072			
5.663474030D+06												-2.763506346D+04	5.518597920D+01	-5.374181990D-03	1.027712880D-06	
-1.052036166D-10												4.455204170D-15	0.000000000D+00	1.513366543D+05	-3.382039840D+02	
C4H9O s-butoxy radical												CH3CH(O*)CH2CH3	HF298=-69.84 kJ	Burcat	G3B3	calc
3	A09/04	C	4.00H	9.000	1.00	0.00	0.00	0	73.1136600		-69843.512					
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18700.128			
-8.398527430D+03												5.333835370D+02	-8.990875130D+00	1.464532558D-01	-5.287278720D-04	
1.032428791D-06												-5.204746190D-10	0.000000000D+00	-1.241129647D+04	6.407518950D+01	
	200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18700.128			
-4.681104270D+05												7.875394340D+03	-4.708385840D+01	1.769408482D-01	-1.955493627D-04	
1.153613644D-07												-2.822006410D-11	0.000000000D+00	-4.715446780D+04	2.863550822D+02	
	1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18700.128			
5.098477150D+06												-2.606787286D+04	5.422400860D+01	-5.279475870D-03	9.730813690D-07	
-9.593376250D-11												3.926501460D-15	0.000000000D+00	1.403982430D+05	-3.292259740D+02	
C4H9O T butoxy radical												(CH3)3CO*	HF298=-20.775 kcal	G3B3	calc	
3	T08/04	C	4.00H	9.000	1.00	0.00	0.00	0	73.1136600		-86922.600					
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18637.211			
-1.717396532D+04												1.071501904D+03	-2.019664831D+01	2.267648553D-01	-7.120666420D-04	
9.160513030D-07												2.134032473D-10	0.000000000D+00	-1.627629243D+04	1.113433077D+02	
	200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18637.211			
-4.061722330D+05												6.490515360D+03	-3.777743090D+01	1.531104200D-01	-1.649137602D-04	
9.523242600D-08												-2.285000359D-11	0.000000000D+00	-4.305931820D+04	2.327956434D+02	
	1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18637.211			
5.090017260D+06												-2.544453448D+04	5.327690810D+01	-4.872635280D-03	9.267027520D-07	
-9.444977570D-11												3.985701710D-15	0.000000000D+00	1.349543358D+05	-3.242474510D+02	

Table 5 (continued)

C4H9O2 Peroxy Tertiary Butyl Radical PM3 HF298=THERGAS, Rough Estimate

```

3 T 9/03 C 4.00H 9.00O 2.00 0.00 0.00 0 89.1130600 -102970.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22335.103
-1.100393866D+04 8.182928240D+02-1.868919042D+01 3.036367605D-01-1.548454315D-03
4.311919030D-06-4.655111830D-09 0.000000000D+00-1.765427685D+04 1.002833326D+02
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22335.103
-4.583899830D+05 8.100963880D+03-5.059379560D+01 2.085014924D-01-2.627033266D-04
1.743871673D-07-4.688058150D-11 0.000000000D+00-5.226206660D+04 3.026472457D+02
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22335.103
6.492427930D+06-2.782951131D+04 5.494859360D+01-3.756283080D-03 5.363665510D-07
-3.916285310D-11 1.098918778D-15 0.000000000D+00 1.499578617D+05-3.318091980D+02

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C4H10FO2P SARIN CH(CH3)2OP(O)FCH3 Melius BACMP4 Q2U

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3 T 9/96 C 4.00H 10.00F 1.00O 2.00P 1.00 0 140.0931642 -963156.800
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 29468.372
-1.010371812D+04 7.578264890D+02-1.785114323D+01 3.256144660D-01-1.574787672D-03
4.314692600D-06-4.660199850D-09 0.000000000D+00-1.217621717D+05 9.773127620D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 29468.372
-3.798268200D+05 6.440533470D+03-3.715121640D+01 1.838942695D-01-2.116282711D-04
1.330137454D-07-3.475614190D-11 0.000000000D+00-1.492836023D+05 2.341630026D+02
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 29468.372
7.348398660D+06-3.454095210D+04 7.212165050D+01-6.630827580D-03 1.256966796D-06
-1.274943916D-10 5.350477200D-15 0.000000000D+00 8.289564360D+04-4.380120750D+02

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C4H10N2 1,4-PIPERAZINE Burcat G3B3 calc HF298=7.66 kcal.

```

3 A03/05 C 4.00H 10.00N 2.00 0.00 0.00 0 86.1356800 32057.808
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16632.540
-4.881574820D+03 3.376099860D+02-4.637502230D+00 9.377332700D-02-3.650278690D-04
1.040975548D-06-9.856816140D-10 0.000000000D+00 7.655835620D+02 4.408221740D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16632.540
-5.676969110D+05 1.012728896D+04-6.624207290D+01 2.365870559D-01-2.745519964D-04
1.706745546D-07-4.369006730D-11 0.000000000D+00-4.440611570D+04 3.839677300D+02
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16632.540
7.914951230D+06-3.607728490D+04 6.552598630D+01-5.989469690D-03 1.059509083D-06
-1.005906816D-10 3.964848110D-15 0.000000000D+00 2.148511031D+05-4.174447130D+02

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C4H10O2 Tert-Butyl Hydroperoxy PM3 HF298=THERGAS

```

3 T 9/03 C 4.00H 10.00O 2.00 0.00 0.00 0 90.1210000 -247780.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22580.912
-1.091897681D+04 8.252909140D+02-1.960590591D+01 2.953223282D-01-1.339680027D-03
3.347644390D-06-3.176156840D-09 0.000000000D+00-3.509468930D+04 1.040024001D+02
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22580.912
-4.411821990D+05 7.684178860D+03-4.862367130D+01 2.095897145D-01-2.649339580D-04
1.764911643D-07-4.752434620D-11 0.000000000D+00-6.786612590D+04 2.895204368D+02
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22580.912
7.303201950D+06-3.012653144D+04 5.827494870D+01-3.699700240D-03 5.262558510D-07
-3.722541270D-11 9.503190340D-16 0.000000000D+00 1.469517795D+05-3.553268080D+02

```

Table 5 (continued)

C4H12Sn Stanumtetramethyl Sn(CH3)4 Allendorf & Melius JPC 109, (2005), 4939.														
3	A	6/05	SN	1.00C	4.00H	12.00	0.00	0.00	0	178.8480800	-20501.600			
		50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	29840.215
		1.871832992D+04		-1.546108104D+03		4.832408560D+01		-4.382585430D-01		2.690379945D-03				
		-7.613144610D-06		8.666986760D-09		0.000000000D+00		-1.310969623D+03		-1.697777403D+02				
		200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	29840.215
		-5.327360760D+04		1.596923617D+03		-8.166177840D+00		9.565197100D-02		-1.035139294D-04				
		6.760353660D-08		-1.890677648D-11		0.000000000D+00		-1.276988485D+04		7.642900020D+01				
		1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	29840.215
		9.336010050D+06		-3.812304390D+04		6.892512180D+01		-7.133019930D-03		1.335540505D-06				
		-1.338932180D-10		5.558226200D-15		0.000000000D+00		2.234984770D+05		-4.229128420D+02				
C4H12Sn Stanumdiethyldihydride (C2H5)2SnH2 Allendorf, Melius JPC 109, (2005), 4939														
3	A	6/05	SN	1.00C	4.00H	12.00	0.00	0.00	0	178.8480800	56484.000			
		50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	26919.764
		-6.439799670D+03		5.407103100D+02		-1.288944289D+01		2.756938960D-01		-1.439830778D-03				
		4.267029290D-06		-4.982513220D-09		0.000000000D+00		1.908336774D+03		7.843920240D+01				
		200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	26919.764
		-2.691631776D+05		4.709199800D+03		-2.657288578D+01		1.440172285D-01		-1.613044607D-04				
		1.013020675D-07		-2.677666648D-11		0.000000000D+00		-1.818131821D+04		1.783879492D+02				
		1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	26919.764
		7.506674460D+06		-3.368470360D+04		6.642847070D+01		-6.082943920D-03		1.028271902D-06				
		-9.406345840D-11		3.613608550D-15		0.000000000D+00		2.027410038D+05		-4.025112000D+02				
C5H2Cl2O 3,4-dichloro-2,4-cyclopentadiene 1-one Janoschek J. Mol. Struct. 2003														
3	T06/03	C		5.00H	2.00O	1.00CL	2.00	0.00	0	148.9741800	-12170.000			
		50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	20679.427
		4.894893050D+03		-3.053973192D+02		9.972406610D+00		-4.053465920D-02		4.325999160D-04				
		-1.221976510D-06		1.345328330D-09		0.000000000D+00		-2.914184172D+03		-1.474346725D+01				
		200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	20679.427
		-8.942206890D+02		4.910508320D+02		-4.612563960D+00		7.848012020D-02		-9.590485280D-05				
		6.081899470D-08		-1.571636737D-11		0.000000000D+00		-5.642931580D+03		5.033298180D+01				
		1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	20679.427
		1.300057118D+06		-9.706310710D+03		3.337364200D+01		-1.690126921D-03		3.069466603D-07				
		-2.993228353D-11		1.211660703D-15		0.000000000D+00		4.819593150D+04		-1.731953904D+02				
C5H2Cl3 1,3,4 trichloro-2,4 cyclopentadienyl radical Janoschek J. Mol. Struct.														
3	T	6/03	C	5.00H	2.00CL	3.00	0.00	0.00	0	168.4274800	152680.000			
		50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22140.278
		4.492557350D+03		-2.591196754D+02		8.023879930D+00		-5.414531780D-03		2.438132366D-04				
		-7.288136340D-07		8.106760140D-10		0.000000000D+00		1.661049747D+04		-6.464199830D+00				
		200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22140.278
		-5.735278540D+04		1.268086427D+03		-8.033228260D+00		9.065262790D-02		-1.147549266D-04				
		7.426288930D-08		-1.939045242D-11		0.000000000D+00		1.018780200D+04		7.162283960D+01				
		1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22140.278
		1.025800922D+06		-8.394112130D+03		3.242990720D+01		-1.320009509D-03		2.259571879D-07				
		-2.068353598D-11		7.834028990D-16		0.000000000D+00		5.990392680D+04		-1.626116422D+02				

Table 5 (continued)

C5H3Cl3O 1-hydroxy-1,2,4 trichloropentadiene Janoschek J.Mol.Struct. 661/2 2003											
3	T06/03	C	5.00H	3.00O	1.00CL	3.00	0.00	0	185.4348200	-104720.000	
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0 25013.899
-1.846806888D+03 8.755028750D+01 2.151474693D+00 2.505682074D-02 3.762001480D-04											
-1.786517442D-06 2.738810375D-09 0.000000000D+00-1.591799676D+04 2.144844988D+01											
	200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0 25013.899
-1.829806402D+04 6.265926310D+02-5.422466950D+00 1.001156622D-01-1.311759810D-04											
8.759419010D-08-2.344264830D-11 0.000000000D+00-1.806251641D+04 5.531019190D+01											
	1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0 25013.899
1.709039638D+06-1.076842308D+04 3.837734690D+01-1.183369393D-03 1.509168394D-07											
-8.565480300D-12 1.049848180D-16 0.000000000D+00 4.266500880D+04-1.988037376D+02											
C5H3N CyanoVinyl Acetylene HCC-CH=CHCN HF298=422.613 kJ Burcat G3B3 calc											
3	A01/05	C	5.00H	3.00N	1.00	0.00	0.00	0	77.0840600	422613.288	
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0 18379.533
6.327507050D+03-4.343616080D+02 1.448032727D+01-1.066716212D-01 8.107196660D-04											
-2.403519285D-06 2.783532101D-09 0.000000000D+00 5.003216470D+04-3.406583470D+01											
	200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0 18379.533
5.489892060D+04-5.651004470D+02 3.384732350D+00 4.319665310D-02-5.106376330D-05											
3.417479510D-08-9.509486410D-12 0.000000000D+00 5.169123730D+04 6.554309860D+00											
	1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0 18379.533
3.174014340D+06-1.406186686D+04 3.243438020D+01-2.222039336D-03 3.820841950D-07											
-3.518619750D-11 1.342747685D-15 0.000000000D+00 1.312041242D+05-1.773293688D+02											
C5H4 1,3 Pentadiyne HCC-CC-CH3 Burcat G3B3 calc HF298=98.431 kcal											
3	A	1/05	C	5.00H	4.00	0.00	0.00	0.00	0	64.0852600	411835.304
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0 17221.176
3.533676890D+03-2.132018561D+02 8.033424250D+00-2.671541317D-02 2.778947653D-04											
-7.079074910D-07 6.414474100D-10 0.000000000D+00 4.819176680D+04-1.082683132D+01											
	200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0 17221.176
2.425426603D+04-2.144595513D+02 2.449079166D+00 3.805198500D-02-3.986458750D-05											
2.547778722D-08-7.033164700D-12 0.000000000D+00 4.871906140D+04 1.071892567D+01											
	1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0 17221.176
4.149705470D+06-1.716521184D+04 3.430642550D+01-2.861076924D-03 5.074662870D-07											
-4.832541320D-11 1.911065091D-15 0.000000000D+00 1.500525075D+05-1.967548828D+02											
C5H4 1,4 Pentadiyne HCC-CH2-CCH Burcat G3B3 calc HF298=108.022 kcal											
3	A	1/05	C	5.00H	4.00	0.00	0.00	0.00	0	64.0852600	451964.048
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0 17191.220
-4.897478810D+02 2.069997749D+01 3.730302400D+00-3.562906980D-03 2.670151528D-04											
-9.096767680D-07 1.097791369D-09 0.000000000D+00 5.221219770D+04 1.061031418D+01											
	200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0 17191.220
8.924367120D+04-1.168102393D+03 6.366308660D+00 3.492976860D-02-4.258373940D-05											
3.043165772D-08-8.944078230D-12 0.000000000D+00 5.818284700D+04-1.174924656D+01											
	1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0 17191.220
3.940830410D+06-1.593839350D+04 3.306892230D+01-2.290054607D-03 3.703726900D-07											
-3.173066510D-11 1.112015426D-15 0.000000000D+00 1.474800597D+05-1.853879322D+02											

Table 5 (continued)

C5H4 Pentane Tetraene H2C=C=C=CH2 Burcat G3B3 calc HF298=106.23 kcal											
3	A	1/05	C	5.00H	4.00	0.00	0.00	0.00	0.00	0	64.0852600
				50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0
											3.0
											4.0
											0.0
											16967.550
				2.582736821D+03	-1.422877024D+02	5.967614290D+00	2.558714324D-03	5.493264800D-05			
				5.714360630D-08	-2.942372677D-10	0.000000000D+00	5.192483970D+04	-3.010917277D+00			
				200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0
											3.0
											4.0
											0.0
											16967.550
				4.926838780D+04	-3.212426460D+02	1.074363788D+00	4.593984030D-02	-5.359785440D-05			
				3.605751320D-08	-1.013252621D-11	0.000000000D+00	5.349712210D+04	1.604084527D+01			
				1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0
											3.0
											4.0
											0.0
											16967.550
				3.836202550D+06	-1.631003855D+04	3.379819420D+01	-2.683534305D-03	4.711397980D-07			
				-4.433093180D-11	1.729875822D-15	0.000000000D+00	1.482942141D+05	-1.930134341D+02			
C5H4 1,2 Pentadiene-4-yne H2C=C=C-CCH Burcat G3B3 calc HF298=103.57 kcal											
3	A	2/05	C	5.00H	4.00	0.00	0.00	0.00	0.00	0	64.0852600
				50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0
											3.0
											4.0
											0.0
											16628.484
				-2.279223761D+03	1.470056673D+02	1.560872648D-01	4.762183050D-02	-1.146897714D-04			
				3.359891810D-07	-3.621925890D-10	0.000000000D+00	4.964027970D+04	2.453136085D+01			
				200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0
											3.0
											4.0
											0.0
											16628.484
				7.917087670D+04	-6.413911950D+02	1.216487759D+00	5.054018240D-02	-6.395015730D-05			
				4.517339250D-08	-1.306591998D-11	0.000000000D+00	5.391293640D+04	1.502655988D+01			
				1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0
											3.0
											4.0
											0.0
											16628.484
				3.434510050D+06	-1.532179945D+04	3.343592920D+01	-2.622537549D-03	4.687424110D-07			
				-4.485886740D-11	1.778989765D-15	0.000000000D+00	1.402569183D+05	-1.877810999D+02			
C5H4N 1,3-pentadiene-4cyano-1-yl Radical *CH=CH-CH=CH-CN G3B3calc HF298=120.206 kcal											
3	A	4/05	C	5.00H	4.00N	1.00	0.00	0.00	0.00	0	78.0920000
				50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0
											3.0
											4.0
											0.0
											19160.396
				3.643701690D+03	-2.364213035D+02	8.701817120D+00	-2.142839574D-02	2.516550313D-04			
				-6.997355670D-07	8.432820120D-10	0.000000000D+00	5.897775550D+04	-9.507791700D+00			
				200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0
											3.0
											4.0
											0.0
											19160.396
				-3.544935340D+04	1.154734196D+03	-7.975315470D+00	7.813851020D-02	-9.728240680D-05			
				6.535736590D-08	-1.793402414D-11	0.000000000D+00	5.343517570D+04	7.068967000D+01			
				1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0
											3.0
											4.0
											0.0
											19160.396
				3.372303630D+06	-1.536249052D+04	3.520524780D+01	-2.066995608D-03	2.979904124D-07			
				-2.341258577D-11	7.716700020D-16	0.000000000D+00	1.480935009D+05	-1.936792408D+02			
C5H4N m-Pyridyl Radical HF298=96.855 kcal Burcat G3B3 calc QCISD/SCF=QC											
3	A	2/05	C	5.00H	4.00N	1.00	0.00	0.00	0.00	0	78.0920000
				50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0
											3.0
											4.0
											0.0
											13634.201
				9.763859540D+01	-3.646424610D+01	6.004422890D+00	-4.234911010D-02	3.691185510D-04			
				-9.984497390D-07	1.228071059D-09	0.000000000D+00	4.718269730D+04	3.468110900D+00			
				200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0
											3.0
											4.0
											0.0
											13634.201
				-2.344890322D+05	4.858150610D+03	-3.549923960D+01	1.476889693D-01	-1.812578286D-04			
				1.160466424D-07	-3.022691849D-11	0.000000000D+00	2.567891478D+04	2.154396681D+02			
				1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0
											3.0
											4.0
											0.0
											13634.201
				2.798127533D+06	-1.571141507D+04	3.644623270D+01	-2.565527863D-03	4.481652550D-07			
				-4.192077690D-11	1.624863173D-15	0.000000000D+00	1.363906010D+05	-2.100547532D+02			

Table 5 (continued)

C5H4O2 Ketene Propylene aldehyde O=CH-CH=CH-CH=C=O Burcat G3B3 HF298=-25.295  
 3 A 4/05 C 5.00H 4.00O 2.00 0.00 0.00 0 96.0840600 -105834.280  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20079.854  
 -6.110160330D-01 2.216186148D+01 2.771172264D+00 4.238695630D-02-7.172711810D-05  
 1.642065466D-07-1.510126424D-10 0.000000000D+00-1.518503304D+04 1.719566953D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20079.854  
 -1.618352509D+05 2.863317145D+03-1.579462582D+01 9.381121470D-02-1.037631658D-04  
 6.245518860D-08-1.570716746D-11 0.000000000D+00-2.824540371D+04 1.183190874D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20079.854  
 3.599323460D+06-1.788642546D+04 4.076934970D+01-3.348243680D-03 6.297841490D-07  
 -6.351672520D-11 2.654460520D-15 0.000000000D+00 8.855571470D+04-2.294050802D+02

C5H5 1-Pentyne-3-ene-5yl HCC-CH=CH-CH2\* Burcat G3B3 calc HF298=92.0 kcal  
 3 A 1/05 C 5.00H 5.00 0.00 0.00 0.00 0 65.0932000 384928.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18195.567  
 5.577086640D+03-4.200457570D+02 1.637373470D+01-1.538400162D-01 1.174752789D-03  
 -3.652500880D-06 4.465053100D-09 0.000000000D+00 4.541575740D+04-3.846431650D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18195.567  
 1.913659338D+04 2.201077166D+02-3.420848310D+00 6.670105980D-02-8.439282910D-05  
 5.777596560D-08-1.605769204D-11 0.000000000D+00 4.380031580D+04 4.275699750D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18195.567  
 3.958301240D+06-1.666427183D+04 3.568862790D+01-2.517312798D-03 4.143888170D-07  
 -3.612300240D-11 1.289916470D-15 0.000000000D+00 1.428445056D+05-2.002457761D+02

C5H5N 1-Cyano-1,3-Butadiene CH2=CH-CH=CH-CN HF298=57.108 kcal Burcat G3B3 calc  
 3 A 2/05 C 5.00H 5.00N 1.00 0.00 0.00 0 79.0999400 238944.056  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19245.910  
 3.655424090D+03-2.391292540D+02 8.873918670D+00-2.420840305D-02 2.622391168D-04  
 -6.986981230D-07 8.368357480D-10 0.000000000D+00 2.722168254D+04-1.071523456D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19245.910  
 -8.499428320D+04 2.061881771D+03-1.421734736D+01 9.651220360D-02-1.171921338D-04  
 7.731496790D-08-2.099078002D-11 0.000000000D+00 1.754710073D+04 1.037448211D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19245.910  
 3.932386020D+06-1.846197711D+04 4.039873410D+01-2.893030802D-03 4.677612650D-07  
 -4.164906130D-11 1.573308390D-15 0.000000000D+00 1.343455299D+05-2.309321352D+02

C5H7 1,3-Pentadiene-5yl Radical Burcat G3B3 calc HF298=49.105 kcal  
 3 A 1/05 C 5.00H 7.00 0.00 0.00 0.00 0 67.1090800 205455.320  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17483.737  
 1.057146240D+02 8.498018390D+01-1.310225228D+00 1.020712436D-01-5.833102680D-04  
 2.030979186D-06-2.598117865D-09 0.000000000D+00 2.243968597D+04 2.957366637D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17483.737  
 -2.724108308D+05 5.170151780D+03-3.384120770D+01 1.468887133D-01-1.793958656D-04  
 1.173753440D-07-3.136860343D-11 0.000000000D+00-7.318381210D+02 2.109869988D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17483.737  
 6.666827780D+06-2.766210575D+04 5.027837710D+01-5.656311540D-03 1.025198586D-06  
 -9.991313750D-11 4.048558400D-15 0.000000000D+00 1.881114575D+05-3.058033965D+02

Table 5 (continued)

C5H7 1,4-Pentadiene-3yl Radical G3B3 calc HF298=49.105 kcal HF0=53.151 kcal  
 3 A 1/05 C 5.00H 7.00 0.00 0.00 0.00 0.00 0 67.1090800 205455.320  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17275.060  
 3.150903378D+01 9.004910150D+01-1.052489251D+00 8.797608550D-02-4.657846540D-04  
 1.673508532D-06-2.202879889D-09 0.000000000D+00 2.244221611D+04 2.918916192D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17275.060  
 -2.452899837D+05 4.758799930D+03-3.228942590D+01 1.455213376D-01-1.785162693D-04  
 1.175636455D-07-3.163419570D-11 0.000000000D+00 1.292936546D+03 2.009958713D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17275.060  
 7.657776920D+06-3.126280959D+04 5.518985360D+01-7.747960350D-03 1.464108391D-06  
 -1.486284663D-10 6.261880720D-15 0.000000000D+00 2.102863539D+05-3.407532400D+02

C5H7 CYCLO-1-penten-1yl Burcat G3B3 calc HF298=41.258 kcal HF0=45.971 kcal  
 3 A 9/04 C 5.00H 7.00 0.00 0.00 0.00 0.00 0 67.1090800 172623.472  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14784.737  
 3.538823030D+03-2.440009026D+02 9.771973370D+00-5.100563600D-02 2.510683834D-04  
 -2.471823601D-07 3.391633880D-11 0.000000000D+00 1.977861756D+04-1.464468362D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14784.737  
 -2.965084546D+05 6.302408040D+03-4.624742910D+01 1.837121001D-01-2.294936632D-04  
 1.511251312D-07-4.044965170D-11 0.000000000D+00-8.770110030D+03 2.727806299D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14784.737  
 5.114072600D+06-2.395655417D+04 4.668382680D+01-3.776485480D-03 6.438796720D-07  
 -5.855063780D-11 2.198044236D-15 0.000000000D+00 1.594680501D+05-2.840180030D+02

C5H7 Cyclo-1-penten-4yl Radical G3B3 calc HF298=53.523 kcal Burcat G3B3 calc  
 3 A 9/04 C 5.00H 7.00 0.00 0.00 0.00 0.00 0 67.1090800 223940.232  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15030.681  
 -4.508033670D+03 3.442201980D+02-6.105054560D+00 1.359300505D-01-7.899604700D-04  
 2.572784249D-06-3.010761435D-09 0.000000000D+00 2.405440983D+04 4.867732470D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15030.681  
 -2.823064058D+05 5.807757430D+03-4.104524180D+01 1.654310359D-01-2.048590748D-04  
 1.358935125D-07-3.680307330D-11 0.000000000D+00-6.599659180D+02 2.453532990D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15030.681  
 6.057717160D+06-2.654669614D+04 4.826803680D+01-4.319849680D-03 7.503905730D-07  
 -6.966522140D-11 2.675946352D-15 0.000000000D+00 1.828320254D+05-2.977196398D+02

C5H7CL 5 Chloro-1,3-Pentadiene Burcat G3B3 calc HF298=13.884 kcal HF0=18.27 kcal  
 3 A08/05 C 5.00H 7.00CL 1.00 0.00 0.00 0.00 0 102.5617800 58090.656  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 21352.429  
 9.422328820D+02-6.486808600D+01 5.113208170D+00 3.298022350D-02-9.257399510D-05  
 3.778940270D-07-3.868473820D-10 0.000000000D+00 4.629974430D+03 7.378723160D+00  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 21352.429  
 -2.489180915D+05 4.957805860D+03-3.259081210D+01 1.544533259D-01-1.930821384D-04  
 1.277522538D-07-3.434857740D-11 0.000000000D+00-1.777418728D+04 2.073782918D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 21352.429  
 5.207941550D+06-2.306789527D+04 4.777750940D+01-3.516409390D-03 5.322779900D-07  
 -4.179353060D-11 1.308680946D-15 0.000000000D+00 1.404342993D+05-2.779106054D+02

Table 5 (continued)

C5H7CL2 1,5-diChloro-3-Pentene-1-yl Burcat G3B3 calc HF298=26.512 kcal  
 3 A08/05 C 5.00H 7.00CL 2.00 0.00 0.00 0 138.0144800 110926.208  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 26257.459  
 -6.632858190D+03 4.157539700D+02-4.841517650D+00 1.590774372D-01-7.399248820D-04  
 2.097303900D-06-2.236185762D-09 0.000000000D+00 8.776176680D+03 5.381465090D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 26257.459  
 -2.918491574D+05 5.695243210D+03-3.639079830D+01 1.795085459D-01-2.350938548D-04  
 1.590559194D-07-4.320891480D-11 0.000000000D+00-1.543234779D+04 2.339136232D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 26257.459  
 4.120477180D+06-1.926988840D+04 4.675008820D+01-2.717435975D-03 4.243399130D-07  
 -3.439899540D-11 1.109393462D-15 0.000000000D+00 1.220296126D+05-2.564677584D+02

C5H7O Cy C5H7-O\* Cy-1-penten-4-oxy Burcat G3B3 calc HF298=22.714 kcal  
 3 A10/04 C 5.00H 7.00O 1.00 0.00 0.00 0 83.1084800 95039.560  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16751.831  
 -4.100764600D+03 2.119501980D+02 4.229186590D-01 3.598645720D-02-5.920233100D-05  
 1.427798063D-07 1.920435265D-10 0.000000000D+00 8.654798070D+03 2.682439883D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16751.831  
 -3.089931775D+05 6.563352380D+03-4.837891050D+01 1.983871925D-01-2.495035338D-04  
 1.649237394D-07-4.428262860D-11 0.000000000D+00-1.949532018D+04 2.846991905D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16751.831  
 4.911479800D+06-2.422401974D+04 5.003834980D+01-3.950713640D-03 6.863693830D-07  
 -6.369143760D-11 2.443949483D-15 0.000000000D+00 1.501416867D+05-3.021527979D+02

C5H8 1,3 Pentadiene CH2=CH-CH=CH-CH3 Burcat G3B3 calc HF298=20.11 kcal  
 3 A12/04 C 5.00H 8.00 0.00 0.00 0.00 0 68.1170200 84156.976  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17527.050  
 -3.596043250D+03 2.674317790D+02-3.941331290D+00 1.067135595D-01-4.656465270D-04  
 1.304267097D-06-1.319036555D-09 0.000000000D+00 7.179632210D+03 4.158727270D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17527.050  
 -3.036927178D+05 5.484369860D+03-3.449387870D+01 1.433408655D-01-1.599516687D-04  
 9.756851910D-08-2.490720330D-11 0.000000000D+00-1.699921257D+04 2.150587000D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17527.050  
 5.503875830D+06-2.675837472D+04 5.271059540D+01-5.688744840D-03 1.074596647D-06  
 -1.092579972D-10 4.620650250D-15 0.000000000D+00 1.646053339D+05-3.218196460D+02

C5H8CL 5 Chloro-3-Pentene-1-yl Burcat G3B3 calc HF298=37.81 kcal  
 3 A04/05 C 5.00H 8.00CL 1.00 0.00 0.00 0 103.5697200 158197.040  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22639.970  
 -2.626281811D+03 1.244377264D+02 3.041206545D+00 1.804485090D-02 2.501066702D-04  
 -1.173277470D-06 1.906100971D-09 0.000000000D+00 1.582612954D+04 2.128728181D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22639.970  
 -2.934016070D+05 5.357295390D+03-3.394865570D+01 1.621561802D-01-2.015398440D-04  
 1.323155755D-07-3.526940360D-11 0.000000000D+00-8.030940670D+03 2.173065392D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22639.970  
 5.879846490D+06-2.539867994D+04 5.206234560D+01-4.469757060D-03 7.719106780D-07  
 -7.057433410D-11 2.654901484D-15 0.000000000D+00 1.665038999D+05-3.037249983D+02



Table 5 (continued)

C5H8O CYCLOPENTANONE IR +B3PW91/6-31G\* NIST HF298 Wiberg JACS 113 (1991),3447.

3 T 7/01 C	5.00H	8.000	1.00	0.00	0.00	0	84.1164200	-197401.120
50.000	200.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.135089410D+03	-2.907539929D+02	1.147322608D+01	-7.765483680D-02	5.458508220D-04				
-1.357500671D-06	1.544141425D-09	0.000000000D+00	-2.489712428D+04	-2.124591194D+01				
200.000	1000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.264231040D+05	6.623230910D+03	-4.743717410D+01	1.938164554D-01	-2.349140233D-04				
1.519931415D-07	-4.034897170D-11	0.000000000D+00	-5.525009790D+04	2.792475493D+02				
1000.000	6000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.629628650D+06	-2.787769786D+04	5.593859690D+01	-5.150069860D-03	9.570587490D-07				
-9.520270320D-11	3.921477740D-15	0.000000000D+00	1.364652318D+05	-3.447310060D+02				

C5H8O 1-Cyclopenten-3-ol Burcat G3B3 calc HF298=30.253 kcal

3 A 4/05 C	5.00H	8.000	1.00	0.00	0.00	0	84.1164200	-126578.552
50.000	200.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.736916150D+03	4.365525070D+02	-6.281815760D+00	1.008616494D-01	-3.460778080D-04				
8.436575030D-07	-5.949213630D-10	0.000000000D+00	-1.865929675D+04	5.419188890D+01				
200.000	1000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.534723160D+05	6.924794370D+03	-4.939521320D+01	2.009027494D-01	-2.485871327D-04				
1.623957244D-07	-4.315864860D-11	0.000000000D+00	-4.817066400D+04	2.903653276D+02				
1000.000	6000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.895931530D+06	-2.714559833D+04	5.334462950D+01	-3.956893990D-03	6.443627430D-07				
-5.559314630D-11	1.963056942D-15	0.000000000D+00	1.420221957D+05	-3.266778720D+02				

C5H9 CycloPentyl Radical Burcat G3B3 calc HF298=26.561 kcal HF0=32.972 kcal

3 A12/04 C	5.00H	9.00	0.00	0.00	0.00	0	69.1249600	111131.224
50.000	200.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.235745989D+03	2.232388990D+02	-4.321285830D+00	1.362070863D-01	-8.753856950D-04				
3.061297947D-06	-3.795802060D-09	0.000000000D+00	1.079128664D+04	4.002914750D+01				
200.000	1000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.554165180D+05	8.722811160D+03	-5.902322950D+01	2.170255366D-01	-2.629057885D-04				
1.699778299D-07	-4.500438050D-11	0.000000000D+00	-2.790083157D+04	3.444870870D+02				
1000.000	6000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.802458670D+06	-3.108353872D+04	5.704291000D+01	-5.278685870D-03	9.404037060D-07				
-8.973422420D-11	3.549279220D-15	0.000000000D+00	1.949821132D+05	-3.576284810D+02				

C5H9 2-penten-5-yl CH3CH=CHCH2CH2\* Burcat G3B3 calc HF298=41.734 kcal

3 A 4/05 C	5.00H	9.00	0.00	0.00	0.00	0	69.1249600	174615.056
50.000	200.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.899727848D+03	2.344296853D+02	-3.750815310D+00	1.239954244D-01	-4.911353450D-04				
1.176901888D-06	-1.012067841D-09	0.000000000D+00	1.775848681D+04	4.165122720D+01				
200.000	1000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.813187931D+05	4.869744010D+03	-2.835996897D+01	1.344067963D-01	-1.578242687D-04				
1.022547901D-07	-2.736907779D-11	0.000000000D+00	-4.001363020D+03	1.854580169D+02				
1000.000	6000.000	7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.472248180D+06	-3.025341770D+04	5.438534860D+01	-4.566805610D-03	7.171177710D-07				
-5.984995930D-11	2.054938818D-15	0.000000000D+00	2.003731977D+05	-3.304077600D+02				

Table 5 (continued)

C5H9 2-penten-1-yl *CH2CH=CHCH2CH3 Burcat G3B3 calc HF298=27.892 kcal										
3 A 4/05 C	5.00H	9.00	0.00	0.00	0.00	0.00	0	69.1249600	116700.128	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.191383890D+03	3.635501000D+02	-5.866948630D+00	1.334159480D-01	-6.060214240D-04						
1.792247383D-06	-2.011683207D-09	0.000000000D+00	1.053002690D+04	5.166136980D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.157438525D+05	4.302435790D+03	-2.954657680D+01	1.453627263D-01	-1.791651418D-04						
1.196059520D-07	-3.259824660D-11	0.000000000D+00	-7.491100120D+03	1.869283394D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.238589700D+06	-2.957859109D+04	5.378201360D+01	-4.295494040D-03	6.482149270D-07						
-5.092801920D-11	1.599798998D-15	0.000000000D+00	1.889620607D+05	-3.273518240D+02						
C5H9 1-buten-3-methyl-3-yl H2C=CHC*(CH3)2 Burcat G3B3 calc HF298=24.493 kcal										
3 A 4/05 C	5.00H	9.00	0.00	0.00	0.00	0.00	0	69.1249600	102478.712	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.047360540D+03	3.984706570D+02	-6.476326210D+00	1.359181756D-01	-5.506562360D-04						
1.422332473D-06	-1.412957408D-09	0.000000000D+00	8.644039460D+03	5.254382330D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.555915130D+05	6.064778580D+03	-3.642038400D+01	1.539887292D-01	-1.744991522D-04						
1.064457184D-07	-2.681868120D-11	0.000000000D+00	-1.806362222D+04	2.269765059D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.811454670D+06	-2.641313115D+04	5.253673380D+01	-4.184978990D-03	7.226692330D-07						
-7.021256020D-11	2.882159942D-15	0.000000000D+00	1.654400090D+05	-3.175491640D+02						
C5H9 1-buten-3-methyl-1-yl *HC=CHCH(CH3)CH3 Burcat G3B3 calc HF298=52.364 kcal										
3 A 4/05 C	5.00H	9.00	0.00	0.00	0.00	0.00	0	69.1249600	219090.976	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.073898395D+04	6.860670010D+02	-1.262478464D+01	1.918339914D-01	-8.291402660D-04						
2.113257756D-06	-2.057099817D-09	0.000000000D+00	2.176511248D+04	7.957155620D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.362171780D+05	5.872129380D+03	-3.644424900D+01	1.557520560D-01	-1.786417202D-04						
1.102754526D-07	-2.809295220D-11	0.000000000D+00	-2.917477582D+03	2.263725719D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.773242880D+06	-2.637369996D+04	5.245112680D+01	-4.079625540D-03	6.718296900D-07						
-6.068891300D-11	2.314634963D-15	0.000000000D+00	1.791525440D+05	-3.169562250D+02						
C5H9 1-buten-3-methyl-4-yl H2C=CHCH(CH3)CH2* Burcat G3B3 calc HF298=43.106 kcal										
3 A 4/05 C	5.00H	9.00	0.00	0.00	0.00	0.00	0	69.1249600	180355.504	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.109913860D+03	5.422509480D+02	-7.260362450D+00	1.080539968D-01	-2.227693355D-04						
7.954828300D-08	5.844762890D-10	0.000000000D+00	1.748328266D+04	6.093178980D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.052738495D+05	5.442633850D+03	-3.491832260D+01	1.567208052D-01	-1.849683130D-04						
1.168471121D-07	-3.030445423D-11	0.000000000D+00	-5.479441280D+03	2.179293723D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.076101250D+06	-2.710855552D+04	5.372603250D+01	-5.000011150D-03	9.043502100D-07						
-8.720846820D-11	3.478742030D-15	0.000000000D+00	1.791880762D+05	-3.235790330D+02						

Table 5 (continued)

C5H10O CYCLO TerahydroPyran Burcat G3B3 calc HF298=-53.605 kcal											
3 A 4/05 C	5.00H	10.000	1.00	0.00	0.00	0	86.1323000	-224283.320			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16709.972
-4.614608040D+03	3.280182380D+02	-4.692107310D+00	9.817276570D-02	-3.900440310D-04							
1.059834900D-06	-9.228266020D-10	0.000000000D+00	-3.003303501D+04	4.466453900D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16709.972
-5.928675290D+05	1.049747910D+04	-6.782520960D+01	2.387566410D-01	-2.755251075D-04							
1.708408222D-07	-4.373808890D-11	0.000000000D+00	-7.704643560D+04	3.942697560D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16709.972
7.884225150D+06	-3.660114200D+04	6.661590220D+01	-6.582255800D-03	1.211670392D-06							
-1.196297366D-10	4.898442320D-15	0.000000000D+00	1.867506649D+05	-4.242550400D+02							
C5H12O MTBE Propane 2-methoxy-2-methyl NIST Webbook IR spectrum + NIST											
3 T08/00 C	5.00H	12.000	1.00	0.00	0.00	0	88.1481800	-283200.000			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	24360.200
-1.127050612D+04	8.949962680D+02	-2.296580622D+01	3.555155390D-01	-1.727562322D-03							
4.676966000D-06	-5.086990510D-09	0.000000000D+00	-3.974496470D+04	1.159137373D+02							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	24360.200
-4.153050370D+05	6.542788530D+03	-3.606592270D+01	1.621976486D-01	-1.752602137D-04							
1.067503952D-07	-2.746740216D-11	0.000000000D+00	-6.783774760D+04	2.262918099D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	24360.200
9.609358610D+06	-4.097350960D+04	7.398355080D+01	-7.628021100D-03	1.427912668D-06							
-1.432583022D-10	5.955212210D-15	0.000000000D+00	2.076139363D+05	-4.661625030D+02							
C6 Cumulenlic Linear Van Orden A. and Saykally R Chem.Rev. 98 (1998),2313.											
3 A09/04 C	6.00	0.00	0.00	0.00	0.00	0	72.0642000	1313776.000			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17770.316
4.716824990D+02	-5.199087720D+01	4.808701290D+00	1.229472338D-02	9.096864180D-05							
-3.112684850D-07	2.350989517D-10	0.000000000D+00	1.560230694D+05	3.141945356D+00							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17770.316
9.405027310D+04	-1.833715346D+03	1.641282701D+01	-9.173991590D-03	2.348849693D-05							
-2.079202033D-08	6.454529930D-12	0.000000000D+00	1.641180429D+05	-6.111908570D+01							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17770.316
5.351395720D+05	-4.708172200D+03	1.990100782D+01	-1.340112044D-03	2.944996672D-07							
-3.375366500D-11	1.567697857D-15	0.000000000D+00	1.808424143D+05	-8.941155990D+01							
C6H2Cl3O 2,4,6-TRICHLOROPHENOXY RADICAL Janoschek G3MP2B3 J. Mol. Struct. 2003											
3 T 6/03 C	6.00H	2.000	1.00CL	3.00	0.00	0	196.4375800	-27480.000			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	25713.698
-8.869752500D+02	9.386464570D+01	-5.773342700D-01	9.873933610D-02	-2.463352265D-04							
4.748714030D-07	-3.587548460D-10	0.000000000D+00	-6.648665670D+03	2.957340691D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	25713.698
-1.215346188D+05	2.177239112D+03	-1.258017318D+01	1.126768903D-01	-1.364613400D-04							
8.487070130D-08	-2.144423622D-11	0.000000000D+00	-1.632705094D+04	9.799712260D+01							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	25713.698
9.845652140D+05	-1.009061105D+04	3.979235270D+01	-1.890354515D-03	3.560494600D-07							
-3.595965040D-11	1.504725707D-15	0.000000000D+00	4.576517260D+04	-2.063949344D+02							

Table 5 (continued)

C6H2OC13 2,4,6 TRICHLOROPHENOL-3-yl RADICAL Janoschek G3MP2B3 calc										
3 T 6/03 C	6.00H	2.00O	1.00CL	3.00	0.00	0	196.4375800		101510.000	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.991599677D+03	1.559682117D+02	-1.103521470D+00	6.275623740D-02	2.073027723D-04						
-1.352279540D-06	2.169476982D-09	0.000000000D+00	8.683371330D+03	3.590110490D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.474519760D+04	5.506621220D+02	-2.159753371D+00	8.669713110D-02	-1.045239352D-04						
6.438833320D-08	-1.605496873D-11	0.000000000D+00	6.515563030D+03	4.148119350D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.017305248D+06	-9.241016630D+03	3.825180810D+01	-1.389815894D-03	2.349947434D-07						
-2.135859248D-11	8.067047810D-16	0.000000000D+00	5.681967070D+04	-1.937692019D+02						
C6H2Cl3O3 2,4,6, trichloro-BiCyclo-2,5-hexadiene-1,4-peroxy 1 phenoxy Janoschek										
3 T07/03 C	6.00H	2.00CL	3.00O	3.00	0.00	0	228.4363800		131420.000	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.345095449D+03	-4.131437670D+01	2.739757401D+00	5.316537980D-02	1.867646851D-04						
-9.057597360D-07	1.325677004D-09	0.000000000D+00	1.239714006D+04	1.725943258D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
8.847047620D+04	-7.867045200D+02	3.452541140D-02	1.126318948D-01	-1.517555223D-04						
1.026182335D-07	-2.774191834D-11	0.000000000D+00	1.671978478D+04	2.168418755D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.591913290D+05	-8.945917230D+03	4.479194560D+01	-1.442838869D-03	2.485477154D-07						
-2.281320112D-11	8.636858980D-16	0.000000000D+00	5.517597890D+04	-2.301122849D+02						
C6H2Cl3O3 2,4,6, trichloro-BiCyclo-2-hexene-1-one-5-yl-4,6peroxy Janoschek										
3 T07/03 C	6.00H	2.00CL	3.00O	3.00	0.00	0	228.4363800		28950.000	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.226054620D+03	3.954545630D+02	-8.457173490D+00	1.953618615D-01	-6.684718630D-04						
1.455261990D-06	-1.147425473D-09	0.000000000D+00	-1.362358588D+03	6.250038210D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.946392520D+04	1.146779633D+03	-1.028946930D+01	1.352500184D-01	-1.782014123D-04						
1.187824735D-07	-3.179800380D-11	0.000000000D+00	-4.739806800D+03	8.099677280D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.073400670D+05	-9.466321780D+03	4.514078520D+01	-1.571321801D-03	2.751591244D-07						
-2.571126213D-11	9.925214480D-16	0.000000000D+00	4.594017660D+04	-2.330105262D+02						
o-C6H3 1,2-Benzyne-3-yl Radical Burcat G3B3 calc HF298=174.214 kcal										
3 A02/05 C	6.00H	3.00	0.00	0.00	0.00	0	75.0880200		728911.376	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.255188640D+03	-2.076355841D+02	1.135550949D+01	-1.248641059D-01	1.007539583D-03						
-3.233595140D-06	4.121903720D-09	0.000000000D+00	8.658543860D+04	-1.720333761D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.638682980D+05	3.311644510D+03	-2.393945296D+01	1.138683684D-01	-1.382459723D-04						
8.735113300D-08	-2.246734194D-11	0.000000000D+00	7.138519080D+04	1.532915397D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.039571436D+06	-1.229599523D+04	3.171025900D+01	-2.075422890D-03	3.701029540D-07						
-3.541112950D-11	1.406111847D-15	0.000000000D+00	1.548720980D+05	-1.754815572D+02						

Table 5 (continued)

C6H3OC13 2,4,6-TRICHLOROPHENOL IR-NIST + Janoschek G3MP2B3 calc											
3 T 6/03 C	6.00H	3.00O	1.00CL	3.00	0.00	0	197.4455200	-189070.000			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	24983.540
-2.491872482D+03	1.869095116D+02	-1.688256093D+00	6.358413620D-02	2.386370369D-04							
-1.622269095D-06	2.761047311D-09	0.000000000D+00	-2.632158489D+04	3.746888240D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	24983.540
-1.545485461D+05	2.398119266D+03	-1.350917090D+01	1.155295131D-01	-1.368663535D-04							
8.377632710D-08	-2.084035729D-11	0.000000000D+00	-3.697531890D+04	1.029394740D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	24983.540
1.895303149D+06	-1.278050197D+04	4.263790790D+01	-1.651880843D-03	2.522717471D-07							
-2.022333569D-11	6.525371510D-16	0.000000000D+00	4.344307920D+04	-2.277204891D+02							
C6H2Cl3OOH 2-Hydroxy-2,4,6,trichloro-3,5-cyclohexadiene 1-one Janoschek G3MP2B3											
3 T 7/03 C	6.00H	3.00CL	3.00O	2.00	0.00	0	213.4449200	-277250.000			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	28218.871
-4.060134540D+03	2.892367144D+02	-4.643198420D+00	1.203325483D-01	-1.410193194D-04							
-2.119719192D-07	7.512088550D-10	0.000000000D+00	-3.764869030D+04	4.876713180D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	28218.871
-2.581287994D+04	5.385987140D+02	-4.011368220D+00	1.060314381D-01	-1.310800807D-04							
8.356778750D-08	-2.159534718D-11	0.000000000D+00	-3.901425790D+04	4.857684860D+01							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	28218.871
1.835429203D+06	-1.297234920D+04	4.623477280D+01	-1.977641663D-03	3.340829140D-07							
-3.020999392D-11	1.131071369D-15	0.000000000D+00	3.271118740D+04	-2.463226468D+02							
o-C6H3I 1,2-Benzyne-3-Iodo Burcat B3LYP/6-311G* HF298=127.8 kcal Wang											
3 A08/05 C	6.00H	3.00I	1.00	0.00	0.00	0	201.9924900	534715.200			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18092.782
2.631400517D+03	-1.409341457D+02	6.153104870D+00	-9.549205940D-03	2.259341401D-04							
-6.475226980D-07	7.697593400D-10	0.000000000D+00	6.263913580D+04	2.440194890D+00							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18092.782
-1.217399193D+05	2.561926812D+03	-1.784798592D+01	1.068580670D-01	-1.307895865D-04							
8.374708720D-08	-2.186241706D-11	0.000000000D+00	5.087815590D+04	1.237848702D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18092.782
2.167924481D+06	-1.284935417D+04	3.507194750D+01	-2.204550395D-03	3.960073200D-07							
-3.814766290D-11	1.524404866D-15	0.000000000D+00	1.340815423D+05	-1.901072814D+02							
1,2-C6H4 o-Benzyne Burcat G3B3 calc HF298=110.2 kcal HF298=115. kcal											
3 A02/05 C	6.00H	4.00	0.00	0.00	0.00	0	76.0959600	461135.376			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14264.819
-8.553660800D+01	-4.459922670D+01	6.952577940D+00	-6.722901090D-02	6.304602250D-04							
-2.039130609D-06	2.708919291D-09	0.000000000D+00	5.383182350D+04	-9.417340960D-01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14264.819
-1.582601802D+05	3.495058470D+03	-2.678828058D+01	1.262093085D-01	-1.552988540D-04							
1.003968734D-07	-2.644599092D-11	0.000000000D+00	3.858073570D+04	1.659654052D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14264.819
3.042561354D+06	-1.603660253D+04	3.659180460D+01	-2.599588679D-03	4.521517280D-07							
-4.209500090D-11	1.623419669D-15	0.000000000D+00	1.456290723D+05	-2.119788160D+02							

Table 5 (continued)

1,3-C<sub>6</sub>H<sub>4</sub> m-Benzyne Burcat G3B3 calc HF298=125.16 kcal;

3 A02/05 C	6.00H	4.00	0.00	0.00	0.00	0.00	0	76.0959600	523690.360	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	
									14450.823	
-5.962720340D+02	2.797758598D+01	3.886415400D+00	-1.167419326D-02	1.662098723D-04						
-2.359088336D-07	1.022839341D-10	0.000000000D+00	6.113950960D+04	1.007977832D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	
									14450.823	
-1.005243716D+05	2.758698647D+03	-2.381474835D+01	1.227113983D-01	-1.543757437D-04						
1.014679076D-07	-2.705773598D-11	0.000000000D+00	4.975238540D+04	1.479404987D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	
									14450.823	
2.871198347D+06	-1.532729404D+04	3.606217420D+01	-2.386081849D-03	4.044516660D-07						
-3.656003320D-11	1.363895828D-15	0.000000000D+00	1.487004355D+05	-2.074973304D+02						

1,4-C<sub>6</sub>H<sub>4</sub> p-Benzyne Burcat G3B3 calc HF298=137.25 kcal

3 A02/05 C	6.00H	4.00	0.00	0.00	0.00	0.00	0	76.0959600	574254.000	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	
									15146.903	
1.697563689D+03	-1.359925869D+02	8.516286520D+00	-7.716810470D-02	6.453008840D-04						
-1.812958141D-06	2.063664871D-09	0.000000000D+00	6.765728980D+04	-8.716114740D+00						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	
									15146.903	
-6.355648550D+04	2.026123897D+03	-1.917516912D+01	1.139102324D-01	-1.456433826D-04						
9.675797660D-08	-2.596090463D-11	0.000000000D+00	5.907119890D+04	1.213434043D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	
									15146.903	
2.790790247D+06	-1.455046813D+04	3.540500760D+01	-2.106384760D-03	3.404144250D-07						
-2.904984787D-11	1.010391194D-15	0.000000000D+00	1.502038266D+05	-2.020359363D+02						

1,5-C<sub>6</sub>H<sub>4</sub> 1,5-Hexadiyne-3-ene trans Burcat G3B3 calc HF298=125.025 kcal

3 A02/05 C	6.00H	4.00	0.00	0.00	0.00	0.00	0	76.0959600	523104.600	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	
									19328.070	
9.002184010D+03	-6.242173290D+02	1.976721262D+01	-1.781858151D-01	1.289390285D-03						
-3.794444380D-06	4.320485500D-09	0.000000000D+00	6.260803930D+04	-5.567455380D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	
									19328.070	
1.178727034D+05	-1.546770011D+03	7.906751040D+00	3.969530050D-02	-4.873543210D-05						
3.414862790D-08	-9.812308930D-12	0.000000000D+00	6.836887590D+04	-2.137711717D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	
									19328.070	
3.923945220D+06	-1.635323760D+04	3.613719460D+01	-2.261784485D-03	3.564901130D-07						
-2.955934850D-11	9.926730940D-16	0.000000000D+00	1.574204144D+05	-2.029390164D+02						

1,5-C<sub>6</sub>H<sub>4</sub> 1,5 Hexadiyne-3-ene cis Burcat G3B3 calc HF298=125.291 kcal

3 A02/05 C	6.00H	4.00	0.00	0.00	0.00	0.00	0	76.0959600	524217.544	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	
									18842.947	
2.876882115D+03	-1.794563775D+02	7.992367380D+00	-3.760668750D-02	3.996716310D-04						
-9.618184040D-07	7.570714680D-10	0.000000000D+00	6.138189830D+04	-7.477818120D+00						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	
									18842.947	
1.597343220D+05	-2.102271959D+03	1.005280808D+01	3.592659400D-02	-4.545602050D-05						
3.286039300D-08	-9.665665450D-12	0.000000000D+00	7.130932570D+04	-3.419793200D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	
									18842.947	
3.893745370D+06	-1.627533278D+04	3.606463850D+01	-2.228091237D-03	3.481982620D-07						
-2.852835379D-11	9.417968510D-16	0.000000000D+00	1.570337206D+05	-2.023884483D+02						

Table 5 (continued)

1,2,3,4,5-C6H4 Hexa-Pentaene H2C=C=C=C=CH2 Burcat G3B3 calc HF298=135.818 kcal  
 3 A02/05 C 6.00H 4.00 0.00 0.00 0.00 0 76.0959600 568262.512  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19359.344  
 6.479585690D+02-5.311225580D+01 4.721125640D+00 1.836610308D-02 1.887637503D-05  
 1.400110423D-07-4.447156080D-10 0.000000000D+00 6.619094090D+04 3.513642240D+00  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19359.344  
 7.378373270D+04-8.271023420D+02 4.827160750D+00 4.192678500D-02-4.599308060D-05  
 3.000914383D-08-8.354356950D-12 0.000000000D+00 7.035410310D+04-3.299872030D+00  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19359.344  
 3.995758370D+06-1.742271231D+04 3.759585500D+01-2.996036633D-03 5.395204150D-07  
 -5.214311760D-11 2.091830619D-15 0.000000000D+00 1.689403716D+05-2.147047773D+02

C6H4 1,2,3-Hexatriene-5-yne H2C=C=C=C-CCH Burcat G3B3 calc HF298=133.773 kcal  
 3 A03/05 C 6.00H 4.00 0.00 0.00 0.00 0 76.0959600 559706.232  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19171.589  
 -5.797433990D+02 5.047626650D+01 2.236054295D+00 3.061101255D-02 3.869162170D-05  
 -9.965187960D-08-6.880149980D-12 0.000000000D+00 6.485984450D+04 1.658089671D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19171.589  
 1.028939981D+05-1.325077373D+03 7.034806180D+00 4.002818030D-02-4.748166150D-05  
 3.281663780D-08-9.428641990D-12 0.000000000D+00 7.169421030D+04-1.494095804D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19171.589  
 3.949219980D+06-1.680736702D+04 3.680440010D+01-2.602180443D-03 4.416292400D-07  
 -4.006832460D-11 1.503790067D-15 0.000000000D+00 1.643877079D+05-2.068777400D+02

C6H4ClO Radical ortho-Chlorophenoxy radical R. Janoschek G3MP2B3  
 3 T06/03 C 6.00H 4.00CL 1.00O 1.00 0.00 0 127.5480600 30600.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19309.065  
 1.146083596D+03-5.570637480D+01 4.522178280D+00 2.793746810D-03 1.926737329D-04  
 -4.996930610D-07 5.332698240D-10 0.000000000D+00 1.566954304D+03 9.492365650D+00  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19309.065  
 -1.880080339D+05 3.827361770D+03-2.778909245D+01 1.449748472D-01-1.777102882D-04  
 1.133279466D-07-2.938289490D-11 0.000000000D+00-1.555541944D+04 1.753004455D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19309.065  
 2.711553967D+06-1.610109134D+04 4.266900630D+01-2.641021843D-03 4.632867030D-07  
 -4.356043290D-11 1.698576822D-15 0.000000000D+00 9.142962200D+04-2.409120947D+02

C6H4ClO Radical 6-chloro-1-one-2-yl-cyclohexa-2-4-diene R. Janoschek  
 3 T06/03 C 6.00H 4.00CL 1.00O 1.00 0.00 0 127.5480600 225910.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20599.351  
 2.144610719D+03-1.280610372D+02 7.013310820D+00-1.602506356D-02 2.835742643D-04  
 -7.571790550D-07 8.598977910D-10 0.000000000D+00 2.512166917D+04 3.548423680D-02  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20599.351  
 -1.357292823D+05 3.043039626D+03-2.249346756D+01 1.308300344D-01-1.596490700D-04  
 1.021373031D-07-2.666139220D-11 0.000000000D+00 1.148999784D+04 1.480604007D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20599.351  
 2.863130272D+06-1.648975979D+04 4.305566100D+01-2.816503706D-03 5.047704780D-07  
 -4.851429290D-11 1.934352964D-15 0.000000000D+00 1.175199716D+05-2.418045822D+02

Table 5 (continued)

C6H4Cl2O 2,4-DICHLOROPHENOL C6H3Cl2OH IR-NIST + Janoschek G3MP2B3 calc

3 T 6/03 C	6.00H	4.00O	1.00CL	2.00	0.00	0	163.0007600	-167010.000			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	21948.568
-3.205428590D+03	1.971867323D+02	-2.456594381D-01	1.966799160D-02	4.616831800D-04							
-2.124938963D-06	3.192096810D-09	0.000000000D+00	-2.338734572D+04	3.279482440D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	21948.568
-8.491271330D+04	1.518236241D+03	-1.085365852D+01	1.041499157D-01	-1.209513897D-04							
7.399145520D-08	-1.853551508D-11	0.000000000D+00	-2.948365987D+04	8.476002170D+01							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	21948.568
3.112058633D+06	-1.675492946D+04	4.489890620D+01	-2.374700545D-03	3.848445560D-07							
-3.322945430D-11	1.180991226D-15	0.000000000D+00	7.180303230D+04	-2.511425118D+02							

o-C6H4I 1,2-Iodobenzene Radical Wang CCSD(T) HF298=102.1 kcal

3 A08/05 C	6.00H	4.00I	1.00	0.00	0.00	0	203.0004300	427186.400			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18009.747
2.356822074D+03	-9.902082460D+01	4.172078610D+00	3.097858697D-02	-1.424311151D-04							
7.852461580D-07	-1.218340024D-09	0.000000000D+00	4.960880270D+04	1.013112997D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18009.747
-1.942475766D+05	4.070618080D+03	-2.907256703D+01	1.415206477D-01	-1.755267119D-04							
1.134019412D-07	-2.976093100D-11	0.000000000D+00	3.125272197D+04	1.845321056D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18009.747
2.704565387D+06	-1.542145060D+04	3.925305270D+01	-2.491184021D-03	4.327009860D-07							
-4.054989460D-11	1.614904728D-15	0.000000000D+00	1.362332474D+05	-2.190815645D+02							

o-C6H4I2 1,2-Diiodobenzene Burcat MOPAC PM3 calc HF298=252+/-5.9 kJ Cox Pilcher

3 A08/05 C	6.00H	4.00I	2.00	0.00	0.00	0	329.9049000	248950.000			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	21777.803
-3.969034050D+02	5.274548090D+01	5.846409970D-01	9.761804240D-02	-5.138039010D-04							
1.862208201D-06	-2.591005990D-09	0.000000000D+00	2.719500096D+04	2.572790125D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	21777.803
-6.177364020D+04	1.194264590D+03	-4.872137120D+00	6.485615180D-02	-5.364060310D-05							
2.356386957D-08	-4.379834660D-12	0.000000000D+00	2.192939172D+04	6.079754310D+01							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	21777.803
3.554426670D+06	-1.965641220D+04	4.633201720D+01	-4.361688050D-03	8.822379780D-07							
-9.483317710D-11	4.188827750D-15	0.000000000D+00	1.398453210D+05	-2.632041533D+02							

m-C6H4I2 1,3-Diiodobenzene Burcat MOPAC PM3 calc HF298=243.5 kJ NIST 94.

3 A08/05 C	6.00H	4.00I	2.00	0.00	0.00	0	329.9049000	243508.800			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22195.574
-3.846147930D+02	6.629796030D+01	-2.881494221D-01	1.103253455D-01	-5.751228190D-04							
1.968938742D-06	-2.521181503D-09	0.000000000D+00	2.646504725D+04	2.838407313D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22195.574
-2.146056948D+05	4.220566260D+03	-2.754065510D+01	1.443329802D-01	-1.779681428D-04							
1.142905657D-07	-2.982988136D-11	0.000000000D+00	7.676992050D+03	1.800746426D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22195.574
2.738901276D+06	-1.571760536D+04	4.240829730D+01	-2.540652080D-03	4.413434100D-07							
-4.103821410D-11	1.580718044D-15	0.000000000D+00	1.149931529D+05	-2.332554626D+02							



Table 5 (continued)

p-C6H4I2 1,4-Diiodobenzene Burcat MOPAC PM3 calc HF298=243.5 kJ NIST 94											
3	A02/05	C	6.00H	4.00I	2.00	0.00	0.00	0	329.9049000	242700.000	
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0 21976.466
-4.594013370D+02 4.374104190D+01 1.721865598D+00 7.259764600D-02-2.774123494D-04											
	8.343576900D-07-8.951162650D-10	0.000000000D+00	2.642690516D+04	1.941783134D+01	200.000	1000.000	7	-2.0	-1.0	0.0	1.0 2.0 3.0 4.0 0.0 21976.466
-1.765950300D+05 3.396985580D+03-2.045707746D+01 1.148559137D-01-1.264136793D-04											
	7.458462080D-08-1.843170223D-11	0.000000000D+00	1.121543480D+04	1.416971986D+02	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0 2.0 3.0 4.0 0.0 21976.466
2.361305920D+06-1.641027810D+04 4.446443290D+01-3.739758320D-03 7.612640750D-07											
	-8.213611480D-11	3.635553260D-15	0.000000000D+00	1.175413656D+05-2.500147358D+02							
C6H4N4O2 4-Nitrophenyl azide O2N-C6H4-N3 Finch et al Thermochim Acta 298, (1997)											
3	A12/04	C	6.00H	4.00N	4.00O	2.00	0.00	0	164.1217200	389700.000	
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0 28254.171
-1.892369502D+03 2.534102470D+01 5.216290420D+00 1.516709242D-02 3.093965647D-04											
	-1.139712401D-06 1.557446409D-09	0.000000000D+00	4.328556190D+04	9.648715920D+00	200.000	1000.000	7	-2.0	-1.0	0.0	1.0 2.0 3.0 4.0 0.0 28254.171
-1.351462847D+05 2.799992892D+03-1.911395041D+01 1.414643427D-01-1.615750014D-04											
	9.763268870D-08-2.444031176D-11	0.000000000D+00	3.112063623D+04	1.322587879D+02	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0 2.0 3.0 4.0 0.0 28254.171
3.294128130D+06-2.140222002D+04 5.927020420D+01-5.527829130D-03 1.110788370D-06											
	-1.175601926D-10	5.103212460D-15	0.000000000D+00	1.621646886D+05-3.395660060D+02							
C6H5 PHENYL RADICAL IUPAC Datasheet April 2003											
3	IU4/03	C	6.00H	5.00	0.00	0.00	0.00	0	77.1039000	339740.000	
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0 13574.581
3.214826430D+03-2.252829191D+02 1.018433298D+01-8.208330490D-02 5.084109440D-04											
	-1.097070527D-06 1.076917989D-09	0.000000000D+00	3.994797490D+04-1.487121217D+01	200.000	1000.000	7	-2.0	-1.0	0.0	1.0 2.0 3.0 4.0 0.0 13574.581	
-1.711304145D+05 4.384413890D+03-3.686779940D+01 1.627977761D-01-2.098588525D-04											
	1.405246379D-07-3.802345410D-11	0.000000000D+00	2.065712124D+04	2.178299890D+02	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0 2.0 3.0 4.0 0.0 13574.581
3.162313720D+06-1.735064407D+04 3.936510220D+01-2.840383215D-03 4.931166590D-07											
	-4.565977650D-11	1.746043182D-15	0.000000000D+00	1.381374161D+05-2.310239347D+02							
C6H5 FULVENYL RAD 5-methylene-2,4-cyclopentadiene-6-yl Burcat G3B3 calc.											
3	A03/05	C	6.00H	5.00	0.00	0.00	0.00	0	77.1039000	467315.144	
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0 15482.080
3.316824940D+02 3.067784772D+01 1.559755915D+00 5.030568540D-02-3.760171460D-04											
	1.877013617D-06-2.896337136D-09	0.000000000D+00	5.430221740D+04	1.786704158D+01	200.000	1000.000	7	-2.0	-1.0	0.0	1.0 2.0 3.0 4.0 0.0 15482.080
-7.895043780D+04 2.737462944D+03-2.572895694D+01 1.363473241D-01-1.755169258D-04											
	1.176781474D-07-3.184489360D-11	0.000000000D+00	4.328704950D+04	1.573216340D+02	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0 2.0 3.0 4.0 0.0 15482.080
3.604871840D+06-1.778066099D+04 3.987599320D+01-2.461168974D-03 3.844976950D-07											
	-3.134854600D-11	1.023613387D-15	0.000000000D+00	1.569287298D+05-2.324047186D+02							

Table 5 (continued)

C6H5BrO 2-Bromophenol C6H4BrOH Burcat B3LYP/6-31G(d) HF298=-15.23+/-4. kcal  
 3 T05/04 C 6.00H 5.00O 1.00BR 1.00 0.00 0 173.0073000 -63722.320  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19459.916  
 -1.747620869D+03 1.277410552D+02 9.818508400D-01 1.362624341D-02 2.923086982D-04  
 -1.104006432D-06 1.548690778D-09 0.000000000D+00 -1.041474309D+04 2.691700107D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19459.916  
 -1.675053269D+05 3.535414460D+03 -2.780108524D+01 1.529644554D-01 -1.891562704D-04  
 1.220652482D-07 -3.200009060D-11 0.000000000D+00 -2.543400169D+04 1.735089357D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19459.916  
 3.435637740D+06 -1.887922188D+04 4.732019480D+01 -2.878401211D-03 4.837348440D-07  
 -4.338409990D-11 1.606401222D-15 0.000000000D+00 9.671759570D+04 -2.722982406D+02

C6H5ClO ortho-Chloro-Phenol C6H4ClOH Janoschek G3MP2B3 J. Mol. Struct. 2003  
 3 T 6/03 C 6.00H 5.00CL 1.00O 1.00 0.00 0 128.5560000 -138380.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19497.467  
 -4.938917780D+03 3.285690260D+02 -3.576046660D+00 5.832055030D-02 9.007950920D-05  
 -6.502371820D-07 1.077330560D-09 0.000000000D+00 -2.006866882D+04 4.492428190D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19497.467  
 -1.459099395D+05 2.796198989D+03 -2.070684789D+01 1.271905948D-01 -1.512906534D-04  
 9.479451580D-08 -2.425007956D-11 0.000000000D+00 -3.138290902D+04 1.357719910D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19497.467  
 3.804837220D+06 -1.917796815D+04 4.603023130D+01 -2.657063978D-03 4.220210580D-07  
 -3.545312780D-11 1.214662798D-15 0.000000000D+00 9.083309920D+04 -2.656917258D+02

C6H5ClO 2,4-cyclohexadiene-6 chloro-1-one Janoschek G3MP2B3 Calc  
 3 T06/03 C 6.00H 5.00CL 1.00O 1.00 0.00 0 128.5560000 -35750.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20479.871  
 3.302254110D+03 -2.089679372D+02 9.137923310D+00 -4.279117110D-02 4.366639980D-04  
 -1.181910863D-06 1.358071935D-09 0.000000000D+00 -6.074540750D+03 -9.216656510D+00  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20479.871  
 -1.953380426D+05 4.112897290D+03 -2.982322122D+01 1.521707966D-01 -1.845977706D-04  
 1.178344569D-07 -3.071527633D-11 0.000000000D+00 -2.484768397D+04 1.868605438D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20479.871  
 3.737950090D+06 -1.999306170D+04 4.782779900D+01 -3.318713270D-03 5.858376200D-07  
 -5.544363280D-11 2.176541314D-15 0.000000000D+00 1.072985195D+05 -2.771580399D+02

C6H5ClO 2,5-cyclohexadiene-6 chloro-1-one Janoschek J. Mol. Struct. 2003  
 3 T06/03 C 6.00H 5.00CL 1.00O 1.00 0.00 0 128.5560000 -55870.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20346.574  
 -3.422149000D+03 2.439546596D+02 -2.920457481D+00 9.579169950D-02 -3.403588790D-04  
 9.967841310D-07 -1.118635311D-09 0.000000000D+00 -9.941143120D+03 3.913540580D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20346.574  
 -2.016606735D+05 3.964261100D+03 -2.733469812D+01 1.420197089D-01 -1.675766013D-04  
 1.049309879D-07 -2.700799741D-11 0.000000000D+00 -2.685928766D+04 1.738537283D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20346.574  
 3.798603010D+06 -2.043279987D+04 4.847620940D+01 -3.656425680D-03 6.719528290D-07  
 -6.624861570D-11 2.709252929D-15 0.000000000D+00 1.074613789D+05 -2.824281378D+02

Table 5 (continued)

C6H5I Iodobenzene HF298=39.4+/-1.5 kcal Cox & Pilcher 1970.

```

3 A08/05 C 6.00H 5.00I 1.00 0.00 0.00 0 204.0083700 165000.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18050.939
7.833708410D+02 9.190751320D+00 1.467466459D+00 6.068734780D-02-3.177664000D-04
1.324720908D-06-1.849084055D-09 0.000000000D+00 1.771931603D+04 1.990610433D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18050.939
-2.085761241D+05 4.398683770D+03-3.185029080D+01 1.506171322D-01-1.836952882D-04
1.180376212D-07-3.099375329D-11 0.000000000D+00-1.710660197D+03 1.975878345D+02
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18050.939
3.482630190D+06-1.903882716D+04 4.469984870D+01-3.402380860D-03 6.228714190D-07
-6.109776430D-11 2.484017118D-15 0.000000000D+00 1.262267988D+05-2.593160901D+02

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C6H5O 2,4-cyclohexadiene-1-one-2-yl Janoschek G3MP2B3 Calc J. Mol. Struct. 2003

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3 T06/03 C 6.00H 5.00O 1.00 0.00 0.00 0 93.1033000 246580.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17987.101
-4.343471070D+02-1.657628147D+01 6.631879990D+00-4.723389520D-02 5.355997000D-04
-1.710131529D-06 2.229914876D-09 0.000000000D+00 2.748212376D+04 3.210698860D+00
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17987.101
-1.876398977D+05 3.919181720D+03-2.847361504D+01 1.391090044D-01-1.662407004D-04
1.053077822D-07-2.735675603D-11 0.000000000D+00 1.027730611D+04 1.793794387D+02
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17987.101
3.789625870D+06-1.982092646D+04 4.499881300D+01-3.458787830D-03 6.270536160D-07
-6.098160790D-11 2.460476304D-15 0.000000000D+00 1.413046605D+05-2.624845568D+02

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C6H6 Benzvalene Gaussian 94 HF/6-31G(d) scal. 0.8929 Wang & Law JPC 1997 3400

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3 T02/04 C 6.00H 6.00 0.00 0.00 0.00 0 78.1118400 384928.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13699.843
3.561934620D+03-2.335628741D+02 9.841611990D+00-6.739794050D-02 3.226430680D-04
-2.446258743D-07-1.386653523D-10 0.000000000D+00 4.541236430D+04-1.435313756D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13699.843
-1.179197598D+05 4.158253730D+03-4.022159100D+01 1.848172749D-01-2.464076309D-04
1.695260951D-07-4.683318760D-11 0.000000000D+00 2.784998446D+04 2.311349949D+02
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13699.843
2.827115721D+06-1.737265577D+04 4.151973000D+01-2.535316393D-03 5.414194420D-07
-6.186157800D-11 2.862994446D-15 0.000000000D+00 1.421736773D+05-2.448740662D+02

```

C6H6 1,3-Hexadiyne HCC-CC-CH2CH3 HF298=93.777 kcal Burcat G3B3 calc.

```

3 A03/05 C 6.00H 6.00 0.00 0.00 0.00 0 78.1118400 392362.968
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19789.658
1.147004078D+03 1.189561572D+01 7.014562150D-01 7.493205750D-02-3.288433530D-04
1.265242396D-06-1.894088300D-09 0.000000000D+00 4.487458430D+04 2.032223132D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19789.658
-2.528865209D+04 7.630195060D+02-5.375980820D+00 7.458868200D-02-8.595359810D-05
5.650127600D-08-1.551151876D-11 0.000000000D+00 4.170062970D+04 5.363035420D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19789.658
5.649528710D+06-2.361299524D+04 4.619641680D+01-3.861623410D-03 6.762796520D-07
-6.348723520D-11 2.471937351D-15 0.000000000D+00 1.855735134D+05-2.740459638D+02

```

Table 5 (continued)

C6H6 2,4-Hexadiyne CH<sub>3</sub>-CC-CC-CH<sub>3</sub> Burcat G3B3 calc. HF298=88.217 kcal.

3 A03/05 C	6.00H	6.00	0.00	0.00	0.00	0	78.1118400	369099.928
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
4.0	0.0	20995.112						
-2.392470028D+03	1.565813899D+02	-3.844771720D-01	9.292981740D-02	-3.943329450D-04				
1.082121102D-06	-1.155585505D-09	0.000000000D+00	4.136499820D+04	2.560477572D+01				
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
4.0	0.0	20995.112						
-1.992394144D+05	3.343543380D+03	-1.647522944D+01	9.022089750D-02	-9.439984410D-05				
5.660281660D-08	-1.450916347D-11	0.000000000D+00	2.630491305D+04	1.211543179D+02				
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
4.0	0.0	20995.112						
5.988941590D+06	-2.556966020D+04	4.809022110D+01	-4.722732140D-03	8.815986680D-07				
-8.824982710D-11	3.661898800D-15	0.000000000D+00	1.946345136D+05	-2.880954029D+02				

C6H6 1,5-Hexadiyne HCC-CH<sub>2</sub>-CH<sub>2</sub>-CCH HF298=99.705 kcal Burcat G3B3 calc.

3 A03/05 C	6.00H	6.00	0.00	0.00	0.00	0	78.1118400	417165.720
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
4.0	0.0	20829.424						
4.194008790D+03	-3.179036550D+02	1.315661954D+01	-1.014432775D-01	8.789362130D-04				
-2.719388046D-06	3.286452290D-09	0.000000000D+00	4.865818740D+04	-2.671440625D+01				
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
4.0	0.0	20829.424						
2.252491657D+04	1.945655521D+02	-3.412201030D+00	7.595114450D-02	-9.389740170D-05				
6.434897700D-08	-1.806905922D-11	0.000000000D+00	4.749271070D+04	4.174024360D+01				
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
4.0	0.0	20829.424						
5.150588830D+06	-2.169643142D+04	4.462393580D+01	-3.484578230D-03	5.976684570D-07				
-5.470247210D-11	2.069148319D-15	0.000000000D+00	1.765084865D+05	-2.602703004D+02				

C6H6 1,2,4,5-Hexatetraene H<sub>2</sub>C=C=CH-CH=C=CH<sub>2</sub> HF298=396.229 kJ Burcat G3B3

3 A03/05 C	6.00H	6.00	0.00	0.00	0.00	0	78.1118400	396228.984
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
4.0	0.0	20011.991						
2.439555764D+03	-1.609426650D+02	8.214525970D+00	-2.027672481D-02	2.491389030D-04				
-6.773864310D-07	8.692925380D-10	0.000000000D+00	4.577158020D+04	-6.691536000D+00				
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
4.0	0.0	20011.991						
-1.146825772D+05	2.724947330D+03	-1.915416773D+01	1.128336297D-01	-1.376789559D-04				
9.117424280D-08	-2.479801815D-11	0.000000000D+00	3.348845190D+04	1.307043398D+02				
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
4.0	0.0	20011.991						
5.112099240D+06	-2.276166585D+04	4.614879870D+01	-4.209447400D-03	7.691903950D-07				
-7.500501080D-11	3.025474099D-15	0.000000000D+00	1.796918137D+05	-2.712306345D+02				

C6H6O 2,4-cyclohexadiene-1-one Janoschek G3MP2B3 Calc

3 T06/03 C	6.00H	6.000	1.00	0.00	0.00	0	94.1112400	-21630.000
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
4.0	0.0	17747.938						
1.425215426D+03	-1.472467810D+02	9.569025790D+00	-7.810300690D-02	6.805651330D-04				
-2.021985201D-06	2.500286476D-09	0.000000000D+00	-4.321698720D+03	-1.015495632D+01				
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
4.0	0.0	17747.938						
-2.393987234D+05	4.882039240D+03	-3.527958180D+01	1.590503561D-01	-1.892130062D-04				
1.196916241D-07	-3.107957583D-11	0.000000000D+00	-2.632117255D+04	2.148696294D+02				
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
4.0	0.0	17747.938						
4.635863810D+06	-2.334241599D+04	4.989436480D+01	-4.035938790D-03	7.282449430D-07				
-7.049345710D-11	2.831386353D-15	0.000000000D+00	1.303012180D+05	-2.990122006D+02				

Table 5 (continued)

C6H7 1,3,5 Hexatriene-6-yl CH<sub>2</sub>=CH-CH=CH-CH=CH\* Burcat G3B3 QCISD/SCF=QC.

```

3 A03/05 C 6.00H 7.00 0.00 0.00 0.00 0 79.1197800 431387.136
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20936.597
-1.844992221D+03 1.159939571D+02 4.823030990D-01 7.945789870D-02-3.557504620D-04
1.219860003D-06-1.504534814D-09 0.000000000D+00 4.898618400D+04 2.569361936D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20936.597
-1.384498230D+05 3.130273110D+03-2.211461091D+01 1.274373856D-01-1.583050612D-04
1.055531528D-07-2.867206137D-11 0.000000000D+00 3.571709180D+04 1.476194111D+02
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20936.597
5.539196730D+06-2.359035065D+04 4.746039000D+01-2.814458595D-03 3.085515999D-07
-1.259156982D-11-1.094836334D-16 0.000000000D+00 1.893110309D+05-2.779038381D+02

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C6H7 2,4-Cyclopentadiene-1-Methynyl 2,4-C5H5-1-CH2\* Melius P72JB

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3 A03/05 C 6.00H 7.00 0.00 0.00 0.00 0 79.1197800 334092.400
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18097.571
6.173084700D+03-3.569241700D+02 1.030448677D+01-2.455608129D-02 5.525066880D-05
5.294370620D-07-1.102260831D-09 0.000000000D+00 3.924522950D+04-1.827368352D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18097.571
-1.640271516D+05 4.292804700D+03-3.498508210D+01 1.677774452D-01-2.145862696D-04
1.447447088D-07-3.960989890D-11 0.000000000D+00 1.977516480D+04 2.103367865D+02
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18097.571
4.722464880D+06-2.320972480D+04 4.927831610D+01-3.961632650D-03 7.046063430D-07
-6.698410090D-11 2.635320184D-15 0.000000000D+00 1.727653319D+05-2.943323600D+02

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C6H7 2,4-Cyclopentadiene-3-Methynyl 2,4-C5H5-3-CH2\*. Melius P72JA

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3 A03/05 C 6.00H 7.00 0.00 0.00 0.00 0 79.1197800 247316.240
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17692.977
3.285710490D+03-2.154552669D+02 8.956672920D+00-4.817649700D-02 3.663592100D-04
-6.811499060D-07 5.163072060D-10 0.000000000D+00 2.832949407D+04-9.933815640D+00
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17692.977
-1.122069508D+05 3.264551860D+03-2.907795979D+01 1.539650074D-01-1.970557354D-04
1.331926470D-07-3.652396770D-11 0.000000000D+00 1.409002905D+04 1.764316671D+02
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17692.977
4.630965970D+06-2.283355831D+04 4.917243630D+01-3.963562500D-03 7.116786900D-07
-6.834073950D-11 2.717062658D-15 0.000000000D+00 1.599138877D+05-2.934959223D+02

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C6H7 2,4-Cyclopentadienyl-1-Methyl 2,4-C5H4\*-1-CH3. Melius P72JC

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3 A03/05 C 6.00H 7.00 0.00 0.00 0.00 0 79.1197800 226772.800
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18093.691
3.911738630D+03-1.900088408D+02 6.445363740D+00-1.956551256D-03 4.710109640D-05
3.819037380D-07-9.278311850D-10 0.000000000D+00 2.579994000D+04-2.584029934D+00
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18093.691
-1.358594607D+05 3.354684370D+03-2.734189218D+01 1.445866703D-01-1.799997701D-04
1.194971707D-07-3.238572740D-11 0.000000000D+00 1.080001758D+04 1.679828466D+02
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18093.691
4.834531030D+06-2.342721456D+04 4.964520410D+01-4.164951020D-03 7.587083750D-07
-7.399094790D-11 2.989273676D-15 0.000000000D+00 1.613241471D+05-2.979896210D+02

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Table 5 (continued)

C6H8 DIHYDROBENZVALENE Gaussian 94 HF/6-31G(d) Wang & Law JPC 1997 p.3400

3	T02/04	C	6.00H	8.00	0.00	0.00	0.00	0.00	0	80.1277200	230120.000	
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15001.499
-1.669187779D+02	6.219366520D+01	7.607740500D-01	6.249625960D-02	-5.081921610D-04								
2.319754936D-06	-3.179131990D-09	0.000000000D+00	2.572816098D+04	2.096973697D+01								
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15001.499
-3.064321990D+05	7.336587400D+03	-5.948058580D+01	2.397992756D-01	-3.088873886D-04								
2.067811367D-07	-5.599481880D-11	0.000000000D+00	-5.729171080D+03	3.376298760D+02								
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15001.499
4.093507460D+06	-2.347385772D+04	5.203878410D+01	-4.072637090D-03	7.288803180D-07								
-6.965527790D-11	2.752573590D-15	0.000000000D+00	1.592261307D+05	-3.173144660D+02								

C6H8 2,4-Cyclopentadiene-1-Methyl 2,4-C5H5-1-CH3. Burcat G3B3 HF298=112.25 kJ

3	A03/05	C	6.00H	8.00	0.00	0.00	0.00	0.00	0	80.1277200	112256.720	
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17183.243
-2.875960621D+03	2.469097333D+02	-4.387184120D+00	1.317210769D-01	-7.954411600D-04								
2.793854031D-06	-3.514530190D-09	0.000000000D+00	1.069851575D+04	4.152451910D+01								
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17183.243
-3.645045300D+05	7.209799600D+03	-5.024069850D+01	1.994114710D-01	-2.436422025D-04								
1.580344971D-07	-4.184366600D-11	0.000000000D+00	-2.082372042D+04	2.958308024D+02								
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17183.243
6.191718350D+06	-2.834419594D+04	5.448381230D+01	-4.461655420D-03	7.618758690D-07								
-6.947762460D-11	2.618662448D-15	0.000000000D+00	1.782315659D+05	-3.359455330D+02								

C6H9 1-3 Hexadiene-5-yl CH2=CHCH=CHCH\*CH3 Burcat G3B3 calc . HF298=41.465 kcal

3	A05/05	C	6.00H	9.00	0.00	0.00	0.00	0.00	0	81.1356600	173489.560	
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22225.137
-1.369191643D+03	1.299400446D+02	-1.578010990D+00	1.161277412D-01	-5.464444920D-04								
1.706714676D-06	-1.998872577D-09	0.000000000D+00	1.782717060D+04	3.252656500D+01								
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22225.137
-2.703216471D+05	5.053181650D+03	-3.213790770D+01	1.552434804D-01	-1.870811826D-04								
1.222147247D-07	-3.273541590D-11	0.000000000D+00	-4.723158580D+03	2.041253631D+02								
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22225.137
7.367500910D+06	-3.064357998D+04	5.747305030D+01	-4.566792130D-03	7.137637540D-07								
-5.939352580D-11	2.009652547D-15	0.000000000D+00	2.012160648D+05	-3.482765730D+02								

C6H9 1-3 Hexadiene-6-yl CH2=CHCH=CHCH2CH2\* Burcat G3B3 calc. HF298=63.464 kcal

3	A05/05	C	6.00H	9.00	0.00	0.00	0.00	0.00	0	81.1356600	265533.376	
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22989.723
7.030950350D+03	-4.477546860D+02	1.284369230D+01	-3.476462460D-02	2.875023320D-04								
-7.179440210D-07	9.312384330D-10	0.000000000D+00	3.067866561D+04	-2.570963527D+01								
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22989.723
-2.682014856D+05	5.277102580D+03	-3.416547980D+01	1.627631998D-01	-1.998792105D-04								
1.323932518D-07	-3.582700420D-11	0.000000000D+00	5.443112080D+03	2.169050846D+02								
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22989.723
7.675185800D+06	-3.156738192D+04	5.858862320D+01	-5.192562670D-03	8.632455400D-07								
-7.619553970D-11	2.743805405D-15	0.000000000D+00	2.181602201D+05	-3.539067710D+02								

Table 5 (continued)

C6H9 1-CycloHexene-3-yl Burcat G3B3 calc. HF298=31.42 kcal											
3 A05/05 C	6.00H	9.00	0.00	0.00	0.00	0.00	0	81.1356600		131469.648	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16885.993
1.898309440D+03	-8.604409920D+01	4.885401220D+00	1.468778987D-03	6.287530380D-05							
1.381635370D-07	-3.138388646D-10	0.000000000D+00	1.410833627D+04	5.788923980D+00							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16885.993
-4.179816370D+05	7.995400700D+03	-5.551898400D+01	2.147766265D-01	-2.574350132D-04							
1.646564477D-07	-4.317650460D-11	0.000000000D+00	-2.216816141D+04	3.245549760D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16885.993
6.881372960D+06	-3.196461740D+04	6.050899560D+01	-5.424523610D-03	9.676142620D-07							
-9.251924690D-11	3.669012750D-15	0.000000000D+00	2.016548125D+05	-3.781271380D+02							
C6H9 Cy C5H6-CH3 Cyclo-1-penten-4-methyl-4yl G3B3 calc HF298=45.045 kcal											
3 A09/04 C	6.00H	9.00	0.00	0.00	0.00	0.00	0	81.1356600		188468.280	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18574.105
-6.584955270D+03	4.676988790D+02	-9.255795250D+00	1.853365741D-01	-1.026425246D-03							
3.235706500D-06	-3.761120940D-09	0.000000000D+00	1.894868737D+04	6.207661090D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18574.105
-4.602793550D+05	8.617745100D+03	-5.738213420D+01	2.190110987D-01	-2.616644419D-04							
1.662936598D-07	-4.335001460D-11	0.000000000D+00	-1.859907311D+04	3.368121510D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18574.105
6.152739670D+06	-2.980779790D+04	5.908308130D+01	-5.220666450D-03	9.465686500D-07							
-9.199971940D-11	3.707939860D-15	0.000000000D+00	1.944875274D+05	-3.652703740D+02							
C6H9 Cy C5H7-CH2 Cyclo-1-penten-4-methynyl G3B3 calc HF298=51.561 kcal											
3 A09/04 C	6.00H	9.00	0.00	0.00	0.00	0.00	0	81.1356600		215731.224	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18624.609
-4.525660890D+03	2.636538204D+02	-1.740123149D+00	6.122781480D-02	-1.016767140D-04							
6.945560310D-08	4.223982840D-10	0.000000000D+00	2.280728290D+04	3.457662270D+01							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18624.609
-4.086890190D+05	7.911290280D+03	-5.526187920D+01	2.226407738D-01	-2.779088038D-04							
1.830239275D-07	-4.897490160D-11	0.000000000D+00	-1.180235414D+04	3.224657630D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18624.609
6.495664850D+06	-2.972565564D+04	5.818025770D+01	-4.648580470D-03	7.886933730D-07							
-7.132284460D-11	2.660813590D-15	0.000000000D+00	1.983704863D+05	-3.586215610D+02							
C6H9 1-Cyclopentene-3-Methenyl 1-C5H7-3-CH2* Burcat G3B3 calc HF298=50.78 kcal											
3 A04/05 C	6.00H	9.00	0.00	0.00	0.00	0.00	0	81.1356600		212463.520	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18926.459
1.670628087D+03	-1.005617520D+02	4.970301740D+00	2.990116866D-02	-1.694166892D-04							
8.749848390D-07	-1.148538192D-09	0.000000000D+00	2.363486910D+04	4.643406200D+00							
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18926.459
-3.980255340D+05	7.803507100D+03	-5.364138460D+01	2.129929543D-01	-2.609240079D-04							
1.700325950D-07	-4.522588060D-11	0.000000000D+00	-1.172598700D+04	3.163612010D+02							
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18926.459
6.931866880D+06	-3.116797582D+04	5.905350940D+01	-4.952658170D-03	8.499975760D-07							
-7.793710960D-11	2.955142242D-15	0.000000000D+00	2.073111485D+05	-3.649591730D+02							

Table 5 (continued)

C6H9I 1-Cyclohexen-3-Iodo Burcat B3LYP/6-311G\* HF298=16.5+/-5 kcal

3	A08/05	C	6.00H	9.00I	1.00	0.00	0.00	0.00	0	208.0401300	69036.000		
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	20730.506
-1.224756230D+03	1.430544300D+02	-2.130806801D+00	1.205656659D-01	-6.619365710D-04									
2.278035429D-06	-2.789024261D-09	0.000000000D+00	5.419344270D+03	3.483712210D+01									
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		20730.506
-4.708422060D+05	8.806282690D+03	-5.856523150D+01	2.299208580D-01	-2.768033155D-04									
1.773311031D-07	-4.653325680D-11	0.000000000D+00	-3.409175430D+04	3.462217160D+02									
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		20730.506
6.819616450D+06	-3.224495130D+04	6.372618310D+01	-5.510581620D-03	9.861513170D-07									
-9.458185390D-11	3.761782970D-15	0.000000000D+00	1.946474165D+05	-3.918991070D+02									

C6H10 1,3-Hexadiene Burcat G3B3 calc HF298=13.985 kcal

3	A09/05	C	6.00H	10.00	0.00	0.00	0.00	0	82.1436000	58513.240			
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22606.364
-1.142913210D+03	9.643927600D+01	1.381039454D-01	9.942135790D-02	-4.828417390D-04									
1.593008935D-06	-1.887420394D-09	0.000000000D+00	4.032888230D+03	2.582919433D+01									
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		22606.364
-2.931079796D+05	5.579776810D+03	-3.578428720D+01	1.645998667D-01	-1.942905382D-04									
1.256113765D-07	-3.350738220D-11	0.000000000D+00	-2.089965281D+04	2.242893167D+02									
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		22606.364
8.720816280D+06	-3.588316500D+04	6.416845620D+01	-5.976479960D-03	9.659185520D-07									
-8.276102590D-11	2.919219972D-15	0.000000000D+00	2.195015449D+05	-3.966471650D+02									

C6H10 Cy C5H7-CH3 Cyclo-1-penten-3-methyl Burcat G3B3 calc HF298=2.022 kcal

3	A09/04	C	6.00H	10.00	0.00	0.00	0.00	0	82.1436000	8460.048			
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17207.712
-9.409729100D+03	6.280672570D+02	-1.159916811D+01	1.704786201D-01	-7.665459530D-04									
2.087271992D-06	-2.026524202D-09	0.000000000D+00	-3.101272421D+03	7.419716660D+01									
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		17207.712
-5.134022040D+05	9.376427400D+03	-6.268687770D+01	2.321422581D-01	-2.721825763D-04									
1.705759839D-07	-4.400786160D-11	0.000000000D+00	-4.366705910D+04	3.644161480D+02									
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		17207.712
7.027251000D+06	-3.369061000D+04	6.435594370D+01	-5.978418070D-03	1.092500691D-06									
-1.070674837D-10	4.351927770D-15	0.000000000D+00	1.961642935D+05	-4.050868480D+02									

C6H11 1-Hexene-6-yl CH2=CHCH2CH2CH2CH2\* HF298=38.839 kcal Burcat G3B3

3	A07/05	C	6.00H	11.00	0.00	0.00	0.00	0	83.1515400	162502.376			
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	24511.574
2.126723347D+03	-2.096614803D+02	9.885668940D+00	-7.622667790D-03	1.567332070D-04									
-3.952073480D-07	7.118838370D-10	0.000000000D+00	1.721616035D+04	-9.312387940D+00									
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		24511.574
-3.552356320D+05	7.078402190D+03	-4.708327990D+01	2.056147666D-01	-2.557545917D-04									
1.708124690D-07	-4.651872230D-11	0.000000000D+00	-1.513398736D+04	2.888967159D+02									
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		24511.574
8.972410620D+06	-3.736855570D+04	6.788507650D+01	-6.735413900D-03	1.139202853D-06									
-1.027519283D-10	3.839801110D-15	0.000000000D+00	2.402221289D+05	-4.158153070D+02									



Table 5 (continued)

C6H11 2-Hexene-6-yl CH3CH=CHCH2CH2CH2* HF298=38.839 kcal Burcat G3B3														
3	A07/05	C	6.00H	11.00	0.00	0.00	0.00	0	83.1515400	153862.416				
			50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	24877.633
-7.900396250D+02 6.550571880D+01 4.394271780D-01 1.165961372D-01-5.698360110D-04														
			1.722421924D-06	-1.869113667D-09	0.000000000D+00	1.533031573D+04	2.537329949D+01							
			200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	24877.633
-4.041342100D+05 7.239024620D+03-4.356114160D+01 1.864160651D-01-2.208752620D-04														
			1.430021069D-07	-3.816271510D-11	0.000000000D+00	-1.770624462D+04	2.718642748D+02							
			1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	24877.633
9.781796730D+06-3.967480670D+04 6.975144040D+01-7.370840320D-03 1.279531379D-06														
			-1.176366642D-10	4.459174510D-15	0.000000000D+00	2.542247262D+05	-4.318178810D+02							
C6H11 trans CH3CH2CH=CHCH2CH2* HF298=36.936 kcal Burcat G3B3 calc.														
3	A07/05	C	6.00H	11.00	0.00	0.00	0.00	0	83.1515400	154540.224				
			50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	25204.464
6.883273510D+02-1.188804495D+02 8.055533510D+00 1.120216811D-02 1.032933378D-04														
			-3.958371870D-07	8.098185100D-10	0.000000000D+00	1.586810638D+04	-2.581840254D+00							
			200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	25204.464
-4.338397580D+05 7.924222050D+03-4.888296770D+01 2.032169576D-01-2.437749553D-04														
			1.577462834D-07	-4.187092340D-11	0.000000000D+00	-2.061344907D+04	3.012831821D+02							
			1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	25204.464
9.290438240D+06-3.823577210D+04 6.876047160D+01-6.979992420D-03 1.193401690D-06														
			-1.077726220D-10	4.002543760D-15	0.000000000D+00	2.448602176D+05	-4.228047030D+02							
C6H11 CH2=C(CH2*)CH2CH2CH3 HF298=22.788 kcal Burcat G3B3 calc.														
3	A07/05	C	6.00H	11.00	0.00	0.00	0.00	0	83.1515400	95344.992				
			50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22942.282
1.249232358D+03-1.539173358D+02 9.238268420D+00-3.025292480D-02 3.367743130D-04														
			-7.873230940D-07	8.281400160D-10	0.000000000D+00	9.135204660D+03	-6.617356690D+00							
			200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22942.282
-2.994048603D+05 5.929467450D+03-4.076454750D+01 1.876182809D-01-2.275099522D-04														
			1.486773214D-07	-3.975344790D-11	0.000000000D+00	-1.777072693D+04	2.505347795D+02							
			1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22942.282
9.234431410D+06-3.807279160D+04 6.870537410D+01-7.102977950D-03 1.244733652D-06														
			-1.154648669D-10	4.412767260D-15	0.000000000D+00	2.366057169D+05	-4.248899440D+02							
C6H11 trans-CH3C(CH2*)=CHCH2CH3 HF298=21.71 kcal Burcat G3B3 calc														
3	A06/05	C	6.00H	11.00	0.00	0.00	0.00	0	83.1515400	90847.192				
			50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22608.673
1.015223656D+03-9.428703190D+01 7.033400510D+00-6.712820550D-03 2.385309404D-04														
			-6.805552740D-07	8.957602360D-10	0.000000000D+00	8.491044010D+03	1.452218229D+00							
			200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22608.673
-3.222209220D+05 6.038055430D+03-3.931194070D+01 1.760852719D-01-2.068297414D-04														
			1.330818416D-07	-3.533701160D-11	0.000000000D+00	-1.908136302D+04	2.441761400D+02							
			1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22608.673
9.501740590D+06-3.902681200D+04 6.869009510D+01-6.853904910D-03 1.200851709D-06														
			-1.120367711D-10	4.320923640D-15	0.000000000D+00	2.423938991D+05	-4.275418730D+02							

Table 5 (continued)

C6H11 (CH3)2C=CHCH*CH3 HF298=17.4 kcal Burcat G3B3 calc											
3	A06/05	C	6.00H	11.00	0.00	0.00	0.00	0	83.1515400		72910.384
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	24237.150
	5.295962040D+01		1.388217122D+02		-5.549506500D+00		2.014956012D-01		-1.068773181D-03		
	3.143540867D-06		-3.591848750D-09		0.000000000D+00		5.588289010D+03		4.395352910D+01		
	200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	24237.150
	-5.071705620D+05		8.129996850D+03		-4.377787850D+01		1.725154081D-01		-1.863121427D-04		
	1.121850641D-07		-2.839383310D-11		0.000000000D+00		-3.243108060D+04		2.749202094D+02		
	1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	24237.150
	1.095343174D+07		-4.437389170D+04		7.532904920D+01		-9.731092920D-03		1.838360835D-06		
	-1.840089689D-10		7.595763330D-15		0.000000000D+00		2.734250058D+05		-4.760876370D+02		
C6H11 (CH3)2CHCH*CH=CH2 HF298=21.805 kcal Burcat G3B3											
3	A06/05	C	6.00H	11.00	0.00	0.00	0.00	0	83.1515400		91232.120
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	24211.927
	-2.013727427D+03		1.486781340D+02		-1.013466780D+00		9.359556120D-02		-2.665490850D-04		
	6.437142300D-07		-5.422879110D-10		0.000000000D+00		7.602071490D+03		3.178590380D+01		
	200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	24211.927
	-4.011553360D+05		7.066796240D+03		-4.459166780D+01		1.979129483D-01		-2.352895228D-04		
	1.495835174D-07		-3.895260010D-11		0.000000000D+00		-2.433664940D+04		2.719060426D+02		
	1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	24211.927
	7.679935740D+06		-3.356555240D+04		6.586418160D+01		-5.474116900D-03		9.002252500D-07		
	-7.925391760D-11		2.896580042D-15		0.000000000D+00		2.065551233D+05		-4.022468300D+02		
C6H11 CH2=C(CH3)CH2CH*CH3 HF298=32.72 kcal REF=Burcat G3B3											
3	A06/05	C	6.00H	11.00	0.00	0.00	0.00	0	83.1515400		136913.032
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	23974.800
	1.373864775D+03		-4.061925090D+01		2.061618375D+00		9.410691600D-02		-4.443646580D-04		
	1.419125439D-06		-1.619252718D-09		0.000000000D+00		1.379007998D+04		1.698304660D+01		
	200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	23974.800
	-3.733791860D+05		6.630358630D+03		-3.983745290D+01		1.736208240D-01		-1.989270922D-04		
	1.259983217D-07		-3.316469050D-11		0.000000000D+00		-1.687786610D+04		2.496504707D+02		
	1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	23974.800
	1.018858291D+07		-4.094168620D+04		7.066722280D+01		-6.917291210D-03		1.023638963D-06		
	-7.569696000D-11		2.119041003D-15		0.000000000D+00		2.602994208D+05		-4.416841300D+02		
C6H11 Cyclohexyl Radical HF298=18.126 kcal Burcat G3B3 calc											
3	A06/05	C	6.00H	11.00	0.00	0.00	0.00	0	83.1515400		75839.184
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	18313.348
	-3.083020735D+03		2.354664682D+02		-3.087750730D+00		9.290732070D-02		-3.606619480D-04		
	9.791993820D-07		-7.842671830D-10		0.000000000D+00		6.190006380D+03		3.781232730D+01		
	200.000		1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	18313.348
	-5.812965830D+05		1.045901294D+04		-6.841362030D+01		2.481550943D-01		-2.905526598D-04		
	1.830479336D-07		-4.754117800D-11		0.000000000D+00		-4.082408480D+04		3.971962190D+02		
	1000.000		6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	18313.348
	8.557741530D+06		-3.904137790D+04		7.082332600D+01		-6.908283460D-03		1.260140243D-06		
	-1.232608586D-10		5.000606090D-15		0.000000000D+00		2.375589118D+05		-4.512219060D+02		

Table 5 (continued)

C6H11I IodoCyclohexane Burcat B3LYP/6-311G* HF298=-50+/-4.7 kJ Pedley et al 1986											
3	A08/05	C	6.00H	11.00I	1.00	0.00	0.00	0	210.0560100	-50000.000	
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0 21419.946
-2.022503393D+03 2.072599568D+02-4.324075070D+00 1.468412022D-01-7.597135640D-04											
	2.374268238D-06	-2.645691571D-09	0.000000000D+00	-9.171169000D+03	4.329505290D+01						
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0 21419.946
-6.284296130D+05 1.125157357D+04-7.243096670D+01 2.669385059D-01-3.153381522D-04											
	1.993744198D-07	-5.183242170D-11	0.000000000D+00	-6.008110150D+04	4.233936630D+02						
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0 21419.946
8.470471180D+06-3.923929850D+04 7.386397670D+01-6.896768350D-03 1.253337369D-06											
	-1.221247544D-10	4.935453680D-15	0.000000000D+00	2.223952494D+05	-4.640383880D+02						
C6H12 trans 3-HEXENE C2H5-CH=CH-C2H5 Burcat G3B3 calc HF298=-50.417 kJ											
3	A03/05	C	6.00H	12.00	0.00	0.00	0.00	0	84.15948	-50417.200	
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0 23930.808
-8.212012100D+03 5.864039460D+02-1.194038510D+01 2.368171879D-01-1.217266301D-03											
	3.597368580D-06	-4.119062640D-09	0.000000000D+00	-1.081810611D+04	7.377868290D+01						
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0 23930.808
-4.409422340D+05 7.708080070D+03-4.671300780D+01 1.934499681D-01-2.229748107D-04											
	1.415448775D-07	-3.726789310D-11	0.000000000D+00	-4.442313790D+04	2.845847526D+02						
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0 23930.808
1.079268011D+07-4.398163230D+04 7.557749190D+01-8.457846940D-03 1.513864853D-06											
	-1.439410290D-10	5.655366470D-15	0.000000000D+00	2.556717121D+05	-4.786662970D+02						
C6H13 2-Hexyl CH3CH*CH2CH2CH2CH3 Burcat G3B3 calc											
3	A07/05	C	6.00H	13.00	0.00	0.00	0.00	0	85.1674200	28158.320	
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0 28212.843
-1.880440377D+03 1.256713705D+02-8.689305310D-01 1.445703828D-01-6.592710100D-04											
	1.790201523D-06	-1.718071786D-09	0.000000000D+00	-4.001809480D+02	3.068715068D+01						
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0 28212.843
-5.038922730D+05 8.739783290D+03-5.104075700D+01 2.126903528D-01-2.497277233D-04											
	1.608880572D-07	-4.285619570D-11	0.000000000D+00	-4.042617680D+04	3.151687118D+02						
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0 28212.843
1.150349709D+07-4.678144520D+04 8.151687110D+01-9.650763540D-03 1.765892250D-06											
	-1.712840368D-10	6.857439380D-15	0.000000000D+00	2.815822214D+05	-5.104594850D+02						
C6H13 2-Methyl-1-Pentyl CH2*CH(CH3)CH2CH2CH3 Burcat G3B3 calc.											
3	A07/05	C	6.00H	13.00	0.00	0.00	0.00	0	85.1674200	35635.128	
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0 26199.739
-4.266677090D+03 2.879462741D+02-4.234718660D+00 1.434075224D-01-4.858239940D-04											
	9.039717000D-07	-3.696658260D-10	0.000000000D+00	2.081313728D+02	4.471705150D+01						
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0 26199.739
-5.398273460D+05 8.983831340D+03-5.188463690D+01 2.100437626D-01-2.432497234D-04											
	1.542967072D-07	-4.048413290D-11	0.000000000D+00	-4.071403430D+04	3.176550850D+02						
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0 26199.739
1.085443572D+07-4.442038350D+04 7.777764170D+01-8.441001480D-03 1.538739158D-06											
	-1.494546501D-10	6.003724330D-15	0.000000000D+00	2.680809380D+05	-4.882772350D+02						

Table 5 (continued)

C6H13 2-Methyl-5-Pentyl (CH3)2CHCH2CH2CH2* Burcat G3B3 calc.												
3 A07/05 C	6.00H	13.00	0.00	0.00	0.00	0	85.1674200		32367.424			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	26304.214	
4.004131470D+02	-4.400652740D+01	4.058258620D+00	6.240944140D-02	-1.138899880D-04								
5.497303320D-08	4.194326560D-10	0.000000000D+00	8.710108870D+02	1.171982835D+01								
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	26304.214	
-4.913970480D+05	8.433666950D+03	-4.948373720D+01	2.039942068D-01	-2.364184195D-04								
1.509366250D-07	-3.991709010D-11	0.000000000D+00	-3.831092170D+04	3.057046663D+02								
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	26304.214	
1.139844501D+07	-4.604948620D+04	7.905359900D+01	-8.783803740D-03	1.580337642D-06								
-1.512185838D-10	5.981610340D-15	0.000000000D+00	2.782413057D+05	-4.965775500D+02								
C6H13 2-Methyl-2Pentyl (tertiary) (CH3)2C*CH2CH2CH3 Burcat G3B3												
3 A07/05 C	6.00H	13.00	0.00	0.00	0.00	0	85.1674200		17208.792			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	26392.058	
-4.918753090D+03	3.960677810D+02	-9.206956030D+00	2.364431926D-01	-1.224679548D-03								
3.569955590D-06	-4.037204170D-09	0.000000000D+00	-2.308202356D+03	6.275383360D+01								
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	26392.058	
-4.907556760D+05	8.168127500D+03	-4.592390870D+01	1.893434371D-01	-2.116348904D-04								
1.319947521D-07	-3.443626530D-11	0.000000000D+00	-3.921328550D+04	2.868050850D+02								
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	26392.058	
1.152969647D+07	-4.690577560D+04	8.027625620D+01	-9.476240790D-03	1.764079871D-06								
-1.746642931D-10	7.144574280D-15	0.000000000D+00	2.814745676D+05	-5.064526350D+02								
C6H13 2Methyl-4-Pentyl (CH3)2CHCH2CH*CH3 Burcat G3B3												
3 A07/05 C	6.00H	13.00	0.00	0.00	0.00	0	85.1674200		20079.016			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	26420.123	
-2.755526026D+03	1.942121532D+02	-2.317269134D+00	1.248732119D-01	-3.741767940D-04								
5.637084730D-07	2.721021189D-11	0.000000000D+00	-1.371973873D+03	3.531538920D+01								
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	26420.123	
-4.878944190D+05	8.031108180D+03	-4.521317030D+01	1.898097043D-01	-2.146199234D-04								
1.350228282D-07	-3.541152780D-11	0.000000000D+00	-3.828958320D+04	2.807015058D+02								
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	26420.123	
1.158601727D+07	-4.658648690D+04	7.966253790D+01	-9.003929540D-03	1.622270617D-06								
-1.554429165D-10	6.158684530D-15	0.000000000D+00	2.802307172D+05	-5.035924270D+02								
C6H13 2Methyl-4-Pentyl (CH3)2CHCH2CH*CH3 Burcat G3B3												
3 T07/05 C	6.00H	13.00	0.00	0.00	0.00	0	85.1674200		20079.016			
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	26420.123	
-2.755563788D+03	1.942146931D+02	-2.317337404D+00	1.248741494D-01	-3.741837310D-04								
5.637347570D-07	2.717029550D-11	0.000000000D+00	-1.371982065D+03	3.670195450D+01								
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	26420.123	
-4.878944290D+05	8.031108280D+03	-4.521317090D+01	1.898097060D-01	-2.146199260D-04								
1.350228302D-07	-3.541152840D-11	0.000000000D+00	-3.828958370D+04	2.820878033D+02								
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	26420.123	
1.158600782D+07	-4.658646570D+04	7.966251860D+01	-9.003920780D-03	1.622268489D-06								
-1.554426544D-10	6.158671690D-15	0.000000000D+00	2.802305767D+05	-5.022059910D+02								

Table 5 (continued)

C6H13 2-Methyl-2Pentyl (tertiary) (CH3)2C*CH2CH2CH3 Burcat G3B3 calc											
3 T07/05 C	6.00H	13.00	0.00	0.00	0.00	0.00	0	85.1674200		17208.792	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	26392.058
-4.918753090D+03 3.960677810D+02-9.206956030D+00 2.364431926D-01-1.224679548D-03											
3.569955590D-06	-4.037204170D-09	0.000000000D+00	-2.308202356D+03	6.275383360D+01	200.000	1000.000	7	-2.0	-1.0	0.0	26392.058
-4.907556760D+05 8.168127500D+03-4.592390870D+01 1.893434371D-01-2.116348904D-04											
1.319947521D-07	-3.443626530D-11	0.000000000D+00	-3.921328550D+04	2.868050850D+02	1000.000	6000.000	7	-2.0	-1.0	0.0	26392.058
1.152969647D+07-4.690577560D+04 8.027625620D+01-9.476240790D-03 1.764079871D-06											
-1.746642931D-10 7.144574280D-15 0.000000000D+00 2.814745676D+05-5.064526350D+02											
C7 Cumulenlic linear Van Orden A. and Saykally R Chem.Rev. 98 (1998),2313.											
3 A09/04 C	7.00	0.00	0.00	0.00	0.00	0	84.0749000		1326328.000		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	20372.204
1.569623753D+03-8.734204320D+01 4.462278960D+00 3.743118050D-02-5.406490400D-05											
1.418263418D-07	-3.374025010D-10	0.000000000D+00	1.573778005D+05	2.700330355D+00	200.000	1000.000	7	-2.0	-1.0	0.0	20372.204
1.171114963D+05-2.277161195D+03 1.999630213D+01-1.272635354D-02 2.942205163D-05											
-2.482684843D-08 7.459919470D-12 0.000000000D+00 1.672761709D+05-8.044044550D+01											
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	20372.204
8.283912770D+05-6.165819420D+03 2.387184105D+01-1.698703943D-03 3.693666370D-07											
-4.199211050D-11 1.938066332D-15 0.000000000D+00 1.904395969D+05-1.136431688D+02											
C7H4 TriEthynylMethane CH(CCH)3 PM3 HF298 est.NIST 94											
3 T08/02 C	7.00H	4.00	0.00	0.00	0.00	0	88.1066600		676134.400		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17859.765
9.698116780D+02 2.130103478D+00 2.214660441D+00 3.074678083D-02-1.887976103D-05											
1.523411186D-07	-1.481309903D-10	0.000000000D+00	7.923546650D+04	1.560613523D+01	200.000	1000.000	7	-2.0	-1.0	0.0	17859.765
8.737363360D+04-1.686938708D+02-6.721320460D+00 9.126338820D-02-1.226901300D-04											
8.765123020D-08	-2.524497999D-11	0.000000000D+00	8.144426820D+04	5.327396380D+01	1000.000	6000.000	7	-2.0	-1.0	0.0	17859.765
3.510856210D+06-1.746681093D+04 4.064396430D+01-2.995858361D-03 5.334570220D-07											
-5.073622090D-11 1.995782250D-15 0.000000000D+00 1.799248161D+05-2.339305098D+02											
C7H5(NO2)3 TRI-NITRO TOLUENE (TNT) HF298=5.76 kcal Lenchitz et al											
3 A 8/05 C	7.00H	5.00N	3.00O	6.00	0.00	0	227.1312200		24099.840		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	37697.748
-3.130260248D+03 2.417103516D+02-4.191966690D+00 1.972660163D-01-8.169652210D-04											
2.628269631D-06	-3.432255230D-09	0.000000000D+00	-2.379373709D+03	4.364410940D+01	200.000	1000.000	7	-2.0	-1.0	0.0	37697.748
-2.767948747D+05 5.004128290D+03-3.149065481D+01 2.037675983D-01-2.279759179D-04											
1.315943223D-07	-3.117539322D-11	0.000000000D+00	-2.444042959D+04	2.008897712D+02	1000.000	6000.000	7	-2.0	-1.0	0.0	37697.748
2.449028304D+06-2.308774411D+04 7.583267350D+01-7.081385590D-03 1.490924088D-06											
-1.635072430D-10 7.299122790D-15 0.000000000D+00 1.206523087D+05-4.349633110D+02											

Table 5 (continued)

C7H7 2,4,6-Cycloheptatriene-1-yl radical Burcat G3B3 calc HF298=67.088 kcal										
3 T09/05 C	7.00H	7.00	0.00	0.00	0.00	0.00	0	91.1304800	280696.192	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.503638402D+03	-1.240988632D+02	7.505636420D+00	-2.600193898D-02	2.743019459D-04						
-5.485967750D-07	5.386028890D-10	0.000000000D+00	3.180629390D+04	-3.787762660D+00						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.109998842D+05	4.729392580D+03	-3.614451010D+01	1.717144270D-01	-2.110986885D-04						
1.374226508D-07	-3.647577220D-11	0.000000000D+00	1.086093918D+04	2.176611157D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.365073310D+06	-2.553334880D+04	5.349973320D+01	-4.022014490D-03	6.874631800D-07						
-6.277706990D-11	2.370363109D-15	0.000000000D+00	1.801889459D+05	-3.225017780D+02						
C7H7 C6H5CH2 BENZYL RADICAL IUPAC Task Group on Selected Radicals										
3 IU3/03 C	7.00H	7.00	0.00	0.00	0.00	0.00	0	91.13048	208000.000	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-0.756495439D+03	0.376311027D+02	0.366107184D+01	-0.150976243D-01	0.357926180D-03						
-0.107968568D-05	0.143603017D-08	0.000000000D+00	0.226915530D+05	0.128978231D+02						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-0.165413161D+06	0.404634790D+04	-0.343823664D+02	0.173587185D+00	-0.218575878D-03						
0.145307561D-06	-0.393164608D-10	0.000000000D+00	0.560557100D+04	0.203565978D+03						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.530285955D+07	-0.265513279D+05	0.567373699D+02	-0.606930760D-02	0.120158407D-05						
-0.125587992D-09	0.538552853D-14	0.000000000D+00	0.176378374D+06	-0.345315385D+03						
C7H7 Quadricyclene Appex Radical A. Burcat G3-B3LYP HF298=127.753 kcal										
3 T05/04 C	7.00H	7.00	0.00	0.00	0.00	0.00	0	91.1304800	534518.552	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.422074463D+02	1.412147237D+01	2.763859989D+00	2.788534482D-02	-2.934922066D-04						
1.820819730D-06	-2.734262143D-09	0.000000000D+00	6.243885320D+04	1.420170628D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.120608964D+05	6.315605780D+03	-5.833731460D+01	2.544292053D-01	-3.436270240D-04						
2.367415798D-07	-6.515186330D-11	0.000000000D+00	3.627593270D+04	3.256392420D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.149339430D+06	-2.213178075D+04	5.046353550D+01	-2.662509770D-03	3.623249820D-07						
-2.323346040D-11	4.522391870D-16	0.000000000D+00	1.883875488D+05	-3.044665248D+02						
C7H7 Quadricyclene Basis Radical A. Burcat G3-B3LYP HF298=138.945 kcal										
3 T05/04 C	7.00H	7.00	0.00	0.00	0.00	0.00	0	91.1304800	581345.880	
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.155028352D+03	-7.580699830D+01	5.901502780D+00	-2.085953701D-02	5.345797870D-05						
5.585533650D-07	-9.619381040D-10	0.000000000D+00	6.841801850D+04	3.057266526D+00						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.916842012D+05	7.467017820D+03	-6.398581500D+01	2.625171319D-01	-3.474780810D-04						
2.360734893D-07	-6.436182710D-11	0.000000000D+00	3.644018270D+04	3.592403930D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.195540580D+06	-2.302933740D+04	5.148237170D+01	-3.154932636D-03	4.835503440D-07						
-3.813853480D-11	1.177548618D-15	0.000000000D+00	1.991247074D+05	-3.123339525D+02						

Table 5 (continued)

C7H7 Quadricyclene Shoulder Radical A. Burcat G3-B3LYP HF298=140.76 kcal										
3 T05/04 C	7.00H	7.00	0.00	0.00	0.00	0	91.1304800	588939.840		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.105879011D+03	-7.265380370D+01	5.816334370D+00	-1.958169339D-02	4.302292280D-05						
5.895477150D-07	-9.805069070D-10	0.000000000D+00	6.932284910D+04	3.392346650D+00						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.877112754D+05	7.470931680D+03	-6.448438540D+01	2.651826323D-01	-3.524176140D-04						
2.400556248D-07	-6.556049230D-11	0.000000000D+00	3.741105910D+04	3.614975300D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.160321190D+06	-2.285173239D+04	5.128311310D+01	-3.058115277D-03	4.595303200D-07						
-3.516295520D-11	1.031786620D-15	0.000000000D+00	1.989581871D+05	-3.108526098D+02						
C7H8 Quadricyclene A. Burcat G3-B3LYP HF298=80.6 kcal										
3 T05/04 C	7.00H	8.00	0.00	0.00	0.00	0	92.1384200	337230.400		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.828067361D+02	-5.950749170D+00	3.908223000D+00	7.566989670D-03	-1.531704185D-04						
1.239331978D-06	-1.757389865D-09	0.000000000D+00	3.884316040D+04	9.544096580D+00						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.602475590D+05	8.819631630D+03	-7.363792030D+01	2.916237373D-01	-3.844601900D-04						
2.607073372D-07	-7.099673800D-11	0.000000000D+00	1.008659302D+03	4.097802610D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.967922840D+06	-2.624272269D+04	5.603284860D+01	-3.564335630D-03	5.430877810D-07						
-4.248572960D-11	1.295256416D-15	0.000000000D+00	1.891156835D+05	-3.464984130D+02						
C7H10 NORBORNENE HF NIST 2001 est moments PM3 vib Shaw JCP 89, (1988) 716										
3 T11/01 C	7.00H	10.00	0.00	0.00	0.00	0	94.1543000	90000.000		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.110637641D+03	1.533971517D+02	-1.328630802D-01	4.863975890D-02	-2.498040125D-04						
1.163849081D-06	-1.330614310D-09	0.000000000D+00	8.375290620D+03	2.709294507D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.341498780D+05	9.563735690D+03	-7.484596560D+01	2.914662548D-01	-3.692882520D-04						
2.455433015D-07	-6.629713930D-11	0.000000000D+00	-3.295274440D+04	4.203653500D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.467961440D+06	-3.353420100D+04	6.767591000D+01	-5.859310610D-03	1.054922465D-06						
-1.015424242D-10	4.045538290D-15	0.000000000D+00	2.025035230D+05	-4.263274730D+02						
C7H10N2O2 Cyclo Pro-Gly C. Lifshitz & Y. Ling J. Mass. Spect. 33, (1998), 25-34.										
3 A03/05 C	7.00H	10.00N	2.00O	2.00	0.00	0	154.1665800	-341190.797		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.982021510D+03	-3.379073370D+02	1.143460359D+01	-3.110822196D-02	3.792792830D-04						
-8.554181730D-07	8.631346830D-10	0.000000000D+00	-4.318856240D+04	-1.983740855D+01						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.065864650D+05	1.082545283D+04	-7.003071070D+01	2.784684426D-01	-3.185686280D-04						
1.939859060D-07	-4.869249440D-11	0.000000000D+00	-9.379237720D+04	4.095718210D+02						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.909249390D+06	-3.989675490D+04	8.325335170D+01	-7.054439010D-03	1.291850465D-06						
-1.270641768D-10	5.188535810D-15	0.000000000D+00	1.867459818D+05	-5.176187150D+02						

Table 5 (continued)

C8H6O 2,3-Benzofuran Zhu &amp; Bozzelli JPCRD 32 (2003),1713

3	T03/04	C	8.00H	6.00O	1.00	0.00	0.00	0	118.1326400	17000.000		
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18124.186
	6.120571560D+02	6.744448040D+00	2.563054215D+00	2.636596846D-02	-1.055846145D-04							
	9.657244540D-07	-1.696466211D-09	0.000000000D+00	-1.066252102D+02	1.629536369D+01							
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18124.186
	-2.538522379D+05	5.770113450D+03	-4.690478290D+01	2.112078229D-01	-2.610578242D-04							
	1.681256173D-07	-4.399891390D-11	0.000000000D+00	-2.509049757D+04	2.716347421D+02							
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	18124.186
	4.185959670D+06	-2.367817181D+04	5.554247110D+01	-3.748695500D-03	6.434240390D-07							
	-5.904937280D-11	2.242373577D-15	0.000000000D+00	1.338140535D+05	-3.341070360D+02							

C8H6O2 2,3-Benzodioxin Zhu &amp; Bozzelli JPCRD 32(2003),1713

3	T02/04	C	8.00H	6.00O	2.00	0.00	0.00	0	134.1320400	-71200.000		
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	21265.442
	4.313381720D+03	-3.274381800D+02	1.332871424D+01	-1.123469477D-01	8.992258640D-04							
	-2.401566381D-06	2.648149068D-09	0.000000000D+00	-1.009855649D+04	-2.567120176D+01							
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	21265.442
	-2.242010022D+05	5.108149750D+03	-4.166502100D+01	2.042234071D-01	-2.501254991D-04							
	1.599735299D-07	-4.165126580D-11	0.000000000D+00	-3.316079020D+04	2.439426739D+02							
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	21265.442
	4.271329680D+06	-2.435294908D+04	5.904574240D+01	-3.952243970D-03	6.891004720D-07							
	-6.437257600D-11	2.492938388D-15	0.000000000D+00	1.262957210D+05	-3.532550880D+02							

C8H9 PhenylEthyl Rad C6H5CH2CH2\* bURCAT G3B3 calc HF298=237.714 kJ

3	A11/04	C	8.00H	9.00	0.00	0.00	0.00	0	105.1570600	237713.960		
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22134.640
	-1.716799165D+03	9.769928730D+01	1.721036180D+00	3.609605920D-02	5.670782600D-05							
	-1.843766930D-07	4.149353980D-10	0.000000000D+00	2.559354856D+04	2.196066977D+01							
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22134.640
	-2.719022184D+05	5.791335390D+03	-4.393540720D+01	2.085497758D-01	-2.596632512D-04							
	1.711649962D-07	-4.589922900D-11	0.000000000D+00	4.890777080D+02	2.600267603D+02							
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22134.640
	7.109893390D+06	-3.231567000D+04	6.534771570D+01	-5.174977140D-03	8.382766300D-07							
	-7.139934980D-11	2.478657356D-15	0.000000000D+00	2.154789095D+05	-4.002130560D+02							

C8H10 EthylBenzene C6H5CH2CH3 G3B3 calc Burcat G3B3 calc. HF298=Rossini 1945

3	A11/04	C	8.00H	10.00	0.00	0.00	0.00	0	106.1650000	29790.080		
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	21750.331
	-3.740940330D+03	2.817148738D+02	-4.279981830D+00	1.263577029D-01	-6.356184950D-04							
	2.297972179D-06	-2.936900705D-09	0.000000000D+00	8.443393790D+01	4.393281760D+01							
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	21750.331
	-3.507522500D+05	7.259581310D+03	-5.382849500D+01	2.343611246D-01	-2.851427699D-04							
	1.847223628D-07	-4.893263500D-11	0.000000000D+00	-3.114607129D+04	3.128782030D+02							
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	21750.331
	8.132749940D+06	-3.727330840D+04	7.268411310D+01	-6.475429290D-03	1.119241224D-06							
	-1.028527304D-10	3.902605830D-15	0.000000000D+00	2.198637297D+05	-4.542512530D+02							



Table 5 (continued)

C8H14 Bicyclo[2,2,2]octane CH(-CH2-CH2-)3CH B3LYP vib PM3 Moments

3 T08/04 C	8.00H	14.00	0.00	0.00	0.00	0.00	0	110.1967600	-99035.280
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0									20374.064
-8.572688610D+03	5.621215870D+02	-9.402059170D+00	1.644030977D-01	-8.165975180D-04					
2.584785628D-06	-2.798320020D-09	0.000000000D+00	-1.621454734D+04	6.479519530D+01					
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0									20374.064
-8.130866860D+05	1.505882135D+04	-1.024746683D+02	3.610998180D-01	-4.290583370D-04					
2.719034185D-07	-7.075338420D-11	0.000000000D+00	-8.264749520D+04	5.783370220D+02					
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0									20374.064
1.068573329D+07	-5.040016980D+04	9.206810420D+01	-8.847434410D-03	1.606405754D-06					
-1.563699735D-10	6.312548280D-15	0.000000000D+00	2.817649637D+05	-5.976148700D+02					

C8H16 CYCLOOCTANE Dorofeeva, Gurvich and Jorish JPCRD 15 (1986),437

3 T11/03 C	8.00H	16.00	0.00	0.00	0.00	0.00	0	112.2126400	-124400.000
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0									22515.219
-5.301902920D+03	4.067331540D+02	-8.277971140D+00	1.719501651D-01	-8.664470580D-04					
2.897519912D-06	-3.422986730D-09	0.000000000D+00	-1.893009632D+04	5.648052070D+01					
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0									22515.219
-7.709983690D+05	1.421047040D+04	-9.680242340D+01	3.527930110D-01	-4.108755830D-04					
2.584841508D-07	-6.733947710D-11	0.000000000D+00	-8.218113030D+04	5.453738150D+02					
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0									22515.219
1.131749961D+07	-5.515749070D+04	1.024840123D+02	-1.080924903D-02	2.066649906D-06					
-2.111925204D-10	8.920783360D-15	0.000000000D+00	3.051557067D+05	-6.680460000D+02					

C8H20Pb (C2h5)4Pb TETRAETHYLLEAD MOPAC HF298 109.6 kJ Webbook 2003

3 T 3/04 C	8.00H	20.00PB	1.00	0.00	0.00	0.00	0	323.4444000	109600.000
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0									40263.977
-6.507246080D+03	6.395749650D+02	-2.100603601D+01	4.588553810D-01	-2.425707216D-03					
7.118154730D-06	-7.994781770D-09	0.000000000D+00	6.516160600D+03	1.031742671D+02					
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0									40263.977
-6.891903490D+05	1.247559370D+04	-7.987371020D+01	3.560930300D-01	-4.458866930D-04					
2.998977658D-07	-8.205486330D-11	0.000000000D+00	-4.883808980D+04	4.616934300D+02					
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0									40263.977
1.544647504D+07	-6.355815340D+04	1.164141112D+02	-9.859657110D-03	1.662937749D-06					
-1.493033351D-10	5.522199440D-15	0.000000000D+00	3.886250960D+05	-7.405022540D+02					

C9H4 Tetraethynylmethane C(CCH)4 PM3 HF298 est NIST 94

3 T08/02 C	9.00H	4.00	0.00	0.00	0.00	0.00	0	112.1280600	913785.600
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0									21768.326
4.129163320D+03	-1.308089958D+02	2.916044814D+00	5.753746030D-02	-2.376005016D-04					
1.201579700D-06	-1.934085591D-09	0.000000000D+00	1.078723722D+05	9.365077630D+00					
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0									21768.326
1.690090576D+05	-1.525418581D+03	1.105774297D+00	8.572842310D-02	-1.145514649D-04					
8.217430160D-08	-2.382919025D-11	0.000000000D+00	1.158814656D+05	8.166221310D+00					
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0									21768.326
3.919590470D+06	-1.973976310D+04	4.796494730D+01	-3.433692250D-03	6.173479610D-07					
-5.935895300D-11	2.362841028D-15	0.000000000D+00	2.205766665D+05	-2.788334914D+02					

Table 5 (continued)

C9H12 TetraVinylMethane C(CH=CH2)4 PM3 HF298 est NIST 94

3 T08/02 C	9.00H	12.00	0.00	0.00	0.00	0.00	0	120.1915800	250621.600
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.269591860D+03	2.469079426D+02	7.787968680D-01	7.428238130D-02	2.516199472D-05					
-4.914838840D-07	1.092434714D-09	0.000000000D+00	2.543864490D+04	2.560715586D+01					
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.849596288D+05	5.535298070D+03	-3.661791800D+01	2.006089836D-01	-2.419098696D-04					
1.593296395D-07	-4.315211430D-11	0.000000000D+00	1.492980176D+03	2.254749937D+02					
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.033013343D+07	-4.318609830D+04	8.193514590D+01	-6.358720910D-03	8.404756900D-07					
-5.295616280D-11	1.079707053D-15	0.000000000D+00	2.838925729D+05	-5.089426440D+02					

C9H18O6 TATP TriacetoneTriperoxide 33,66,99-hexamethyl-1,4,7-cyclonanotriperoxan

3 A07/05 C	9.00H	18.000	6.00	0.00	0.00	0	222.2356200	-395471.680
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
-8.983038840D+03	8.568395130D+02	-2.544501222D+01	3.923783830D-01	-1.025489631D-03				
1.390897517D-06	-4.453419720D-10	0.000000000D+00	-5.580805090D+04	1.250666288D+02				
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
-4.231713840D+05	5.740762420D+03	-3.102960889D+01	2.451758948D-01	-2.732409002D-04				
1.693987614D-07	-4.394875670D-11	0.000000000D+00	-8.123768330D+04	1.913901503D+02				
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
1.392477978D+07	-6.222851900D+04	1.295409937D+02	-1.150500865D-02	2.146500542D-06				
-2.146599722D-10	8.895415420D-15	0.000000000D+00	3.122113043D+05	-8.140519860D+02				

C9H20 N-NONANE D.W.Scott buletin 666 Bartlesville 1974

2 T 5/99 C	9.00H	20.00	0.00	0.00	0.00	0	128.2551000	-228906.640
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
-7.527507450D+05	1.453853987D+04	-9.160169700D+01	3.580460820D-01	-4.068209830D-04				
2.455842574D-07	-6.107471180D-11	0.000000000D+00	-9.835568990D+04	5.366288170D+02				
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
1.385167225D+07	-5.989490080D+04	1.146043343D+02	-1.365865201D-02	3.431599780D-06				
-4.373950790D-10	2.207813511D-14	0.000000000D+00	3.225982560D+05	-7.216117510D+02				

C10H8O NAPHTOL IR spectrum + Gaussian 94 HF NIST 97

3 T 7/98 C	10.00H	8.000	1.00	0.00	0.00	0	144.1699200	-30794.240
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
-4.271804770D+02	9.192652290D+01	-1.301937813D-02	5.140168880D-02	3.947047070D-05				
9.569798230D-08	-4.021274000D-10	0.000000000D+00	-6.859066070D+03	2.759052285D+01				
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
-8.650664240D+04	2.316292927D+03	-2.205531480D+01	1.542466620D-01	-1.625016124D-04				
9.249922040D-08	-2.217194182D-11	0.000000000D+00	-1.620774833D+04	1.377504331D+02				
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
5.113458320D+06	-3.041141944D+04	7.258331480D+01	-6.108939460D-03	1.188788511D-06				
-1.237227210D-10	5.319661710D-15	0.000000000D+00	1.647632321D+05	-4.422773900D+02				

C10H9 1-methyl-1-indenyl Radical Lifshitz Dubnikova JPC A 108, (2004), 3430

3 A03/05 C	10.00H	9.00	0.00	0.00	0.00	0	129.1784600	262336.800
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
4.865786910D+03	-2.283496143D+02	6.123975930D+00	2.244682532D-02	-4.396319300D-05				
7.661337900D-07	-1.446371103D-09	0.000000000D+00	2.959706797D+04	9.485593710D-02				
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
-3.743473950D+05	7.583026550D+03	-5.637249010D+01	2.509752048D-01	-3.053497851D-04				
1.958211844D-07	-5.124398670D-11	0.000000000D+00	-4.921554490D+03	3.260225220D+02				
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
6.641093230D+06	-3.357560080D+04	7.261703630D+01	-5.525914740D-03	9.698239510D-07				
-9.118544110D-11	3.554144170D-15	0.000000000D+00	2.222906930D+05	-4.468229140D+02				

Table 5 (continued)

C10H9 1-methylene-indene Radical													Lifshitz Dubnikova JPC A 108, (2004), 3430
3	A03/05	C	10.00H	9.00	0.00	0.00	0.00	0	129.1784600	337648.800			
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22770.594
4.890992770D+03	-3.023988623D+02	1.040338146D+01	-5.978337070D-02	5.522461220D-04									
-1.221937193D-06	1.188391358D-09	0.000000000D+00	3.889142180D+04	-1.470393768D+01									
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22770.594	
-3.230094300D+05	7.127764320D+03	-5.728279870D+01	2.623541654D-01	-3.275886660D-04									
	2.145055661D-07	-5.709799240D-11	0.000000000D+00	6.830402720D+03	3.268078570D+02								
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22770.594	
	6.860121190D+06	-3.500968970D+04	7.572448150D+01	-7.096539420D-03	1.346802325D-06								
-1.357900116D-10	5.643521400D-15	0.000000000D+00	2.394012816D+05	-4.682655930D+02									
C10H10 1,1'-bicyclo-2,4-pentadiene HF298=69.7 kcal NIST 94													
3	A05/05	C	10.00H	10.00	0.00	0.00	0.00	0	130.1864000	291624.800			
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	24164.381
-1.654390909D+03	1.118769311D+02	6.274964770D-01	9.974267540D-02	-6.340976910D-04									
	2.656463384D-06	-3.468737800D-09	0.000000000D+00	3.180857550D+04	2.496058688D+01								
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	24164.381	
-4.563676710D+05	1.012283050D+04	-7.792781160D+01	3.226342040D-01	-4.107897600D-04									
	2.720035146D-07	-7.284516100D-11	0.000000000D+00	-1.211201004D+04	4.414981300D+02								
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	24164.381	
	6.628256430D+06	-3.428327680D+04	7.476044700D+01	-5.138422990D-03	8.454446750D-07								
-7.362218230D-11	2.622965182D-15	0.000000000D+00	2.291551837D+05	-4.596633320D+02									
C10H10 2,2'-bicyclo-2,4-pentadiene HF298=69.56 kcal Melius P81BZ													
3	A05/05	C	10.00H	10.00	0.00	0.00	0.00	0	130.1864000	291055.776			
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	25158.649
-4.062848550D+03	2.077755786D+02	1.518739496D-02	6.831405650D-02	-1.209092200D-04									
	2.520008933D-07	2.804795540D-10	0.000000000D+00	3.123815930D+04	2.941801529D+01								
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	25158.649	
-3.930492080D+05	8.571682430D+03	-6.537016720D+01	2.851481825D-01	-3.554058180D-04									
	2.335555006D-07	-6.259470520D-11	0.000000000D+00	-5.626357850D+03	3.743171040D+02								
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	25158.649	
	6.905914560D+06	-3.643513260D+04	7.906148410D+01	-7.239042990D-03	1.346166106D-06								
-1.332081413D-10	5.444921520D-15	0.000000000D+00	2.413154508D+05	-4.884812990D+02									
C10H10 1-methyl-indene Lifshitz Dubnikova JPC A 108, (2004), 3430 HF298=44.2 kcal													
3	A03/05	C	10.00H	10.00	0.00	0.00	0.00	0	130.1864000	184932.800			
	50.000		200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	23112.953
-1.762719063D+02	1.117241507D+02	-2.220629951D+00	1.120805330D-01	-5.415210230D-04									
	2.130139113D-06	-2.885833445D-09	0.000000000D+00	1.921629424D+04	3.388771620D+01								
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	23112.953	
-4.538223630D+05	8.982633390D+03	-6.570635320D+01	2.775221666D-01	-3.373660510D-04									
	2.165488908D-07	-5.675499890D-11	0.000000000D+00	-2.062455491D+04	3.757390460D+02								
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	23112.953	
	7.439743420D+06	-3.707391630D+04	7.755961630D+01	-6.134659690D-03	1.079459995D-06								
-1.017547304D-10	3.976269030D-15	0.000000000D+00	2.339745247D+05	-4.835557690D+02									

Table 5 (continued)

C10H10 2-methyl-indene														Lifshitz Dubnikova JPC A 108, (2004), 3430														HF298=41.5 kc																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
3	A03/05	C	10.00H	10.00	0.00	0.00	0.00	0.00	0	130.1864000	173636.000																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													

Table 5 (continued)

## C11H24 N-UNDECANE TRC 10/1975

2	T	5/99	C	11.00H	24.00	0.00	0.00	0.00	0.00	0	156.3082600	-270286.400										
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	51463.200											
-1.414609949D+06	2.508860204D+04	-1.545373088D+02	5.602534050D-01	-6.831134610D-04	4.398324080D-07	-1.161148169D-10	0.000000000D+00	-1.538024784D+05	8.866980310D+02	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	51463.200	
1.584298461D+07	-6.551034980D+04	1.290624474D+02	-1.200300106D-02	2.951101989D-06	-3.670844840D-10	1.811980374D-14	0.000000000D+00	3.499540490D+05	-8.073857820D+02													

## C12H4Cl4O2 1,3,6,8 Tetra-Chloro-Dibenzo Dioxin JPC 107 (2003), 2848

3	T	8/03	C	12.00H	4.000	2.00CL	4.00	0.00	0	321.9697600	-128700.000											
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	41467.422											
7.201763120D+03	-4.175173020D+02	1.162930670D+01	1.295022278D-02	4.181004880D-04	-1.177260708D-06	1.126699685D-09	0.000000000D+00	-1.901939953D+04	-1.919045392D+01	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	41467.422	
-2.165758025D+05	4.086179370D+03	-2.792987458D+01	2.170548191D-01	-2.566465152D-04	1.563562340D-07	-3.882382230D-11	0.000000000D+00	-3.883008530D+04	1.797118254D+02	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	41467.422	
2.217029481D+06	-2.140006822D+04	7.649766620D+01	-4.151625760D-03	7.956620510D-07	-8.168963200D-11	3.470558600D-15	0.000000000D+00	9.136192620D+04	-4.309930080D+02													

## C12H4CL4O2 2,3,7,8 Tetra-Chloro-Dibenzo Dioxin Dorofeeva JPC 107 (2003), 2848

3	T	8/03	C	12.00H	4.000	2.00CL	4.00	0.00	0	321.9697600	-136100.000											
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	41226.470											
5.018192140D+03	-2.604811129D+02	7.642708890D+00	5.697596850D-02	1.462718227D-04	-2.872262591D-07	-5.590492780D-11	0.000000000D+00	-2.038531439D+04	-3.554091920D+00	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	41226.470	
-2.008414735D+05	3.820725250D+03	-2.662470206D+01	2.140791652D-01	-2.530147130D-04	1.540785037D-07	-3.824570080D-11	0.000000000D+00	-3.843960900D+04	1.712195276D+02	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	41226.470	
2.214482640D+06	-2.140256552D+04	7.653007450D+01	-4.171810000D-03	8.011489410D-07	-8.239975140D-11	3.506187720D-15	0.000000000D+00	9.046784320D+04	-4.321963430D+02													

## C12H6Cl2O 1,6-DiChloroDibenzoFuran Zhu &amp; Bozzelli JPCRD 32 (2003), 1713-1735.

3	T	03/04	C	12.00H	6.00CL	2.000	1.00	0.00	0	237.0808400	5200.000											
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	31522.166											
3.272938200D+03	-2.195308573D+02	8.343914690D+00	-1.767911848D-04	3.329314840D-04	-6.511226440D-07	4.059816640D-10	0.000000000D+00	-2.438051701D+03	-5.220941220D+00	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	31522.166	
-3.098903226D+05	6.345115490D+03	-4.805278320D+01	2.545562532D-01	-3.058977547D-04	1.909292059D-07	-4.858487330D-11	0.000000000D+00	-3.120495291D+04	2.822616845D+02	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	31522.166	
3.934546960D+06	-2.707726786D+04	7.613681930D+01	-4.806967500D-03	8.813460050D-07	-8.674702740D-11	3.543103100D-15	0.000000000D+00	1.451817420D+05	-4.494113120D+02													

## C12H6Cl2O2 1,6-DiChloroDibenzoDioxin Zhu &amp; Bozzelli JPCRD 32 (2003), 1713-1735.

3	T	02/04	C	12.00H	6.00CL	2.000	2.00	0.00	0	253.0802400	-89300.000											
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	34529.122											
3.195646640D+03	-1.774203395D+02	7.506600510D+00	1.268887651D-02	3.369871740D-04	-7.322623420D-07	4.792658890D-10	0.000000000D+00	-1.427908506D+04	-1.100944654D+00	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	34529.122	
-2.859118702D+05	5.789930370D+03	-4.381531280D+01	2.511933854D-01	-3.004251604D-04	1.866000114D-07	-4.727132510D-11	0.000000000D+00	-4.048132840D+04	2.598494097D+02	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	34529.122	
3.932355850D+06	-2.747207937D+04	7.942876700D+01	-4.925281540D-03	9.080407570D-07	-8.987706740D-11	3.691279550D-15	0.000000000D+00	1.350910848D+05	-4.667801340D+02													

Table 5 (continued)

C12H8O p-dibenzo-dioxine hf298 Dorofeeva JPC 107 (2003), 2848.

```

3 T 8/03 C 12.00H 8.000 2.00 0.00 0.00 0 184.1907200 -50100.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 28336.217
-4.066160210D+02 2.818490566D+01 3.521621740D+00 1.872633784D-02 2.551919316D-04
-4.695209430D-07 2.952742473D-10 0.000000000D+00 -9.531884880D+03 1.438685890D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 28336.217
-3.765034490D+05 7.744986190D+03 -6.002703070D+01 2.856349785D-01 -3.432350790D-04
2.159491388D-07 -5.556420130D-11 0.000000000D+00 -4.358280260D+04 3.418698110D+02
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 28336.217
5.215014850D+06 -3.301658160D+04 8.313860450D+01 -6.283026000D-03 1.187366183D-06
-1.201183666D-10 5.029310500D-15 0.000000000D+00 1.744690042D+05 -5.072116100D+02

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C12H26 N-DODECANE TRC 10/1975

```

2 T 5/99 C 12.00H 26.00 0.00 0.00 0.00 0 170.3348400 -290871.680
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 56023.760
-1.583387502D+07 2.318455011D+05 -1.301084838D+03 3.729278890D+00 -5.271624900D-03
3.786419430D-06 -1.083032706D-09 0.000000000D+00 -1.147286089D+06 7.267799460D+03
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 56023.760
-3.430560260D+06 -1.980348190D+04 9.213423780D+01 9.023954470D-03 -2.219973580D-06
2.770463188D-10 -1.372073196D-14 0.000000000D+00 4.381869880D+04 -5.248191040D+02

```

C14H6N6O12 trans-HexaNitroStilbene (HNS) HF298=238.4 kJ Maranz and Amertrout

```

3 A 8/05 C 14.00H 6.00N 6.00O 12.00 0.00 0 450.2306800 238400.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 71248.066
7.428609660D+03 -6.594848450D+02 1.921105028D+01 9.536736120D-02 -6.835355700D-05
9.280239120D-07 -1.921120039D-09 0.000000000D+00 2.214827691D+04 -4.844072700D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 71248.066
-6.182717800D+05 1.129345362D+04 -7.153799300D+01 4.211113360D-01 -4.740413700D-04
2.694612316D-07 -6.232022250D-11 0.000000000D+00 -3.144946127D+04 4.282975510D+02
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 71248.066
-1.323373898D+06 -2.688631881D+04 1.306897335D+02 -1.141603560D-02 2.565264385D-06
-2.947326071D-10 1.362698952D-14 0.000000000D+00 1.417212635D+05 -7.386151710D+02

```

C14H12 t-Stilbene C6H5-CH=CH-C6H5 HF298=223.3 kJ Maranz & Amertrout JCEng.Data

```

3 A 8/05 C 14.00H 12.00 0.00 0.00 0.00 0 180.2450800 223300.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 32900.821
4.103776720D+03 -3.103340588D+02 1.195018715D+01 -2.582149656D-02 3.195307680D-04
-1.008703099D-07 -5.717031610D-10 0.000000000D+00 2.387350493D+04 -1.970133447D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 32900.821
-3.371309790D+05 7.858837290D+03 -6.398836650D+01 3.148698866D-01 -3.830914180D-04
2.465587391D-07 -6.498802700D-11 0.000000000D+00 -1.103939044D+04 3.640106490D+02
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 32900.821
7.821067180D+06 -4.325577560D+04 9.914582860D+01 -8.224047220D-03 1.544005746D-06
-1.549957767D-10 6.437603700D-15 0.000000000D+00 2.690865496D+05 -6.131504450D+02

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C14H14 BiBenzyl C6H5-CH2CH2-C6H5 Burcat G3B3 calc

```

3 T 5/04 C 14.00H 14.00 0.00 0.00 0.00 0 182.2609600 135600.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 33684.348
-3.600227110D+03 1.744828384D+02 3.278407950D+00 5.866950290D-02 -1.175658044D-04
9.085341360D-07 -1.295000216D-09 0.000000000D+00 1.158470911D+04 2.159424226D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 33684.348
-5.392574680D+05 1.153216199D+04 -8.786169510D+01 3.827970090D-01 -4.729311040D-04
3.073218182D-07 -8.128295630D-11 0.000000000D+00 -3.841424750D+04 4.979756640D+02
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 33684.348
1.002163109D+07 -4.985862230D+04 1.056178959D+02 -8.003196680D-03 1.380728960D-06
-1.273179935D-10 4.857265380D-15 0.000000000D+00 3.006404442D+05 -6.588389610D+02

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Table 5 (continued)

C16H33 Hexadecyl secondary radical Bozzelli-THERM Rough Approximation											
2	S05/01	C	16.00H	33.00	0.00	0.00	0.00	0.00	0	225.4332200	-181669.280
	298.150	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.000
1.827083553D+06-1.950059770D+04 8.939625110D+01-5.605686890D-02 2.493302389D-04											
-2.503181615D-07 8.488360950D-11 0.000000000D+00 6.947478810D+04-4.582974610D+02											
	1000.000	5000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.000
6.443724500D+07-2.144224469D+05 3.136586982D+02-8.394163950D-02 2.284531144D-05											
-3.194913360D-09 1.793002595D-13 0.000000000D+00 1.298892346D+06-2.091135437D+03											
C16H34 Hexadecane-n NIST 94 Thergas Bozzelli-THERM Rough Approximation											
2	S	5/01	C	16.00H	34.00	0.00	0.00	0.00	0	226.4411600	-374509.840
	298.150	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.000
4.728669390D+06-5.460779630D+04 2.518403493D+02-4.252167510D-01 6.993759680D-04											
-5.256682290D-07 1.512889624D-10 0.000000000D+00 2.205521194D+05-1.397478825D+03											
	1000.000	5000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.000
6.222594360D+07-2.080574798D+05 3.060130671D+02-7.633945790D-02 2.061691656D-05											
-2.879523588D-09 1.617069880D-13 0.000000000D+00 1.235212182D+06-2.042370604D+03											
C20H10 CORANNULENE Burcat AM1 HF298=473.7+/-7.3 kj											
3	A	5/05	C	20.00H	10.00	0.00	0.00	0.00	0	250.2934000	463700.000
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.000
3.179486920D+03-2.158297189D+02 8.784901350D+00-4.796946480D-02 6.877701990D-04											
-1.374806852D-06 9.237781340D-10 0.000000000D+00 5.272175860D+04-7.058936060D+00											
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.000
-5.155206520D+05 1.013334577D+04-7.801382980D+01 3.504981710D-01-3.845332990D-04											
2.230270620D-07-5.353522100D-11 0.000000000D+00 6.968325670D+03 4.359729920D+02											
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.000
8.326299200D+06-5.092561730D+04 1.179195096D+02-9.994960990D-03 1.925679492D-06											
-1.986811592D-10 8.479135240D-15 0.000000000D+00 3.381817830D+05-7.458383220D+02											
C20H12 Perylene Melius BAC/MP2 calc HF298=47.01+/-4.89 kcal											
3	T03/05	C	20.00H	12.00	0.00	0.00	0.00	0.00	0	252.3092800	205057.840
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.000
4.331323690D+03-2.878440529D+02 1.154430714D+01-6.295360980D-02 9.096541600D-04											
-2.343611982D-06 2.635934396D-09 0.000000000D+00 2.104955100D+04-1.560054503D+01											
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.000
-5.291240510D+05 1.155367692D+04-9.469708040D+01 4.436874760D-01-5.434847650D-04											
3.476594070D-07-9.073074930D-11 0.000000000D+00-3.026937115D+04 5.214879600D+02											
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.000
7.372902570D+06-4.831790410D+04 1.220333427D+02-9.196565800D-03 1.734820837D-06											
-1.750640993D-10 7.308950700D-15 0.000000000D+00 2.879936273D+05-7.580187740D+02											
C24CL12 PerChloroCORONENE PM3 HF298=146.6 kJ ESTIMATED											
3	T	8/03	C	24.00CL	12.00	0.00	0.00	0.00	0	713.6892000	146600.000
	50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.000
-2.931324989D+04 2.248326000D+03-5.962766600D+01 1.042239627D+00-5.363632480D-03											
1.634035565D-05-2.067263912D-08 0.000000000D+00 9.247436940D+02 2.675464885D+02											
	200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.000
-1.087486467D+05 6.433080850D+02 7.871071130D+00 2.048673786D-01-1.886480271D-04											
8.183111970D-08-1.294838999D-11 0.000000000D+00 3.660389610D+03-3.432487740D-02											
	1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.000
-3.510192490D+05-2.445877018D+04 1.241632401D+02-7.288682490D-03 1.621652143D-06											
-1.874692738D-10 8.760888230D-15 0.000000000D+00 1.210929848D+05-6.874539190D+02											

Table 5 (continued)

C24H12 CORONENE AM1 HF298=307.5+/-10 kJ Chickos et al J Chem Thermo 34, (2002)  
 3 T 8/03 C 24.00H 12.00 0.00 0.00 0.00 0 300.3520800 307500.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 38330.783  
 -6.954094190D+02-2.833972449D+01 6.016401240D+00-1.049987188D-02 6.323878080D-04  
 -1.328586862D-06 9.663161370D-10 0.000000000D+00 3.239197340D+04 4.954457850D+00  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 38330.783  
 -6.172987910D+05 1.183957629D+04-8.904941200D+01 4.035587430D-01-4.334074440D-04  
 2.464788196D-07-5.813426080D-11 0.000000000D+00-2.056137947D+04 4.949891320D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 38330.783  
 1.032704675D+07-6.219746880D+04 1.427143168D+02-1.232405258D-02 2.385475016D-06  
 -2.471841636D-10 1.059037873D-14 0.000000000D+00 3.827786490D+05-9.088507370D+02

C70 FULLERENE, FOOTBALLENE HF298=2652+/-34 kJ Kolesov et al J Chem Thermo 2003  
 3 T 1/03 C 70.00 0.00 0.00 0.00 0.00 0 840.7490000 2652000.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 65411.012  
 -2.523873455D+03 3.762648660D+01 1.013164685D+01-2.536314210D-01 3.255047920D-03  
 -8.052923480D-06 7.066304250D-09 0.000000000D+00 3.107852356D+05 1.318890603D+00  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 65411.012  
 -1.369565189D+06 2.748888688D+04-2.361616009D+02 1.064531120D+00-1.217396106D-03  
 7.030871040D-07-1.648539942D-10 0.000000000D+00 1.902868453D+05 1.231786442D+03  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 65411.012  
 -6.212767350D+06-5.321113830D+04 2.473713773D+02-1.571900800D-02 3.478985130D-06  
 -4.002268180D-10 1.862269589D-14 0.000000000D+00 5.354307000D+05-1.528372462D+03

CrCl HF298=129.9+/-2.7 kJ REF=Ebbinghaus C&F 101, (1995), 311-338  
 2 A11/04 CR 1.00CL 1.00 0.00 0.00 0.00 0 87.4488000 129900.000  
 298.150 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9389.000  
 -1.563944072D+06 1.703092989D+04-7.118120800D+01 1.728973461D-01-2.148883444D-04  
 1.381417460D-07-3.597399784D-11 0.000000000D+00-7.147712880D+04 4.407821460D+02  
 1000.000 3000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9389.000  
 -3.226484010D+05 1.707239509D+01 5.523661370D+00-1.077335054D-03 3.328900720D-07  
 -1.235314024D-11 1.240433739D-15 0.000000000D+00 1.317726761D+04-2.047909245D+00

CrO2Cl2 HF298=-519.2+/-4.2 kJ Ebbinghaus C&F 101, (1995), 311-338  
 2 A12/04 CR 1.00CL 2.00O 2.00 0.00 0.00 0 154.9003000 -519200.000  
 298.150 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18066.000  
 -1.976046731D+05 8.276494510D+02 6.821971410D+00 1.193144208D-02-1.062131235D-05  
 4.895279740D-09-1.111690159D-12 0.000000000D+00-7.030302970D+04-6.975667050D-01  
 1000.000 5000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18066.000  
 -1.083752828D+07 2.870715956D+04-1.671515199D+01 1.448861640D-02-3.485190010D-06  
 4.057870070D-10-1.795718506D-14 0.000000000D+00-2.527443311D+05 1.795484989D+02

CrCl6 HF298=345.3+/-50.? kJ REF=Ebbinghaus C&F 101, (1995), 311-338  
 2 A12/04 CR 1.00CL 6.00 0.00 0.00 0.00 0 264.7123000 -345300.000  
 298.150 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 30878.000  
 -2.230202809D+05 9.629667860D+02 1.440836593D+01 1.007195775D-02-1.166582330D-05  
 7.032569410D-09-1.761731990D-12 0.000000000D+00-5.241793810D+04-3.275404360D+01  
 1000.000 5000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 30878.000  
 -2.896015485D+05 3.112387481D+02 1.867350220D+01 1.721495643D-04-4.858506300D-08  
 6.980890950D-12-4.004861497D-16 0.000000000D+00-4.976605570D+04-5.690886080D+01



Table 5 (continued)

## DS IUPAC Task Group for Selected Radicals

3 T02/03 S 1.00D 1.00 0.00 0.00 0.00 0 34.0801020 140139.744  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8666.295  
 -1.539559428D+02 1.050128590D+01 3.216567870D+00 3.918507030D-03-2.893874423D-05  
 1.096305041D-07-1.660683730D-10 0.000000000D+00 1.577635327D+04 5.016118310D+00  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8666.295  
 -5.716458130D+03 9.285021760D+00 4.114928250D+00-4.473639710D-03 1.134507130D-05  
 -9.971466360D-09 3.104121310D-12 0.000000000D+00 1.567274601D+04 1.304729962D+00  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8666.295  
 2.225673004D+05-1.265344575D+03 5.378395410D+00-2.779601670D-04 7.370836460D-08  
 -9.359635200D-12 5.766725640D-16 0.000000000D+00 2.323185538D+04-9.688293840D+00

## GeCL2 singlet Wang &amp; Zhang JPC A 108, (2004), 10346-353. HF298=-166.9 kJ

3 A 1/05 GE 1.00CL 2.00 0.00 0.00 0.00 0 143.5154000 -166900.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13307.060  
 -6.443369600D+02 2.211654282D+01 3.746301170D+00-1.543355479D-03 2.085569256D-04  
 -1.077054775D-06 1.717158313D-09 0.000000000D+00-2.176290571D+04 1.171865866D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13307.060  
 2.130446197D+04-6.210828380D+02 9.375389520D+00-5.063281510D-03 6.131634470D-06  
 -3.931736140D-09 1.034015320D-12 0.000000000D+00-1.908032290D+04-1.847039550D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13307.060  
 -3.472463640D+04-4.594880270D+01 7.042321650D+00-1.969935890D-05 4.873417180D-09  
 -6.091993000D-13 3.020479735D-17 0.000000000D+00-2.203169140D+04-4.839095120D+00

## GeCL2 triplet Wang &amp; Zhang JPC A 108, (2004), 10346-353. HF298=102.3 kJ

3 A 1/05 GE 1.00CL 2.00 0.00 0.00 0.00 0 143.5154000 102300.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13592.644  
 -2.190094319D+03 9.527521750D+01 2.712904426D+00 9.524835510D-03 1.453827797D-04  
 -8.988119950D-07 1.519257976D-09 0.000000000D+00 1.030745811D+04 1.755031492D+01  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13592.644  
 1.875234626D+04-5.607550430D+02 9.156019680D+00-4.614089430D-03 5.604687840D-06  
 -3.602255190D-09 9.490875670D-13 0.000000000D+00 1.299401174D+04-1.576228091D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13592.644  
 -3.109360300D+04-4.222251260D+01 7.038955820D+00-1.815127685D-05 4.493440810D-09  
 -5.619597030D-13 2.787188277D-17 0.000000000D+00 1.033748484D+04-3.403652730D+00

## GeCL3 Wang &amp; Zhang JPC A 108, (2004), 10346-353.

3 A 1/05 GE 1.00CL 3.00 0.00 0.00 0.00 0 178.9681000 -234400.000  
 50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17700.309  
 1.993164289D+03-1.791040134D+02 8.420519160D+00-3.183078450D-02 4.612458820D-04  
 -2.009379050D-06 3.006547255D-09 0.000000000D+00-2.976518473D+04-7.022555240D+00  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17700.309  
 3.109623418D+04-9.664892410D+02 1.368146505D+01-7.823656330D-03 9.453058090D-06  
 -6.051102000D-09 1.589285443D-12 0.000000000D+00-2.638441730D+04-3.837564780D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17700.309  
 -5.704616110D+04-7.063336340D+01 1.006496933D+01-3.021651190D-05 7.471310620D-09  
 -9.336109770D-13 4.627758550D-17 0.000000000D+00-3.098730240D+04-1.723205513D+01

Table 5 (continued)

GeCl4 Wang & Zhang JPC A 108, (2004), 10346-353. HF298=500.9+/-5 kJ														
3	A	1/05	GE	1.00CL	4.00	0.00	0.00	0.00	0	214.4208000	-500400.000			
				50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
				1.003597109D+04	-6.660737230D+02	1.864448909D+01	-1.232065231D-01	1.011301916D-03						
				-3.576397210D-06	4.737079300D-09	0.000000000D+00	-6.052075170D+04	-5.239369310D+01						
				200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
				6.907038690D+04	-1.714292277D+03	1.919338745D+01	-1.262863103D-02	1.477364880D-05						
				-9.220288530D-09	2.373619557D-12	0.000000000D+00	-5.545956340D+04	-6.960869600D+01						
				1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
				-1.086322169D+05	-1.059185691D+02	1.309539027D+01	-4.379337450D-05	1.073602083D-08						
				-1.333605550D-12	6.581999430D-17	0.000000000D+00	-6.385099670D+04	-3.364867920D+01						
GeH3Cl Wang & Zhang JPC A 108, (2004), 10346-353.														
3	A	1/05	GE	1.00H	3.00CL	1.00	0.00	0.00	0	111.0865200	57700.000			
				50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
				2.184787150D+03	-1.620960793D+02	8.768885430D+00	-6.899433140D-02	4.822067850D-04						
				-1.317463960D-06	1.416678151D-09	0.000000000D+00	6.004478980D+03	-1.033500031D+01						
				200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
				1.622887659D+05	-2.253499701D+03	1.320144303D+01	-6.076545300D-03	1.320333827D-05						
				-9.829638930D-09	2.532605529D-12	0.000000000D+00	1.655917921D+04	-4.840067050D+01						
				1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
				7.678812180D+05	-5.382100110D+03	1.667650224D+01	-1.384488635D-03	2.933705728D-07						
				-3.265490270D-11	1.481260411D-15	0.000000000D+00	3.531559150D+04	-7.610128640D+01						
GeH4 Wang & Zhang JPC A 108, (2004), 10346-353.														
3	A	1/05	GE	1.00H	4.00	0.00	0.00	0.00	0	76.6417600	90300.000			
				50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
				-3.156788902D+02	3.403778100D+01	2.647293383D+00	2.592076116D-02	-2.519498956D-04						
				1.138926426D-06	-1.639566166D-09	0.000000000D+00	9.472510740D+03	7.812066350D+00						
				200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
				1.049104471D+05	-1.052376243D+03	5.458520110D+00	8.228255340D-03	-1.204064419D-06						
				-1.741095174D-09	5.577895180D-13	0.000000000D+00	1.522905596D+04	-1.029013357D+01						
				1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
				1.060382381D+06	-7.057102240D+03	1.781872709D+01	-1.813156135D-03	3.838377570D-07						
				-4.268369810D-11	1.934429875D-15	0.000000000D+00	4.948147180D+04	-9.237812160D+01						
HNO3 NITRIC ACID DOROFEEVA et al JPCRD 32 (2003), 879. HF298=-134.3 kJ														
3	T	8/03	H	1.00N	1.00O	3.00	0.00	0.00	0	63.0128800	-134300.000			
				50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
				3.896390790D+03	-2.672567061D+02	1.124681780D+01	-9.695005260D-02	6.376184300D-04						
				-1.744244584D-06	1.858474449D-09	0.000000000D+00	-1.672129609D+04	-2.055112260D+01						
				200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
				1.357944536D+04	6.147355410D+01	-3.012491167D-01	2.970185124D-02	-3.189407280D-05						
				1.726915160D-08	-3.807611860D-12	0.000000000D+00	-1.743807552D+04	2.650630251D+01						
				1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
				-9.937687770D+04	-2.720152239D+03	1.449411507D+01	-7.836990890D-04	1.706976852D-07						
				-1.935111600D-11	8.886380460D-16	0.000000000D+00	-5.016661870D+03	-5.927068230D+01						
OH HYDROXYL RADICAL IUPAC Task Group 2003 B. Ruscic et al JPCRD														
2	IU3/03	O	1.00H	1.00	0.00	0.00	0.00	0.00	0	17.0073400	37300.000			
				200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
				-2.511760119D+03	1.002006472D+02	3.011762224D+00	1.634983432D-03	-3.308462450D-06						
				3.424029200D-09	-1.169850479D-12	0.000000000D+00	2.959215595D+03	4.892238240D+00						
				1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
				1.015060999D+06	-2.503983925D+03	5.110686670D+00	1.333625308D-04	-8.357298310D-08						
				2.015935847D-11	-1.561827375D-15	0.000000000D+00	2.016009065D+04	-1.097028908D+01						

Table 5 (continued)

## HS IUPAC Task Group for Selected Radicals

```

3 IU2/03 S 1.00H 1.00 0.00 0.00 0.00 0 33.0739400 141870.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9274.323
-1.738481592D+03 9.446963120D+01 1.904579777D+00 3.941303750D-03 1.175452952D-04
-7.414244380D-07 1.275123362D-09 0.000000000D+00 1.560965889D+04 1.066095056D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9274.323
4.344401220D+03-3.345731060D+02 7.336632610D+00-1.245991513D-02 1.866574730D-05
-1.247847446D-08 3.215091460D-12 0.000000000D+00 1.720839423D+04-1.636622481D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9274.323
7.665873370D+05-2.386001905D+03 5.897909410D+00-4.103508210D-04 9.006711800D-08
-9.863233120D-12 5.051707900D-16 0.000000000D+00 3.127300418D+04-1.421246575D+01

```

## HS2 Hydrothiosulfeno radical IUPAC Datasheet April 2003

```

3 T 3/03 H 1.00S 2.00 0.00 0.00 0.00 0 65.1399400 103420.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10493.906
1.345569979D+03-8.995746970D+01 6.332221980D+00-2.909648212D-02 1.736859452D-04
-4.175198450D-07 3.925801950D-10 0.000000000D+00 1.146826211D+04-1.868847993D+00
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10493.906
5.831001330D+04-7.370499410D+02 6.411603770D+00 1.057542173D-03-2.071663832D-06
2.648588061D-09-1.093855933D-12 0.000000000D+00 1.488844348D+04-8.291476950D+00
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10493.906
4.824719310D+05-2.323891830D+03 8.387332580D+00-3.625956180D-04 9.886131820D-08
-9.096416320D-12 3.923358010D-16 0.000000000D+00 2.473052400D+04-2.236688103D+01

```

## H2O2 Hydrogen Peroxide DOROFEEVA JPCRD 32 (2003), 879. HF298=-135.88/-0.2 kJ

```

3 T 8/03 H 2.00O 2.00 0.00 0.00 0.00 0 34.0146800 -135880.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11162.000
-2.948812406D+03 2.106424628D+02-1.663695094D+00 7.089191870D-02-4.018655710D-04
1.182472127D-06-1.369197008D-09 0.000000000D+00-1.835181920D+04 2.734727038D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11162.000
-9.147349230D+04 1.541838551D+03-5.830038900D+00 3.228622620D-02-3.869929140D-05
2.464650495D-08-6.339102100D-12 0.000000000D+00-2.483469541D+04 5.797150880D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11162.000
1.505950346D+06-5.241735310D+03 1.138415930D+01-1.333635318D-04-5.533679760D-09
5.604149320D-12-4.174609100D-16 0.000000000D+00 1.461216226D+04-4.722314830D+01

```

## H2SO4 Sulfuric Acid DOROFEEVA et al JPCRD 32 (2003), 879. HF298=-732.7+/-2.0 kJ

```

3 T 8/03 H 2.00S 1.00O 4.00 0.00 0.00 0 98.0794800 -732700.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18391.000
-1.100629097D+04 6.677243560D+02-9.943680310D+00 9.040051790D-02 4.092587870D-04
-3.690315340D-06 7.017483530D-09 0.000000000D+00-9.259383190D+04 7.007470540D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18391.000
-2.426702872D+05 3.135846707D+03-1.087285248D+01 6.764100880D-02-8.529344360D-05
5.533143610D-08-1.440574325D-11 0.000000000D+00-1.059174346D+05 9.170987700D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18391.000
1.505546796D+06-6.228600290D+03 2.044421293D+01-4.584346860D-04 2.892017368D-08
2.218984815D-12-2.819213472D-16 0.000000000D+00-5.423882900D+04-9.283111670D+01

```

Table 5 (continued)

NHD Amidogen-D Hf:est. from NH <sub>2</sub> ,H,&D data. Burcat G3B3 calc HF298=178.165 kJ										
3 A 1/05 N	1.00H	1.00D	1.00	0.00	0.00	0	17.0287820	185158.760		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.993418090D+01	3.417799340D+00	3.916046030D+00	1.017433770D-03	-6.156388660D-06						
1.588714872D-08	-7.586315070D-12	0.000000000D+00	2.106313014D+04	2.270520198D+00						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.083051790D+04	3.070085577D+02	2.482160531D+00	2.329635542D-03	1.323745060D-06						
-1.474807279D-09	3.488389320D-13	0.000000000D+00	1.959773000D+04	1.075697860D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.839178663D+06	-6.541639790D+03	1.166075210D+01	-2.216506017D-03	6.344897290D-07						
-8.475754160D-11	4.233668440D-15	0.000000000D+00	6.181216560D+04	-5.405155890D+01						
ND2 Amidogen-D2 Hf:est. from NH <sub>2</sub> ,H,&D data. Jacox,1998 p133. HF298=181.937 kJ										
3 g 4/01 N	1.00D	2.00	0.00	0.00	0.00	0	18.0349440	181936.570		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.795829930D+01	-3.698834590D+00	4.101646560D+00	-1.496950578D-03	1.301372256D-05						
-6.557967160D-08	1.511998205D-10	0.000000000D+00	2.069347884D+04	1.355220369D+00						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
8.579595290D+03	-5.586479350D+01	3.957972620D+00	-3.403516880D-05	3.943531620D-06						
-2.725271565D-09	4.824243360D-13	0.000000000D+00	2.102064664D+04	1.743637134D+00						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.640698700D+06	-6.601936980D+03	1.285462910D+01	-3.124045000D-03	9.271249180D-07						
-1.254362422D-10	6.302121810D-15	0.000000000D+00	6.097051340D+04	-6.159166930D+01						
ND3 Hf:est. from NH <sub>3</sub> ,H,&D data. Active Tables HF298=-54.583 kJ.										
2 g 4/01 N	1.00D	3.00	0.00	0.00	0.00	0	20.0490460	-54500.706		
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.045120370D+04	1.610166943D+02	8.574963230D-01	1.319688794D-02	-1.153090144D-05						
7.142495560D-09	-2.109194351D-12	0.000000000D+00	-8.190712600D+03	1.675921598D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.599516958D+06	-1.013420124D+04	1.798028169D+01	-3.582609800D-03	1.009922000D-06						
-1.537638609D-10	9.106175650D-15	0.000000000D+00	5.400229290D+04	-9.810988270D+01						
NH2 AMIDOGEN RADICAL IUPAC Task Group for Selected Radicals B. Ruscic et al										
2 IU3/03 N	1.00H	2.00	0.00	0.00	0.00	0	16.0225800	186200.000		
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.790344587D+04	4.257719860D+02	1.652609880D+00	5.526463870D-03	-5.221624350D-06						
4.112340910D-09	-1.338074002D-12	0.000000000D+00	1.917549990D+04	1.384308120D+01						
1000.000	3000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.056033680D+06	6.015369960D+03	-9.565892000D+00	1.524740935D-02	-6.986589490D-06						
1.626762810D-09	-1.514421193D-13	0.000000000D+00	-1.313378631D+04	8.810668480D+01						
ND2H Burcat G3B3 calc. HF298=-48.697 kJ										
3 A12/04 N	1.00D	2.00H	1.00	0.00	0.00	0	19.0428840	-52748.069		
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.675051301D+02	1.912189409D+01	3.453371740D+00	7.922547840D-03	-6.018665970D-05						
2.164430437D-07	-2.438122173D-10	0.000000000D+00	-7.616270260D+03	4.441096640D+00						
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.856971580D+04	8.950405450D+02	-2.011305094D+00	1.657256689D-02	-1.408934397D-05						
7.944224480D-09	-2.104119381D-12	0.000000000D+00	-1.163373730D+04	3.497786790D+01						
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.221289980D+06	-8.451971330D+03	1.456423783D+01	-1.400743752D-03	2.484261636D-07						
-2.368354311D-11	9.384194950D-16	0.000000000D+00	4.440581420D+04	-7.479987780D+01						

Table 5 (continued)

NH2D Burcat G3B3 calc

```

3 A12/04 N 1.00H 2.00D 1.00 0.00 0.00 0 18.0367220 -48696.635
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10018.070
-3.596897510D+02 2.456032332D+01 3.333047520D+00 9.157442470D-03-6.618807380D-05
2.317196007D-07-2.816644226D-10 0.000000000D+00-7.140678420D+03 4.531549450D+00
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10018.070
-6.498046530D+04 1.072265729D+03-2.475622837D+00 1.624376724D-02-1.322401021D-05
6.948773350D-09-1.663273766D-12 0.000000000D+00-1.206409971D+04 3.774933800D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10018.070
2.640864229D+06-9.102278180D+03 1.424052433D+01-1.084511410D-03 1.528003771D-07
-1.075585489D-11 2.755828878D-16 0.000000000D+00 4.982123210D+04-7.399950830D+01

```

NH3 Amonia RRHO G3B3 Calculations Burcat HF298=-45.567+/-0.03 kJ (Active Tables)

```

3 T12/04 H 3.00N 1.00 0.00 0.00 0.00 0 17.0305600 -45567.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9983.512
-3.969656020D+02 2.677465300D+01 3.282598830D+00 9.726799600D-03-6.982624560D-05
2.473738169D-07-3.241769680D-10 0.000000000D+00-6.767587620D+03 3.180647630D+00
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9983.512
-6.923097090D+04 1.082323341D+03-2.164172163D+00 1.457535955D-02-1.142793378D-05
5.828056060D-09-1.302402573D-12 0.000000000D+00-1.179178109D+04 3.483398130D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9983.512
3.068093467D+06-9.742221370D+03 1.389618631D+01-7.560524970D-04 5.377927410D-08
2.624956558D-12-4.106593360D-16 0.000000000D+00 5.509291850D+04-7.415605930D+01

```

N2D2,cis Hf:Use NASA data for N2H2,H,&amp;D. Chase,1998 p1044 6/77.

```

3 g 6/01 N 2.00D 2.00 0.00 0.00 0.00 0 32.0416840 202857.330
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10308.037
-2.399940286D+01 5.661644780D+00 3.701912170D+00 6.686652450D-03-7.208786370D-05
3.472000350D-07-4.863829910D-10 0.000000000D+00 2.314464021D+04 4.982392220D+00
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10308.037
-3.633597520D+04 8.446286860D+02-2.953508975D+00 2.293369706D-02-2.124650911D-05
1.110642386D-08-2.588542391D-12 0.000000000D+00 1.949200768D+04 4.042235700D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10308.037
8.688501880D+05-5.279214660D+03 1.353694086D+01-1.312935472D-03 2.752278757D-07
-3.038522963D-11 1.369584169D-15 0.000000000D+00 5.342437900D+04-6.261032940D+01

```

N2H3 Hydrazine radical ATcT A value HF298=220.58+/-1.34 kJ

```

3 T09/04 H 3.00N 2.00 0.00 0.00 0.00 0 31.0373000 220580.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10634.472
8.157102650D+02-4.932918440D+01 5.077126960D+00-9.344061150D-03 9.532433580D-06
2.411763653D-07-5.715122470D-10 0.000000000D+00 2.541687619D+04 7.273686190D-01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10634.472
-7.716894960D+04 1.486591345D+03-7.361159420D+00 3.908582880D-02-4.490416760D-05
2.830850914D-08-7.306539970D-12 0.000000000D+00 1.860242020D+04 6.507887110D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10634.472
2.741023776D+06-9.835142340D+03 1.711965196D+01-8.763115550D-04 8.397231870D-08
-1.067412578D-12-2.334067790D-16 0.000000000D+00 8.574872350D+04-8.886320100D+01

```

Table 5 (continued)

N3 Azide Radical HF298=453.54+/-3.5 kJ REF=Ruscic ATcT A

```

3 tpi89 N 3.00 0.00 0.00 0.00 0.00 0.00 0 42.0202200 453540.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9570.906
-1.372959871D+03 6.039838280D+01 3.316425290D+00 -1.240715437D-04 -3.153248619D-05
3.201640360D-07 -6.306278650D-10 0.000000000D+00 5.315495460D+04 7.968782060D+00
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9570.906
3.152079651D+04 -2.688627772D+02 3.155651604D+00 7.170607130D-03 -4.848774420D-06
1.360573627D-09 -7.844587670D-14 0.000000000D+00 5.496622430D+04 6.190791060D+00
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9570.906
2.682811514D+05 -2.405151025D+03 9.179447060D+00 -6.438433210D-04 1.384085209D-07
-1.558595317D-11 7.136659610D-16 0.000000000D+00 6.650918450D+04 -3.167823290D+01

```

N3H Azidic Acid HF298=291.713+/-0.65 kJ REF=Ruscic ATcT A.

```

3 g 4/99 N 3.00H 1.00 0.00 0.00 0.00 0.00 0 43.0281600 291713.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10947.183
2.602919261D+03 -1.839146088D+02 9.102623920D+00 -6.941018410D-02 4.669767910D-04
-1.366963819D-06 1.563364495D-09 0.000000000D+00 3.435376860D+04 -1.474289413D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10947.183
-6.848907990D+02 1.239410173D+02 1.445266741D+00 1.577468680D-02 -1.672882036D-05
1.017709930D-08 -2.637237240D-12 0.000000000D+00 3.337323610D+04 1.691755788D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10947.183
1.134067359D+06 -5.010576890D+03 1.269359027D+01 -7.979768110D-04 1.483515826D-07
-1.374547570D-11 5.413497620D-16 0.000000000D+00 6.340842140D+04 -5.447866890D+01

```

PH2 Phosphino Radical Burcat G3B3 calc HF298=135.47+/-8 kJ

```

3 A 5/05 P 1.00H 2.00 0.00 0.00 0.00 0.00 0 32.9896410 135474.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9969.346
1.844257498D+01 -1.331752200D+00 4.041097760D+00 -7.143785530D-04 7.485978430D-06
-4.427380030D-08 1.128189125D-10 0.000000000D+00 1.509882539D+04 2.611514683D+00
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9969.346
3.665434070D+03 -1.774304789D+01 4.043830630D+00 -1.415691707D-03 7.512214300D-06
-6.109729410D-09 1.599821477D-12 0.000000000D+00 1.520927473D+04 2.643020700D+00
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9969.346
1.175949763D+06 -4.844891530D+03 1.025668626D+01 -1.168701795D-03 2.127219563D-07
-1.574155835D-11 3.445818380D-16 0.000000000D+00 4.461953140D+04 -4.274357570D+01

```

PH3 Phosphine RRHO Burcat G3B3 calc HF298=11.79+/-8. kJ

```

3 A 6/05 P 1.00H 3.00 0.00 0.00 0.00 0.00 0 33.9975810 11786.000
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10136.622
-1.997631912D+02 1.437034650D+01 3.591816030D+00 5.731398880D-03 -3.993756510D-05
1.125487238D-07 -1.549261746D-11 0.000000000D+00 1.529073240D+02 3.992733270D+00
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10136.622
-2.496968335D+04 6.768677200D+02 -1.684504087D+00 1.766581039D-02 -1.461125828D-05
7.751844680D-09 -2.041550254D-12 0.000000000D+00 -2.690966759D+03 3.233188410D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10136.622
1.290688225D+06 -6.624214330D+03 1.436871146D+01 -1.599887211D-03 3.315817320D-07
-3.626095670D-11 1.621585251D-15 0.000000000D+00 3.919585790D+04 -7.132353360D+01

```

Table 5 (continued)

SiF2 Vibrations from Jacox HF298 from Melius JPC 94 (1990) 5123

3	T	8/03	SI	1.00F	2.00	0.00	0.00	0.00	0.00	0	66.0823064	-627014.240
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11228.401	
-2.612868424D+03	1.699432257D+02	-9.855340240D-02	4.392885770D-02	-2.047783816D-04								
5.511750460D-07	-5.656069360D-10	0.000000000D+00	-7.732183060D+04	2.425733482D+01								
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11228.401	
3.027526741D+04	-2.596159623D+02	3.279639420D+00	1.392582327D-02	-2.141935170D-05								
1.565148774D-08	-4.460762910D-12	0.000000000D+00	-7.526768830D+04	8.158933520D+00								
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11228.401	
-2.409073517D+05	1.290156232D+01	6.950763580D+00	3.335750310D-05	-9.932589800D-09								
1.386301516D-12	-7.390044840D-17	0.000000000D+00	-7.826233200D+04	-9.774083140D+00								

SiF3 Vibrations from Jacox HF298 from Melius JPC 94 (1990), 5123.

3	T	8/03	SI	1.00F	3.00	0.00	0.00	0.00	0.00	0	85.0807096	-993365.280
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13398.025	
-6.853434760D+03	4.693277650D+02	-7.990155790D+00	1.355760348D-01	-6.353811430D-04								
1.588222943D-06	-1.548648305D-09	0.000000000D+00	-1.226038521D+05	5.789460340D+01								
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13398.025	
1.473940151D+04	-7.041861360D+01	2.209760900D+00	2.604532175D-02	-3.816278440D-05								
2.705289324D-08	-7.546451810D-12	0.000000000D+00	-1.205522542D+05	1.493184105D+01								
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13398.025	
-3.897167530D+05	-8.295019110D+01	1.000400947D+01	1.831099544D-05	-7.771324540D-09								
1.250173076D-12	-7.192685720D-17	0.000000000D+00	-1.231155913D+05	-2.504355673D+01								

SiF4 Vibrations from Shimanouchi HF298 from Melius JPC 94 (1990), 5123.

3	T	8/03	SI	1.00F	4.00	0.00	0.00	0.00	0.00	0	104.0791128	-1614982.160
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15324.718	
-8.927449120D+03	5.921542850D+02	-1.044006878D+01	1.489156114D-01	-5.297925280D-04								
8.525365910D-07	-2.498093599D-10	0.000000000D+00	-1.980178046D+05	6.757360640D+01								
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15324.718	
-1.208770804D+04	2.292267512D+02	6.907436770D-01	3.821665930D-02	-5.369763900D-05								
3.694244180D-08	-1.007202400D-11	0.000000000D+00	-1.970815760D+05	2.144180397D+01								
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15324.718	
-5.129981080D+05	-3.256768930D+02	1.317944442D+01	-5.005634870D-05	7.020865220D-09								
-4.173960100D-13	4.302095550D-18	0.000000000D+00	-1.977849349D+05	-4.442177830D+01								

SiHF3 Vibrations from Shimanouchi HF298 from Melius JPC 94 (1990), 5123.

3	T	8/03	SI	1.00F	3.00H	1.00	0.00	0.00	0.00	0	86.0886496	-1207669.760
50.000	200.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13544.634	
-6.494284900D+03	4.334084980D+02	-6.729120470D+00	1.167798744D-01	-5.250563680D-04								
1.310904467D-06	-1.214630637D-09	0.000000000D+00	-1.482923422D+05	5.248965900D+01								
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13544.634	
4.568571630D+04	-2.684393830D+02	9.380593170D-01	3.598012520D-02	-5.081347560D-05								
3.598533650D-08	-1.016389772D-11	0.000000000D+00	-1.450620363D+05	1.860260743D+01								
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13544.634	
-9.223805920D+04	-2.174306276D+03	1.435362766D+01	-4.651489700D-04	9.034408770D-08								
-9.275145060D-12	3.907325120D-16	0.000000000D+00	-1.372297739D+05	-5.559318830D+01								

Table 5 (continued)

SnCL4 Stanumtetrachloride Allendorf & Melius JPC 109, (2005), 4939.

```

3 A 6/05 SN 1.00CL 4.00 0.00 0.00 0.00 0 260.5208000 -478649.600
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22339.906
4.052889830D+03-3.901594540D+02 1.476661908D+01-8.848303030D-02 8.948798460D-04
-3.538422030D-06 5.070000510D-09 0.000000000D+00-5.907895180D+04-3.362654360D+01
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22339.906
4.372851470D+04-1.322590485D+03 1.801333204D+01-1.061416211D-02 1.278773128D-05
-8.167383540D-09 2.141354311D-12 0.000000000D+00-5.488249130D+04-6.031366920D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22339.906
-7.848945480D+04-9.507538700D+01 1.308730527D+01-4.056363360D-05 1.002309004D-08
-1.251906142D-12 6.203440850D-17 0.000000000D+00-6.119889410D+04-3.149094085D+01

```

SnH3 ThreeHydrostanum Radical Allendorf & Melius JPC 109, (2005), 4939.

```

3 A 6/03 SN 1.00H 3.00 0.00 0.00 0.00 0 121.7338200 258152.800
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10926.377
1.995514639D+03-1.264989794D+02 7.016426500D+00-3.239068320D-02 1.343577214D-04
2.101594000D-08-5.741711250D-10 0.000000000D+00 3.015317094D+04-6.911369200D+00
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10926.377
6.792644600D+04-1.058993544D+03 8.963136900D+00-7.625674110D-03 2.233954118D-05
-2.074390583D-08 6.637184050D-12 0.000000000D+00 3.481708280D+04-2.389759685D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10926.377
4.231388230D+05-3.706116540D+03 1.274632622D+01-1.102792147D-03 2.458020973D-07
-2.847702570D-11 1.333668111D-15 0.000000000D+00 4.992623530D+04-5.322265240D+01

```

SnH4 Stanumtetrahydride Allendorf & Melius JPC 109, (2005), 4939.

```

3 A 6/05 SN 1.00H 4.00 0.00 0.00 0.00 0 122.7417600 162757.600
50.000 200.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11423.210
2.462714883D+03-1.486892416D+02 7.269170010D+00-2.952330300D-02 5.436032380D-05
5.558972660D-07-1.536187669D-09 0.000000000D+00 1.870256692D+04-9.917038380D+00
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11423.210
1.303548583D+05-1.849510009D+03 1.161873017D+01-8.056259590D-03 2.507659513D-05
-2.343676464D-08 7.470334540D-12 0.000000000D+00 2.726529239D+04-4.264814710D+01
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11423.210
5.250456390D+05-5.129447320D+03 1.675956489D+01-1.496587070D-03 3.312996710D-07
-3.817552330D-11 1.780217039D-15 0.000000000D+00 4.578881190D+04-8.136178310D+01

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Table 6. Enthalpy of formation,  $\Delta_f H_{298}$  and  $\Delta_f H_0$ , heat capacity and entropy at 298 K, and  $H_{298}-H_0$  from the original calculations. *September 2005.*

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
Air (standard mixture)	28.96518	-0.126	-0.125		29.104	198.824	8.649	†
AL(cr) REFERENCE ELEMENT	26.98154	0	0		24.2	28.3	4.540	*‡
AL	26.98154	329.7		±4.2	21.391	164.555	6.919	†
ALH	27.98948	259.4		±20	29.348	187.857		*†
ALO	42.98094	66.944		±8	30.874	218.385		*†
ALOH	43.98888	-179.92		±13	31.877	216.419		*†
ALO2	58.98034	-86.192		±32	49.893	251.834		*†
ALO2H	59.98828	-460.247		±63	50.197	254.389		*†
AL2O	69.96248	-145.186		±17	52.035	252.336		*†
AL2O2	85.96188	-394.554		±32	67.192	280.996		*†
AL2O3(S)	101.96128	-1675.709			79.075	50.972		*†
AL2O3(G)	101.96128	-546.891	-544.39		86.990	316.662		†
AR REFERENCE ELEMENT	39.948	0	0		20.786	154.847	6.197	*‡
Ar+	39.94745	1526.778	1520.6	±0.001	20.984	166.406	6.206	†
B	10.811	560		±12	20.797	153.438		
B(S) REFERENCE ELEMENT	10.81	0.001			11.521	5.899		*‡
BCL	46.2637	141.417			31.675	213.246		*
BCLF	65.2621	-313.792		±29	42.557	264.655		*
BCL2	81.7164	-79.493		±12.6	47.438	272.691		*
BCL3	117.1691	-402.945		±2.1	62.476	290.188		*
BF	29.8094	-115.896		±13.8	29.567	200.473		*
BF2	48.80781	-589.959		±13	40.558	247.161		*
BF3	67.80621	-1135.646		±1.7	50.492	254.367		*
BH	11.81894	442.657		±8.4	29.178	171.849		*
BHF2	49.81575	-733.858		±3.3	42.341	244.025		*
BH2	12.82688	200.83		±63	34.062	180.211		*
BH3	13.83482	106.689		±10	36.211	187.886		*
BO	26.8104	-0.001		±8	29.179	203.472		*
BOCL OBCl	62.2631	-316.298		±29	45.102	237.435		*
BOF OBF	45.8088	-602		±13	40.996	224.806		
BOF2 OBF2	64.80721	-836.817		±15	50.253	267.853		*
BO2	42.8098	-284.518		±8	43.293	229.817		*
B2	21.622	829.687		±33.5	31.595	202.076		
B2O	37.6214	96.234		±105	38.402	227.747		*
B2O2 (BO)2	53.6208	-456.037		±8.4	57.4	242.629		*
B2O3(L)	69.6182	-1253.249			61.795	78.83		*
B2O3	69.6202	-835.975		±4.2	66.969	283.799		*
B3O3CL3 (BOCl)3	186.7893	-1631.706		±8	131.737	382.418		*
B3O3F3 (BOF)3	137.42641	-2365.152		±4.2	115.13	342.475		*
B3O3H3 BOROXIN	83.45502	-1217.544		±42	87.833	291.912		
H3B3O6 BORIC ACID	131.45322	-2271.833		±13	137.613	347.631		*
BaO	153.32640	-117.95	-		32.898	235.460		†
Br	79.904	111.86	117.93	±0.06	20.789	175.017	6.167	†
BrCl	115.35670	14.789	22.233		35.011	240.049	9.407	†
DBr	81.918102	-37.036	-29.160		29.228	204.484	8.668	†
BrF	98.902403	-58.851	-51.200	± 1.0	32.959	228.988	9.021	†
BrF3	136.89921	-255.6	-244.81	± 3.0	67.354	295.775	14.712	†
BrF5	174.89602	-428.8	-413.65	± 2.0	101.335	323.253	19.175	†
BRO	95.9034	125.8	133.333	±2.4	34.17	232.921	9.061	#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
BrO2 Br-O-O	111.9028	108	116.091	$\pm 40$	48.873	288.83	12.851	#
BrO2 O-Br-O	111.9028	152	161.545	$\pm 25$	45.364	271.112	11.395	#
BrO3	127.9022	221	233.180	$\pm 50$	59.995	284.507	13.101	#
Br2 (L) REFERENCE ELEMENT	159.8080	0	0		75.680	152.210	24.520	†
Br2 gas	159.8080	30.91	45.705	$\pm 0.11$	36.057	245.469	9.725	†
Br2O BrBrO	175.8074	168	183.722	$\pm 20$	51.385	312.704	13.137	†#
Br2O Br-O-Br	175.8074	107.6	124.061	$\pm 3.5$	50.168	290.823	12.399	†#
Br2Pb Br-Pb-Br	367.008	-103.9	-87.54		56.966	339.673	15.022	†
C(GR) REFERENCE ELEMENT	12.011	0	0		8.528	5.734	1.054	*‡
C	12.011	716.67	711.198	$\pm 0.45$	20.839	158.102	6.536	†
C+	12.01045	1809.444	1797.65	$\pm 0.8$	20.974	154.664	6.649	†
CBr	91.91470	495.85	500.2		32.370	230.888	8.946	#†
CBrClF2	165.36421	-435.	-423.8	$\pm 15$	74.650	318.724	15.528	†
CBrF3 Freon 1301	148.90991	-650.59	-638.48	$\pm 1.97$	69.270	297.695	14.444	†
CBr2	171.81870	343.51	356.89		49.273	288.706	12.192	#†
CBr2F2	209.81581	-380	-366.88	$\pm 15$	77.000	325.413	16.280	†
CBr3	251.72270	266.44	288.26		69.174	337.229	16.015	#†
CBr4	331.62670	119.20	148.90	$\pm 1.5$	91.162	358.185	20.396	#
CCL	47.46340	432.611	428.860		32.268	224.556	9.395	†
CCLF	66.46180	25.846	25.0	$\pm 30.$	42.962	259.150	10.902	†
COCLF	82.4615	-426.779		$\pm 33$	52.402	277.019		*
CCLF2	85.460206	-275.	-272.96	$\pm 25.$	55.172	287.353	12.432	†
CCLF3 FC-13	104.45861	-710.02	-704.93	$\pm 2.19$	66.887	285.424	13.791	†
CLCN Cyanogen Chloride	61.47044	137.952			45.333	236.344		*
COCL Carbonyl Chloride	63.4631	-62.756		$\pm 42$	45.103	265.974		*
CCL2	82.91670	231.7	230.5	$\pm 1.7$	51.028	266.112	11.728	#
CCL2F	101.91450	-105.	-103.57	$\pm 20.$	59.121	298.917	13.217	†
CCL2F2 FREON-12	120.91291	-490.8	-486.62		72.477	300.908	14.881	†
COCL2 PHOSGEN	98.9158	-219.5	-217.80		57.761	283.752	12.879	†
CCL3	118.3697	71.128	71.553	$\pm 2.5$	63.500	303.100	14.400	†
CCL3F FC-11	137.36720	-283.700	-280.53		78.071	309.785	16.064	†
CCL3O	134.36850	-18.41	-16.48		83.245	322.749		#
CCL4 liquid	153.823	-127.792		$\pm 0.55$				X
CCL4	153.823	-95.815			83.618	309.995		†
CD	14.0251	593.303			29.174	189.049		*
CDH3	17.0489	-78.469			36.395	200.027		*
CDO Formyl – D Radical	30.0245	40.945	40.0		35.920	228.610		#
CD2	16.0392	382.601			36.282	204.302		*
CD2O	32.0386	-114.903			38.048	225.057		*
CD3	18.0533	137.537			41.845	207.031		*
CD3NO2	64.05885	-61.789	-48.423		63.166	291.669	13.556	#
CD4 RRHO	20.0674	-89.022			40.479	198.995		*
CD4 * ANHARMONIC	20.0674	-89.022			40.519	199.003		*
CD4O CD3OD	36.06651	-217.670	-207.07		49.478	249.248	11.932	#
CF	31.009103	246.932	243.333	$\pm 0.7$	30.056	213.034	9.065	†
CF+	31.008554	1131.292	1121.86	$\pm 0.92$	29.642	201.509	8.697	†
FCN	45.01614	35.987		$\pm 16.7$	42.359	225.416		*
COF	47.0088	-171.539		$\pm 63$	38.943	248.48		*
CF2	50.007506	-191.26	-191.73	$\pm 1.35$	38.915	240.831	10.351	†
CF2+	50.006958	917.03	910.37	$\pm 1.6$	38.541	246.731	10.342	†
COF2	66.00721	-640	-636.92	$\pm 5.$	47.365	258.971	11.134	†
CF3	69.00591	-467.4	-464.6	$\pm 1.97$	49.642	264.521	11.491	†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
CF3+	69.00536	411.627	408.179	$\pm 1.96$	49.339	254.540	11.541	†
CF3I	195.91068	-589.11		$\pm 3.3$	70.941	307.633		
CF3O Radical	85.005309	-630.696	-625.69	$\pm 8.$	64.550	283.750	13.622	#
CF3OO RADICAL	101.00501	-627.349			79.392	315.015		
CF4 FC-14	88.00461	-933.4	-927.15	$\pm 0.53$	61.052	261.459	12.730	†
CH	13.01894	595.8	592.5	$\pm 0.6$	29.175	183.037	8.625	#
CHBr	92.92264	377.857	384.99	$\pm 2.$	39.789	252.872	10.416	#
CHBrClF	137.37374	-230.000	-217.24	$\pm 15$	62.869	304.928	13.787	#
CHBrF2 HBFC-22B1	130.91975	-425.46	-412.26	$\pm 1.07$	58.767	295.230	13.170	†
CHBr2	172.82664	198.489	215.446		54.834	298.588	12.851	#
CHBr3 Bromoform	252.73064	54.266	80.419		71.026	330.864	15.915	#
CHCL	48.47189	297.10	296.78		37.787	235.062	10.200	†
CHCLF	67.4703	-83.681			50.466	280.878		†
CHCLF2 HCFC-22	86.46845	-490.72	-484.38	$\pm 2.28$	55.851	280.895	12.362	†
CHCL2	83.92487	95.8	97.469		53.900	285.500	12.800	†
CHCL2F FC-21	102.9233	-284.934			61.077	293.204		†
CHCL2O CCl <sub>2</sub> OH	99.92374	-94.977	-91.0		69.410	307.164		#
CHCL3 liquid Chloroform	119.3779	-133.784		$\pm 0.72$				X
CHCL3 CHLOROFORM	119.3779	-102.928			65.5	295.666		†
CHCL3O CCl <sub>3</sub> OH	135.37644	-275.977	-270.06.	$\pm 3.2$	86.644	323.540		#
CHD2NO2	63.05268	-57.716	-44.135		60.806	289.264	13.290	#
CHD3	19.0612	-85.305			38.893	208.581		*
CHF RADICAL	32.01734	163.176			34.585	228.715		†
CHF2	51.01575	-254			45.279	258.506		†
CHF3 FLUOROFORM HFC-23	70.01385	-693.289	-686.34		51.139	259.375	11.573	†#
CHI3 IODOFORM	393.73205	210.874	218.799	$\pm 4.2$	75.072	355.672	17.157	†
HCN anharmonic	27.02568	129.799	180.136	$\pm 0.38$	35.857	201.824	9.235	†
HNC	27.02568	191.908	191.530	$\pm 0.69$	40.271	205.511	10.001	†
HNCO Isocyanic acid	43.02478	-118.600	-115.60	$\pm 4.2$	45.078	238.265	10.966	†
HOCN Cyanic acid	43.02478	-15.456	-12.76	$\pm 20.$	46.047	241.244	11.268	#
HCNO Fulminic acid	43.02478	167.603	171.042	$\pm 12$	48.395	225.025	10.623	#
HONC	43.02478	234.164	235.73	$\pm 17.$	49.654	248.364	12.400	#
CHN2	41.03242	319.796		$\pm 23.4$	48.059	248.503		
CH(NO2)3	151.03556	-13.389	+4.976		134.09	435.569	25.968	
CHO FORMYL RADICAL	29.01804	42.3	41.928	$\pm 0.3$	34.680	224.28	10.000	#
CHO+	29.0178	833.059			36.015	203.32		*
COH	29.01804	218.10	217.72	$\pm 0.83$	34.970	225.030	10.008	#
COOH equilibrium	45.01744	-181.32	-178.16	$\pm 2.30$	43.610	251.736	10.813	†
HCOO* Radical	45.01744	-150.624			39.748	239.743		
HCS	45.08494	300.47			37.059	236.148		
CH2 Methylene Equilibrium	14.02658	391.2	390.7	$\pm 1.6$	35.130	194.436	10.032	#
CH2 Methylene SINGLET	14.02658	428.8	428.3	$\pm 1.6$	33.781	189.220	9.940	#
CH2 Methylene Triplet only	14.02658	391.2	390.7	$\pm 1.6$	35.014	194.418	10.027	#
CH2BrCl HALON101	129.38358	-45		$\pm 15$	52.726	287.29		
CH2Br2	173.83458	4.937	26.329	$\pm 2.$	54.554	293.767	12.650	#
CH2CL	49.47979	116.875			43.201	243.375		*†
CH2CLF GC-31	68.4782	-264.432			47.038	264.307		†
CH2CL2	84.93198	-95.396	-88.547	$\pm 0.74$	50.951	270.365	11.854	†
CH2DNO2	62.04652	-52.532	-38.81		58.983	286.942	13.098	#
CH2D2	18.0551	-81.769			37.51	207.911	10.151	*
CH2F	33.02528	-32			40.292	236.529		†
CH2F2 FC-32	52.02339	-452.709	-444.65	$\pm 1.0$	42.869	246.347	10.693	†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
H2CN RADICAL	28.03362	240.162			37.768	224.304		
HCNH trans	28.03362	298.738			38.072	229.017		
HCNH cis	28.03362	319.658			38.892	229.493		
H2NCO	44.03302	-23.305		$\pm 9.9$	52.926	256.458		
CH2NO CH <sub>2</sub> =N-O*	44.03302	173.427		$\pm 21$	49.153	249.913		
H2CNO H <sub>2</sub> C*N=O	44.03302	223.928		$\pm 8.4$	42.388	244.644		
CH2NO2 NITRO-METHYL RAD	60.03242	152.465	161.86		58.862	288.218	13.143	#
CH2NO3 Methyl Nitrate Radical	76.03182	98.952	109.481		76.78	312.169	16.347	
CH2N2 CYANAMIDE	42.04036	135.888		$\pm 20$	51.505	247.641		
H2CN2 HN=C=NH	42.04036	149.005		$\pm 15$	50.223	247.113		
CH2N2 H <sub>2</sub> C=N=N	42.04036	286.382		$\pm 25$	51.144	240.982		
H2CN2 CY DIAZIRENE	42.04036	320.143		$\pm 20$	41.383	236.962		
CH2(NO2)2	106.03796	-61.505	-43.674		86.352	358.098	17.721	
CH2O FORMALDEHYDE	30.02628	-108.58			35.388	218.764		
HCOOH FORMIC ACID	46.02568	-378.57			41.305	247.148		
H2CS	46.09288	114.683			38.196	236.949		
CH3	15.03452	146.7	150.0	$\pm 0.3$	38.417	194.008	10.366	#
CH3+	15.03397	1101.792	1099.37	$\pm 0.097$	34.749	186.827	9.983	#
CH3BR	94.93852	-36.443	-21.034	$\pm 2.$	42.312	245.954	10.607	#
CH3CL	50.48722	-81.87	-73.94	$\pm 0.6$	40.741	234.396	10.416	†
CH3F FC-41	34.032923	-239.55	-231.52	$\pm 2.65$	37.504	222.826	10.135	†
CH3Hg Methyl Mercury	215.62452	188.28	200.21	$\pm 8.4$	46.073	260.58	11.165	#
CH3I Methyl Iodide	141.93899	14.30	23.838	$\pm 1.4$	44.084	253.007	10.816	†#
CH3N (H <sub>2</sub> C=NH) Methanamine	29.04126	84.015	91.93	$\pm 4.5$	38.084	221.567	10.176	#
CH3N Methyl-N Radical	29.04126	319.950	327.711	$\pm 4.5$	39.990	226.694	10.330	#
CH3NO NITROSOMETHYL	45.04096	79.002		$\pm 7.3$	50.77	260.833		
OCHNH2 FORMAMIDE	45.04096	-195.263		$\pm 10.5$	48.473	253.646		
CH2NOH	45.04096	29.288			53.359	248.547		
NCH3O FORMIMIDIC ACID	45.04096	-148.436		$\pm 10.9$	43.477	254.079		
H3CNO CH <sub>2</sub> -NH=O	45.04096	59.032		$\pm 11.5$	44.542	250.67		
CH3NO2 NITRO-METHANE	61.04036	-80.751	-66.85		55.528	282.863	12.610	#
CH3NO2 Methyl Nitrite CH3ONO	61.04036	-65.44	-54.015	$\pm 1.$	64.891	302.910	15.345	#
CH3NO3 METHYL-NITRATE	77.03976	-122.005	-107.13	$\pm 4.2$	76.597	305.793	16.234	
CH3N2 CH <sub>3</sub> N=N*	43.0483	247.651		$\pm 12$	53.694	257.186		
CH3N3 CH <sub>3</sub> -N=N=N MethylAzide	57.05474	297.29	309.93	$\pm 8.$	63.015	279.531	14.118	#
CH3O	31.03392	21.0	28.4	$\pm 2.1$	42.541	234.278	10.719	#
CH2OH	31.03392	-17.0	-10.7	$\pm 0.7$	47.401	244.170	11.781	†
CH2OH+	31.03337	716.400	718.149	$\pm 0.3$	37.835	228.047	10.149	†
CH3OD	33.04832	-205.331	-194.49		44.142	242.751	11.543	#
CH3O2 Peroxymethyl Radical	47.034	9.0		$\pm 5.1$	52.257	268.762		
CH3S Thiomethoxy Radical	47.10082	124.6		$\pm 1.7$	46.64	242.040		#
CH4 RRHO	16.04276	-74.6	-66.633	$\pm 0.3$	35.613	186.314	10.023	
CH4 ANHARMONIC	16.04276	-74.6	-66.626	$\pm 0.3$	35.691	186.371	10.016	†
CH4N CH <sub>3</sub> NH*	30.0492	187.569		$\pm 4.8$	47.372	235.967		
CH4N *CH <sub>2</sub> NH <sub>2</sub>	30.0492	153.49	164.62	$\pm 8.$	48.597	244.694		#
(NH2)2C=O Urea	60.05564	-235.5			79.088	282.953		
CH4N4O2 Nitroguanidine, Picrite	104.06852	1.		$\pm 20$	114.92	352		
CH3OH(L)	32.04216	-238.91	-235.57		81.080	127.269	18.995	†
CH3OH	32.04216	-200.94	-190.11		44.039	239.81	11.444	#
CH4O2 (CH <sub>3</sub> OOH)	48.04126	-126.733	-114.22	$\pm 4.2$	66.753	275.904	14.160	#
CH4S (CH <sub>3</sub> SH)	48.10876	-22.525			50.415	258.382		
CH5N CH <sub>3</sub> -NH <sub>2</sub>	31.0574	-23.025			50.505	240.75		*

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
CH5N2 CH <sub>3</sub> N*NH <sub>2</sub>	45.06418	215.183		±5.5	63.575	260.107		
CH5N3 GUANIDINE	59.07092	-15.		±10.	80.489	278.706		
CH6N2 MethylHydrazine	46.07182	109.41	130.443	±8.	68.911	274.188		#
CH6Sn CH <sub>3</sub> SnH <sub>3</sub>	136.76834	118.407	136.091	±4.2	73.750	285.712	15.907	#
Cl4 TetralodoMethane	519.62858	260.41	265.53		95.819	391.347	22.327	#
CN	26.01774	438.68	435.4	±2	29.156	202.643		#
CNO (NCO)	42.01684	128.040	127.57	±4.2	39.989	232.229	10.198	†#
CNN	40.02418	591.87	591.216	±3.19.	42.656	232.398	10.378	†#
NCN (NCN)	40.02418	465.89	465.433	±1.78	41.946	225.814	10.180	†#
C(NO <sub>2</sub> ) <sub>4</sub> TetraNitroMethane	196.03316	82.383	101.856		176.119	503.723	33.993	
CO	28.0104	-110.53		±0.17	29.141	197.657		†
COS	60.0764	-138.399		±1	41.556	231.475		*†
CO <sub>2</sub>	44.0098	-393.51		±0.13	37.135	213.787		†
CP	42.984461	520.162	517.860	±10.	29.910	216.257	8.715	†
CS	44.0767	278.550	275.307	±3.8	29.799	210.559	8.708	†
CS <sub>2</sub> Anharmonic	76.143	116.70	115.913	±1.	45.482	237.889	10.664	†
C <sub>2</sub>	24.0214	824.35	816.288	±1.6	43.549	197.097	10.169	†
C <sub>2</sub> Br	103.9260	623.667	626.39	±2.	45.103	295.017	11.648	#
C <sub>2</sub> Br <sub>2</sub>	183.8300	335.31	346.51	±2.	68.067	294.448	15.427	#
C <sub>2</sub> Br <sub>2</sub> F <sub>4</sub> HALON 2402	259.82361	-790.776		±4.2	120.019	252.529		
C <sub>2</sub> Br <sub>3</sub>	263.7340	385.388	405.674		83.269	369.892	18.602	#
C <sub>2</sub> Br <sub>4</sub>	343.638	215.584	218.816		102.196	387.413	22.410	#
C <sub>2</sub> Br <sub>5</sub>	423.54200	283.257	318.915		126.162	444.694	27.749	#
C <sub>2</sub> Br <sub>6</sub>	503.44600	165.480	209.480		146.665	459.134	31.667	#
C <sub>2</sub> CL	59.4747	494.09			45.046	241.948		†
C <sub>2</sub> CL <sub>2</sub>	94.9274	226.6		±14	65.668	271.942		*†
C <sub>2</sub> CL <sub>2</sub> F <sub>2</sub> CCLF=CFCL E(trans)	132.92361	-341.486	-339.3	±8.	87.333	327.192	17.925	#
C <sub>2</sub> CL <sub>2</sub> F <sub>2</sub> CCLF=CCLF Z(cis)	132.92361	-339.548	-337.37	±8.	87.632	327.213	17.934	#
C <sub>2</sub> CL <sub>2</sub> F <sub>4</sub> FC-114	170.92101	-900.4			116.6	364.2		
C <sub>2</sub> CL <sub>3</sub>	130.3801	190.28			76.033	328.166		†
CCl <sub>2</sub> F-CCLF <sub>2</sub> FC-113	187.37531	-705.8			121	386.9		
C <sub>2</sub> CL <sub>3</sub> F <sub>3</sub> FC-113A	187.37531	-740.6			120.3	369.3		
C <sub>2</sub> CL <sub>4</sub>	165.834	-24.2	-23.336	±8.0	94.92	340.925	19.606	†
C <sub>2</sub> CL <sub>5</sub>	201.2855	39			118.832	397.906		
C <sub>2</sub> CL <sub>6</sub>	236.7376	-162.110	-159.69	±8	136.326	407.696	27.235	†#
C <sub>2</sub> D <sub>2</sub>	28.0502	222.194	222.675		49.556	208.92		*
C <sub>2</sub> D <sub>2</sub> O	44.0496	39.932			55.669	249.614	12.388	*
C <sub>2</sub> D <sub>4</sub>	32.0784	30.279			52.064	230.672		*
C <sub>2</sub> OD <sub>4</sub>	48.0778	-180.582			64.697	275.315	14.042	*
C <sub>2</sub> D <sub>6</sub>	36.1066	-110.676			64.743	244.479	13.228	*
C <sub>2</sub> D <sub>6</sub> N <sub>2</sub> Azomethane-D <sub>6</sub>	64.12001	119.248			92.1	312.346		*
C <sub>2</sub> D <sub>6</sub> O DimethylEther-D <sub>6</sub>	52.10601	-209.49	-192.04		77.528	283.259	15.875	*
C <sub>2</sub> F	43.019803	353.847	350.00	±50.	42.6	231.036	10.367	†
C <sub>2</sub> F <sub>2</sub>	62.018206	-144.666	-147.	±20	60.114	249.570	13.266	†
C <sub>2</sub> F <sub>3</sub>	81.01661	-228.175	-227.0	±20.	66.178	297.643	14.164	†
C <sub>2</sub> F <sub>4</sub> FC-1114	100.01501	-675.34	-671.91	±2.0	80.459	300.128	16.331	†#
C <sub>2</sub> F <sub>5</sub>	119.01402	-891.192			94.111	341.49		
C <sub>2</sub> F <sub>6</sub> FC-116	138.01182	-1347.38	-1339.0	±0.31	106.294	341.033	20.229	†#
CF <sub>3</sub> -O-O-CF <sub>3</sub>	170.01122	-1507.077		±12.5	137.807	433.17		
C <sub>2</sub> H ETHYNYL	25.02994	568.522		±4	41.999	213.304		†
C <sub>2</sub> HBr	104.93394	282.43	289.073	±2	55.087	252.719	11.948	#
C <sub>2</sub> HBr <sub>2</sub>	184.83794	333.590	348.909		68.272	326.691		#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C2HBr3	264.74194	144.13	168.884		85.590	359.979		#
C2HBr4 1,1,2,2-CHBr2CBr2	344.64534	218.823	250.685	$\pm 8.4$	107.701	425.045	23.519	#
C2HBr4 1,1,1,2-CBr3CHBr	344.64534	243.634	274.593	$\pm 8.4$	113.967	417.090	24.422	#
C2HBr5	424.54994	113.09	153.50		126.586	439.181		#
C2HCL	60.48264	226.4		$\pm 10.$	54.32	241.999		†
C2HCLF 1,1-CLF Radical	79.48074	101.87	103.90	$\pm 8.$	63.592	289.422	13.317	#
C2HCLF2-1,1 FC-1122	98.478846	-333.654	-329.16		76.650	304.242	15.263	†
C2HCLF2 cis FC-1131	98.478846	-323.569			75.394	305.096		
C2HCLF2 trans	98.478846	-323.103			75.149	304.318		
CF2H-CCLF2 FC-124A	136.47625	-903.3			100.4	351.1		
CF3-CHCLF HCFC124	136.47625	-924.7			99.06	349.6		
C2HCL2F-1,1+cis+trans	114.93314	-168.648	-164.97		77.324	320.190	16.259	†
CF3-CHCL2 HCFC123	152.93055	-743.9			102.6	352.6		
CF2CL-CHFCL FC123A	152.93055	-710			104.5	368.1		
CFCL2-CHF2	152.93055	-702.1			104.5	361.7		
C2HCL3	131.38804	-17.5	-14.0	$\pm 3.0$	80.016	324.941	16.605	†
C2HCL4	166.84014	21.824	26.108	$\pm 8.$	100.608	375.159	20.419	#
C2HCL5	202.29284	-160.410	-153.83	$\pm 8.$	113.348	379.920	22.716	#
C2HF	44.027743	41.692	41.	$\pm 25$	52.268	231.573	11.446	†
C2HF2	63.02615	-42.5	-40.52	$\pm 17.9$	59.249	279.393		#
C2HF3	82.02455	-490.78	-485.53	$\pm 8.24$	69.191	292.665	14.328	†
C2HF5 FC-125	120.02136	-1120.00	-1110.4	$\pm 8.$	95.808	334.635	18.776	#
HCCN	39.03668	610.431		$\pm 100$	54.238	240.596		
C2HNO NC-CHO	55.03548	44.120	46.152	$\pm 8.$	55.793	270.935		#
C2HNO2 HCC-NO2	71.03488	278.654	283.597	$\pm 8.$	69.580	289.604	14.414	#
HCCO Ketyl Radical	41.02934	177.402		$\pm 8.8$	48.417	245.287		
H2C2 VINYLIDENE	26.03728	414.788	414.489		42.614	221.021	10.874	†
C2H2 ACETYLENE	26.03728	228.20	228.769	$\pm 0.8$	44.001	200.917	10.006	†
C2H2Br2 1,2-DiBromoEthylene	185.84528	101.9	121.55	$\pm 8.$	69.521	315.102	15.447	#
C2H2Br4 CHBr2CHBr2	345.6532	53.35	89.89		107.863	398.747		#
C2H2CL CHCL=CH* Radical	61.48998	274.767	277.937	$\pm 8$	53.700	270.153	11.996	#
C2H2CLF	80.48868	-165.393	-159.0	$\pm 15$	64.216	283.339		†
C2H2CL2 CCL2=CH2	96.94328	2.2	8.084	$\pm 1.4$	67.722	288.285		#
C2H2CL3 CH2-CCL3	132.39538	82.81	88.908	$\pm 5.$	94.764	329.695		#
C2H2F2-1,1+cis+trans equilib.	64.03409	-336.4	-329.48	$\pm 4.$	60.237	266.054	12.480	†
C2H2F2-1,1 FC-1132A	64.03409	-336.4	-329.48	$\pm 4.$	60.123	266.041	12.476	#
H2C2F2 cis	64.03409	-306.5	-299.80	$\pm 5.$	58.349	268.723	12.701	#
F2C2H2 trans FC-1132	64.03409	-303.73	-297.15	$\pm 5.$	60.074	267.847	12.955	#
C2F3H2	83.03309	-517.142			79.499	303.093		
CF3-CFH2	102.03089	-913.3	-902.01	$\pm 17.5$	86.273	315.752	16.937	#
CHF2-CHF2 HFC-134	102.03089	-883.3	-872.21	$\pm 5.5$	84.129	313.143	17.130	#
C2H2N CH2CN Methyl-Cyanide	40.04402	257.78	260.54		54.345	255.826	12.356	#
C2H2N CH2NC Methyl Isocyanide	40.04402	358.23	360.59	$\pm 8.$	53.971	256.71	12.550	#
C2H2NO NC-CH2-O*	56.04342	175.619	181.426	$\pm 8.$	61.512	281.028	13.444	#
C2H2NO2 NC-CH2-O-O*	72.04282	177.987	185.371	$\pm 8.$	74.150	312.514	16.207	#
1,2-C2H2(NO2)2 trans	118.04896	40.953	56.131	$\pm 8.$	108.234	360.962	21.428	#
CH2CO Ketene	42.03728	-47.698		$\pm 1.7$	51.744	241.896		†
HCCOH ETHYNOL	42.03728	93.186		$\pm 18.3$	57.403	249.142		
C2H2O2 trans & cis GLYOXAL	58.03608	-212.082	-206.51	$\pm 0.8$	60.409	272.483	13.682	†
C2H2O2 CIS GLYOXAL	58.03668	-193.35		$\pm 0.8$				X
C2H2O2 Oxyranone	58.03608	-177.916	-170.37	$\pm 8.$	53.635	263.960	11.713	#
C2H2O4 Oxalic Acid	90.03488	-731.8	-721.2	$\pm 2.0$	86.149	320.662		#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C2H3 VINYL RADICAL	27.04522	296.580	300.867	$\pm 0.92$	42.071	233.663	10.522	†#
C2H3+ Vinylum Ion	27.04467	1122.34	1119.2	$\pm 1.17$	50.714	225.350	11.780	#
C2H3BrO2 Bromoacetic Acid	138.94802	-383.5	-364.61	$\pm 3.1$	80.542	337.015		#
CH3CBr3 1,1,1-Tribromoethane	266.75722	-26.3	+5.258		97.982	355.210		#
C2H3CL	62.49792	37.872	45.452	$\pm 8.$	53.681	264.024	11.820	#
C2H3CLO3	94.49672	-427.6	-416.0	$\pm 1.0$	78.839	325.918		#
C2H3CL3 CH3-CCL3	133.40332	-144.6	-133.98	$\pm 2.0$	92.410	320.413	18.025	#
C2H3F	46.043623	-140.1	-132.21	$\pm 2.5$	50.407	252.674	11.336	#
C2H3F2	65.04263	-302.503			67.256	288.291		
CH3CF3 FC-143A	84.04043	-755.655	-742.91	$\pm 1.0$	78.074	287.652	15.298	#
CH3CD3 1,1,1-Ethane-D3	33.087526	-107.57	-92.313	$\pm 3.3$	57.385	241.997	12.406	#
C2H3I Ethyl-Iodide	153.94969	128.867	137.906		56.071	299.640	12.368	#
C2H3N CH3CN Methylcyanide	41.05196	74.04	81.09	$\pm 0.37$	52.249	243.267	12.094	#
C2H3N CH3NC Methylcyanate	41.05196	163.5	169.982	$\pm 7.2$	52.947	246.658	12.660	#
C2H3NO NCCH2OH	57.05136	-49.910	-39.97	$\pm 8.$	64.965	280.796		#
C2H3NO2 NCCH2-O-OH	73.05136	29.476	39.641	$\pm 8.$	82.503	323.081	17.659	#
C2H3NO2 Nitroethylene	73.05136	33.284	46.001	$\pm 8.6$	73.68	300.503	15.108	
C2H3O (CH3CO) RADICAL	43.04522	-10.3	-3.6	$\pm 1.8$	50.785	267.448	12.385	#
C2H3O+ (CH3CO+) ion	43.044714	669.952	670.921	$\pm 0.85$	52.589	243.392	11.977	#
OH3C2 (*CH2CHO) RADICAL	43.04522	25.102			54.974	267.919	12.910	*
C2H3O OXYRANE RADICAL	43.04522	164.473	172.900	$\pm 8.0$	45.741	252.528	10.723	#
C2H4 ETHYLENE	28.0536	52.500	61.025		42.887	219.322	10.519	†
C2H4Br2 CH2Br-CH2Br	187.8611	-37.5	-10.491		75.948	329.088	16.422	#
C2H4Br2 CH3-CHBr2	187.8611	-41.	-13.725		79.452	327.355	16.288	#
C2H4CL RADICAL	63.50646	90.12			58.635	281.459		
C2H4CL2 CH2CL-CH2CL	98.95856	-130.069	-117.37	$\pm 0.6$	72.544	303.542	15.531	#
C2H4CL2 CH3-CHCL2	98.95856	-127.6		$\pm 1.1$				X
C2H4O2CL2 Cl2-Peroxyethane	130.95796	-231.375	-215.17		109.993	362.046	20.697	#
C2H4F RADICAL	47.05216	-72.216			58.857	273.845		
C2H4F2 CH2F-CH2F HFC-152	66.04997	-447.55	-433.78		64.238	279.918		#
C2H4F2 CH3-CHF2 HFC-152a	66.04997	-497.0	-473.07	$\pm 8.0$	87.266	282.502		#
C2H4O VINYL-ALCOHOL	44.05316	-124.683			61	289.996		
C2H4O OXYRANE	44.05316	-52.635	-40.082	$\pm 0.63$	47.624	242.870	10.831	†
CH3CHO ACETALDEHYDE	44.05316	-166.19	-155.70		55.319	263.952	12.897	†
CH3COOH liquid Acetic Acid	60.0524	-484.216		$\pm 0.17$				X
CH3COOH ACETIC ACID	60.0524	-432.253	-418.12		63.439	283.473	13.597	†
(HCOOH)2 Formic Acid dimer	92.0512	-820.951			96.177	332.671		*
C2H5 ETHYL RADICAL	29.06110	118.658	129.75	$\pm 2$	50.484	247.118	12.185	†
C2H5Br BROMOETHANE	108.9651	-61.60	-39.65	$\pm 1.01$	64.206	287.668	13.584	††
C2H5CL CHLOROETHANE	64.5138	-106.827	-92.25	$\pm 0.41$	62.738	276.274	13.294	#
C2H5CLO2 Chloroperoxyethane	96.5132	-212.966	-194.27		92.223	336.239	17.853	#
C2H5F FLUOROETHANE	48.0595	-275.21	-260.41	$\pm 4.9$	59.575	270.530	12.888	#
C2H5I IODOETHANE	155.96557	-7.047	8.253	$\pm 0.56$	71.670	298.362	14.575	#
C2H5NO2 NITROETHANE	75.06724	-103.784	-83.506	$\pm 5.$	79.018	320.512	16.015	
C2H5ONO2 ETHYLNITRATE	91.06664	-154.975	-132.82	$\pm 8.$	95.103	328.863	18.480	
C2H5N3 Ethyl Azide	71.081320	266.872	287.394	$\pm 8.$	80.026	303.042	15.761	#
C2H5O* ETHOXY RADICAL	45.0609	-13.6	-0.2	$\pm 8.0$	66.321	277.642	14.325	#
CH2CH2OH RADICAL	45.0609	-23.849	-11.640	$\pm 8.0$	68.668	291.708	15.564	
CH3CH*OH RADICAL	45.0609	-54.030	-40.776	$\pm 8.0$	64.038	288.991	14.263	#
C2H5O Dimethylether Radical	45.0609	0.960	14.079	$\pm 8.0$	66.124	281.519		#
C2H5O2 EthylPeroxy Radical	61.06050	-28.70	-12.450	$\pm 8.4$	73.721	299.991		#
C2H6 ETHANE	30.0694	-83.852	-68.232	$\pm 0.2$	52.501	229.221	11.892	†



Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C2H6N (CH3)2N Dimethylazide	44.07578	159.854	177.58	$\pm 8.$	66.912	270.641		#
C2H6N *CH2-NH-CH3	44.07578	156.58	174.07	$\pm 8.$	70.233	279.671		#
C2H6N2 AZOMETHANE	58.0828	148.684			77.872	289.777		*
(CH3)2N-NO2	90.08192	-4.8			103.204	328.138		
C2H5OH(L) ETHANOL LIQUID	46.06904	-277.51	-269.74		112.250	160.100	24.082	†
C2H5OH ETHANOL	46.06904	-234.95			65.309	280.593		†
CH3OCH3 DIMETHYLETHER	46.06904	-184.054			65.823	267.381		
C2H6O2 PEROXYETHANE	62.06844	-173.636			82.969	314.534		
CH3OOCH3 Dimethylperoxyde	62.0682	-125.5	-106.5	$\pm 5.0$	80.717	308.409		#
C2H6S C2H5SH Ethanethiol	62.13564	-46.108			72.676	296.102		
C2H6S (CH3SCH3)Methylsulfide	62.13564	-37.53			74.099	285.851		
C2H6S2 CH3-SS-CH3	94.20164	-24.142			94.307	336.645		
C2H7N CH3-NH-CH3	45.08372	-15.259	+6.501	$\pm 8.$	68.541	267.185		#
C2H7N2 (CH3)2N-NH*	59.09046	207.685	232.276	$\pm 8.$	81.384	284.772		#
C2H8N2 SYM Dimethylhydrazine	60.099	94.491		$\pm 7.5$	82.347	287.346		
C2H8N2 UNSYM	60.099	53.22			91.524	302.186		
CCN	38.02814	679.07	674.474	$\pm 6.23$	44.231	237.159	11.089	#†
CNC	38.02814	675.85	670.935	$\pm 5.89$	45.042	233.804	11.357	#†
C2NO	54.02754	210.00	207.188	$\pm 10.$	56.145	278.187	13.594	#†
C2N2	52.03488	309.28	307.342	$\pm 1.03$	57.085	242.204	12.715	†
C2N2O2Hg(s) Hg- Fulminate	284.6	386.						X
C2(NO2)2 Dinitroacetylene	116.03248	349.046	356.251	$\pm 8$	102.603	353.895	20.933	#
C2(NO2)4 Tetranitroethylene	208.04356	N/A	N/A		184.031	468.771	35.016	#
C2(NO2)6 Hexanitroethane	300.05524	179		$\pm 5.9$	273.376	667.098		
C2O	40.02080	291.039	287.000	$\pm 12.$	43.134	233.624	10.486	†
C2S2	88.15340	376.660	373.831		62.030	274.120	13.760	†
C3	36.03210	839.949	831.0		42.202	237.613	12.109	†
C3D4	44.0894	262.675			64.125	254.286	12.650	*
C3D6	48.1176	32.885			72.411	251.394	13.152	*
C3F Radical	55.030503	564.957	559.052	$\pm 8$	55.612	277.062	13.479	#
C3F3 FCC-CF2*	93.02731	-134.419	-135.23	$\pm 8$	81.990	326.463	17.210	#
C3F3 *CC-CF3	93.02731	-79.078	-79.609	$\pm 8$	80.749	313.306	16.929	#
C3F4 PerFluoroAllene	112.02571	-553.685	-551.89	$\pm 8$	92.135	336.733	19.021	#
C3F6 Hexafluoropropene	150.02252	-1157.253	-1150.95	$\pm 8$	121.759	373.675	23.337	#
C3F7 RADICAL	169.02182	-1347.122	-1339.5	$\pm 8$	135.964	416.386	26.401	#
C3F8 FC-218	188.02023	-1760.121			147.248	406.145		
C3H HC≡C-C	37.04004	719.393	714.091	$\pm 8$	53.430	247.795	12.696	#
C3HF7 FC-227EA	169.02092	-1564.816	-1552.4	$\pm 8$	136.690	399.058	25.901	#
C3HN CyanoAcetylene	51.04678	368.414	367.225	$\pm 8$	62.633	247.991	12.918	#
C3H2(1) CyPropenylidene	38.04888	476.976	477.960		44.222	236.204	10.645	
C3H2(3) H2C*-C≡C*	38.04888	651.030	650.361		54.719	254.549	12.298	
C3H2(3) *HC=C=CH*	38.04888	755.254	751.668	$\pm 62.7$	67.953	260.782	15.215	
C3H2(1) HC-C≡CH*	38.04888	817.972	816.374	$\pm 62.7$	58.770	251.691	13.227	
C3H2F3 CF3-CH=CH*	95.04319	-376.895	-369.47	$\pm 8$	90.727	323.105	17.442	#
C3H2F3 CF3-C*=CH2	95.04319	-374.941	-367.82	$\pm 8$	91.100	125.439	17.741	#
C3H2N HC*=CH-CN	52.05472	442.855	445.486	$\pm 8$	59.531	272.030	13.333	#
C3H3 PROPARGYL RADICAL	39.05682	346—349		$\pm 8$	64.891	256.659		†
CLC3H3 1-Chloro-1-propyne	74.50862	184.711	189.553	$\pm 8$	71.364	283.822	15.611	#
C3H3Cl CH2Cl-CCH	74.50952	162.729	167.78		73.747	296.899		
3-C3H3Cl CY	74.50952	218.333	225.43		66.257	281.203		
C3H3Cl CHCl=C=CH2	74.50952	160.851	163.18		70.089	290.465		
C3H3F2 *CF2-CH=CH2	77.052726	-224.438	-216.93	$\pm 8$	89.452	316.769		#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C3H3F3 CF <sub>3</sub> -CH=CH <sub>2</sub>	96.051130	-631.131	-619.51	±6.	90.704	319.468		#
C3H3I CH <sub>2</sub> ICCH Propargyl Iod.	163.96039	269.072	276.353	±12.5	74.028	354.081	15.180	#
C3H3I CH <sub>2</sub> =C=CHI Allenyl Iod.	163.96039	264.117	272.127	±12.5	70.463	305.857	14.451	#
C3H3N CH <sub>2</sub> =CHCN	53.06266	184.037	190.874	±8	59.387	263.290	13.361	#
C3H3O CH <sub>2</sub> =CHC*=O	55.05532	88.530	94.601	±8	61.410	300.654		#
C3H3O *CH <sub>2</sub> -CH=C=O	55.05532	93.560	98.877	±8	68.927	293.760		#
H4C3 PROPYNE	40.06386	184.9	191.966		60.731	248.429	13.031	†
C3H4 ALLENE	40.06386	190.92	198.412		58.88	243.630	12.605	†
C3H4 CYCLOPROPENE	40.06386	277.1	285.823		52.883	243.605	11.374	†
C3H4CL *CH=CH-CH <sub>2</sub> CL	75.51656	250.253	259.680	±8.	73.850	303.749	15.261	#
CLC3H4 *CH <sub>2</sub> -CH=CHCL	75.51656	137.444	147.12	±8.	71.705	303.390	15.012	#
C3H4N CH <sub>3</sub> -CH*-CN	54.07060	222.706	232.213	±8.	72.044	298.672	14.925	#
C3H4N <sub>2</sub> 1,3-DIAZOLE	68.07824	140.959		±28	65.701	273.426		
1,3,3 TRI-NITRO-AZETIDINE	192.08812	128.449	171.220	±8.	134.987	357.315	20.706	
C3H4O ACROLEIN	56.06416	-68.065	-57.913	±8	64.332	297.025		#
C3H4O <sub>2</sub> CH <sub>2</sub> =CH-C(O)-OH	72.06266	-326.051	-312.52	±8	79.301	313.570	15.243	#
C3H5 Symmetric Allyl Radical	41.0727	163.594			63.387	258.886		†
T-C3H5 CH <sub>3</sub> C*=CH <sub>2</sub> “ “	41.0727	237.651			61.663	266.064		
S-C3H5 CH <sub>3</sub> CH=CH* “ “	41.07180	265.533	276.287	±8.	63.362	271.305	13.577	#
C3H5 Cyclo	41.07180	279.91	292.716	±10.5	55.701	251.486		#
C3H5Cl 1-Chloro-1-propene	76.5245	-8.100	+4.937	±8.	76.450	299.193	15.884	#
C3H5Cl 3-Chloro-1-propene	76.5245	0.369	14.052	±8.	74.210	307.919	15.239	#
C3H5N PROPIONITRILE	55.07944	53.191	66.974	±8.	72.039	285.205	14.883	#
CH <sub>3</sub> CH=CHNO <sub>2</sub> Nitropropylene	87.07824	9.987	29.046	±8.9	93.59	330.004	18.288	
C3H5NO <sub>2</sub> NitroCycloPropane	87.07824	21.033	41.466	±8.	90.786	311.278	16.913	#
C3H5N <sub>3</sub> O <sub>9</sub> NITROGLYCERINE	227.08752	-279.073	-246.14	±2.7	234.24	545.865	43.458	
C <sub>2</sub> H <sub>5</sub> CO Propanal	57.0712	-32.83	-19.862	±8.	67.859	314.290		#
CH <sub>2</sub> COCH <sub>3</sub> Acetone Radical	57.0712	-33.34	-20.617	± 8.	72.843	307.518		#
C3H5O Propylene Oxide Radical	57.0712	104.069	118.072	± 8.	71.197	293.196		#
C3H6 PROPYLENE	42.07974	20.000	35.014		64.433	266.668	13.551	†
C3H6 CYCLOPROPANE	42.07974	53.30	70.455		55.572	237.488	11.410	†
C3H6N <sub>2</sub> O <sub>2</sub> N-NITRO-AZETIDIN	102.09292	114.123	141.198		100.656	328.954	18.840	
C3H6N <sub>6</sub> O <sub>6</sub> RDX Solid	222.11748	79.078	--		284.884	146.189	--	
C3H6N <sub>6</sub> O <sub>6</sub> RDX 135 Triazine	222.11748	192.000	233.285		230.174	482.441	39.331	
C <sub>2</sub> H <sub>5</sub> CHO Propionaldehyde	58.08004	-192.046			80.73	304.51		
CH <sub>3</sub> COCH <sub>3</sub> ACETONE	58.08004	-214.814	-198.10	±0.26	74.207	295.660	16.193	†#
C3H6O PROPYLENE OXIDE	58.07914	-92.760	-74.271	±8.	72.671	281.487	14.415	#
C3H6O CY OXETANE	58.07914	-81.086	-61.49	±8.	61.826	274.672	13.499	#
C3H6O Vinylmethylether	58.07914	-100.378	-83.824	±8.	76.313	308.229	16.351	#
C3H6O Cyclopropanol	58.08004	-101.504	-81.907	±8.	70.158	277.454	13.308	#
C3H6S THIETHANE	74.14664	60.584			70.418	278.343		
N-C3H7 PROPYL RADICAL	43.0883	101.32	119.149	±1	71.309	290.460	14.970	†#
I-C3H7 ISOPROPYL RADICAL	43.0883	90.19	108.237	±2	65.545	290.109	14.725	†#
1-C3H7I Iodopropane	169.99305	-31.999		±2	85.883	332.737		
2-C3H7I “	169.99305	-40.865		±2	91.193	334.082		
C3H5NH <sub>2</sub> CY-PROPYLAMINE	57.09499	77.389			89.045	285.464	16.956	*
C3H7N AZETIDINE	57.09532	98.198			67.14	267.274		
C3H7NO <sub>2</sub> Nitropropane	89.09412	-124.265	-97.795	±0.4	104.085	350.046	19.344	
C3H7NO <sub>3</sub> NPN PropylNitrate	105.09352	-174.054	-146.91	±1.3	123.239	362.601	23.008	
C3H7O N-PROPOXY RAD.	59.08798	-37.656			81.634	309.616		
C3H8 PROPANE	44.09562	-104.68	-82.388	±0.6	73.589	270.315	14.741	†
C3H7OH PROPANOL	60.09592	-255.2	-231.35		84.978	323.367	17.519	†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
(CH <sub>3</sub> ) <sub>2</sub> CHOH 2-Propanol	60.09592	-272.7	-248.59		89.594	309.226	17.265	†
C <sub>3</sub> H <sub>8</sub> O <sub>2</sub> CH <sub>3</sub> -O-CH <sub>2</sub> -O-CH <sub>3</sub>	76.0953	-346.967	-321.13	±8.	100.842	347.098		#
C <sub>3</sub> N <sub>2</sub> O NC-CO-CN	80.0449	247.5	246.523	±6.4	80.854	310.032	17.148	#
C <sub>3</sub> O <sub>2</sub>	68.0318	-93.64			67.37	276.816		†
C <sub>4</sub>	48.044	1033.904	1025.0		57.272	252.862	13.118	†
C <sub>4</sub> Cl <sub>2</sub> Cl-CC-CCl	118.94820	453.592	447.208	±8.	93.858	319.209	19.779	#
C <sub>4</sub> CL <sub>6</sub> Perchloro-1,3-Butadiene	162.0343	-96.65	-97.33		38.364	110.307		
C <sub>4</sub> F <sub>2</sub> FCC-CCF	86.03961	215.309	210.191	±8.	88.863	294.682	18.157	#
C <sub>4</sub> F <sub>6</sub> Perfluoro 1,3-Butadiene	162.0343	-1004.122			137.272	388.442	24.949	*
F <sub>6</sub> C <sub>4</sub> Perfluorocyclobutene	162.03439	-1210.843			131.589	379.256	25.135	*
C <sub>4</sub> F <sub>8</sub> Perfluorocyclobutane	200.03123	-1513.6			145.483	405.3		
C <sub>4</sub> F <sub>10</sub> FC-3110 Perfluorobutane	238.02803	-2137.417			189.038	480.624		
C <sub>4</sub> H	49.05194	803.328			66.759	265.569		
C <sub>4</sub> H <sub>2</sub> Butadiyne	50.05988	458.299	456.653	±8	73.738	249.613	14.328	#†
C <sub>4</sub> H <sub>2</sub> N <sub>2</sub> Fumaronitrile	78.072160	330.996	334.8	±8..	85.445	308.998	17.549	#
C <sub>4</sub> H <sub>3</sub> E,1-butene-3-yne-1-yl	51.06662	543.104	545.65	±8	71.773	281.767	14.371	#
C <sub>4</sub> H <sub>3</sub> i,1-butene-3-yne-2-yl	51.06662	501.829	502.00	±8..	77.383	305.368	16.739	#
C <sub>4</sub> H <sub>4</sub> 1-Butene 3-yne	52.07456	287.859	294.717	±8.	71612	277.319	14.292	#
C <sub>4</sub> H <sub>4</sub> Cyclobutadiene	52.07456	385.000	394.047		60.969	251.442	12.104	†
C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> PYRAZINE	80.08804	195.811	212.069	±1.3	73.945	280.378	13.562	#
C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> PYRIMIDINE	80.08804	196.648	212.864	±1.	73.69	280.677	13.645	#
C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> SUCCINONITRILE	80.08804	209.7	221.172	±0.9	92.458	325.114	18.349	#
C <sub>4</sub> H <sub>4</sub> O FURAN	68.07516	-34.685			65.407	267.251		
C <sub>4</sub> H <sub>4</sub> O VINYL-KETENE	68.07516	22.719	31.98	±8.	81.797	309.171	16.229	#
C <sub>4</sub> H <sub>4</sub> O <sub>2</sub> 1,4-DIOXIN	84.07456	-86.0	-71.5	±7.	81.291	284.693		#
C <sub>4</sub> H <sub>4</sub> S Thiophene	84.14176	114.9			72.818	278.778		
E-C <sub>4</sub> H <sub>5</sub> 1,3-butadiene 1-yl	53.08250	363.339	373.360	±8.	74.144	303.589	15.362	#
I-C <sub>4</sub> H <sub>5</sub> 1,3-butadiene-2-yl	53.08250	315.223	325.419	±8.	77.138	290.119	15.188	#
T-C <sub>4</sub> H <sub>5</sub> 1,2-butadiene-4-yl	53.08250	315.223	325.299	±8.	78.273	293.833	15.308	#
C <sub>4</sub> H <sub>5</sub> 1-butyne-3-yl	53.08250	316.530	325.987	±8.	81.528	293.864	15.928	#
C <sub>4</sub> H <sub>5</sub> N PYRROLE	67.09044	108.18		±0.81	71.6	270.722		
C <sub>4</sub> H <sub>5</sub> N Cyclopropanecarbonitrile	67.09044	184.096		±0.84	78.734	321.389		
C <sub>4</sub> H <sub>6</sub> 1-Butayn Ethylacetylen	67.09044	165.2	178.798	±0.88	81.820	291210	16.020	†
C <sub>4</sub> H <sub>6</sub> 2-ButaynDimethylacetylen	54.09044	146.314	159.388	±8.	77.886	291.909	16.544	†#
1,3-C <sub>4</sub> H <sub>6</sub> Butadiene	54.09044	110.834	125.118	±8.	74.219	293.330	15.335	†#
1,2-C <sub>4</sub> H <sub>6</sub> Butadiene	54.09044	161.314	175.436	±2.	78.663	290.993	15.496	#
C <sub>4</sub> H <sub>6</sub> Cyclobutene	54.09164	156.7	173.761		64.414	262.076	12.558	†
C <sub>4</sub> H <sub>6</sub> CL <sub>2</sub> 1,4-Dichlorobutene	124.99584	-51.882	-34.587	±8.	108.341	386.083	21.505	#
CL <sub>2</sub> C <sub>4</sub> H <sub>6</sub> 3,4-Dichlorobutene	124.99584	-53.572	-36.121	±8.	109.803	379.398	21.349	#
C <sub>4</sub> H <sub>6</sub> O 2,5 Di-Hydro FURAN	70.09104	-108.78			75.6	284.25		
C <sub>4</sub> H <sub>6</sub> O <sub>4</sub> CH <sub>3</sub> -CO-OO-CO-CH <sub>3</sub>	118.08804	-500.	-477.02	±10	122.291	390.682	23.944	#
2,5 C <sub>4</sub> H <sub>6</sub> S Dihydrothiophene	86.15764	86.9			83.306	297.089		
C <sub>4</sub> H <sub>7</sub> tt-1-Butene-1-yl	55.09838	245.871	262.755	±8.	83.705	311.281	16.968	#
C <sub>4</sub> H <sub>7</sub> cc-1-Butene-1-yl	55.09838		264.85	±8.	-	-		X
C <sub>4</sub> H <sub>7</sub> trans 1-Butene-2-yl	55.09838	231.162	248.45	±8.	83.973	300.371	16.425	#
C <sub>4</sub> H <sub>7</sub> cis 1-Butne-2-yl	55.09838		248.11	±8.	-	-		X
C <sub>4</sub> H <sub>7</sub> trans-2-Butene-2-yl	55.09838	223.853	239.743	±8.	83.237	313.256	17.962	#
C <sub>4</sub> H <sub>7</sub> cis-2-Butene-2-yl	55.09838		243.09	±8.	-	-		X
C <sub>4</sub> H <sub>7</sub> trans 3-Butene 1-yl Rad.	55.09838	204.595	220.915	±8.	84.719	317.348*	17.533	#
C <sub>4</sub> H <sub>7</sub> cis 3-Butene-1-yl Radical	55.09838		223.01	±8.	-	-		X
C <sub>4</sub> H <sub>7</sub> trans (CH <sub>2</sub> =CH*CHCH <sub>3</sub> )	55.09838	136.111	153.553	±8	80.787	306.087*	16.411	#
C <sub>4</sub> H <sub>7</sub> cis -1-Methylallyl Radical	55.09838		156.48	±8.	-	-		X

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C4H7 2-Methyl-Allyl Radical	55.09838	137.603	155.226	$\pm 5.$	82.196	300.803	16.229	#
C4H7 Cyclobutyl Radical	55.09838	230.306	249.366	$\pm 8.$	73.070	286.490	14.792	#
C4H7O 2-Butanone Radical	71.09778	-75.994	-57.670	$\pm 8.$	97.420	344.655	19.868	#
C4H7O CH <sub>2</sub> =C(CH <sub>3</sub> )CH <sub>2</sub> O*	71.09778	55.748	75.378	$\pm 8.$	96.143	334.259	18.562	#
C4H8 CH <sub>2</sub> =CH-CH <sub>2</sub> -CH <sub>3</sub>	56.107	-0.544			85.362	307.923	16.929	*
H8C4 CH <sub>2</sub> =C(CH <sub>3</sub> ) <sub>2</sub>	56.107	-17.161			87.976	296.668	17.470	*†
C4H8 2-Butene trans	56.107	-10.975			81.112	300.751	17.023	*†
C4H8 2-Butene cis	56.107	-7.426			85.227	295.879	17.242	*†
C4H8 CYCLOBUTANE	56.10752	28.4			70.564	264.396		†
C4H8CL <sub>2</sub> S Mustard	159.07772	-124.77	-100.66		136.283	420.586	27.569	#
beta HMX solid	296.15664	74.894	--		307.302	145.101	--	
C4H8N <sub>8</sub> O <sub>8</sub> HMX	296.15664	187.862	245.304	$\pm 25.1$	275.455	568.833	50.045	
C4H <sub>8</sub> O 2-Methyl-Allyl Alcohol	72.10572	-161.143	-137.34	$\pm 2$	100.007	316.183	18.622	#
C4H <sub>8</sub> O 2-BUTANONE	72.10572	-238.362			102.432	339.991		
H <sub>8</sub> C <sub>4</sub> O 2,3-Dimethyloxirane	72.10572	-137.658	-113.00	$\pm 8.$	95.471	303.780	17.777	#
OC <sub>4</sub> H <sub>8</sub> ETHYL-OXYRANE	72.10572	-115.960	-91.115	$\pm 8$	91.134	316.499	17.582	#
C4H <sub>8</sub> O Tetrahydrofuran, Oxolan	72.10572	-184.18			76.25	302.41		
C4H <sub>8</sub> O <sub>2</sub> 1,4 DIOXANE	88.10632	-314.428		$\pm 7.$	92.568	294.582		
(CH <sub>3</sub> COOH) <sub>2</sub> Acetic Acid dimer	120.1048	-929.015	-901.62		137.254	414.396	28.053	†
C4H <sub>8</sub> O <sub>4</sub> Tetraoxocan	120.10512	-620.2			116.255	340.343		
C4H <sub>8</sub> S Tetrahydrothiophen	88.17352	-34.1			92.55	309.627		
1,4-C4H <sub>8</sub> S <sub>2</sub> Dithiane	120.23952	0			109.655	326.252		*
1,3-C4H <sub>8</sub> S <sub>2</sub> Dithiane	120.23952	-10			110.434	333.542		
C4H <sub>9</sub> ,n-Butyl Radical	57.11426	81.80	105.91	$\pm 8.$	94.555	307.628		#†
i-C4H <sub>9</sub> iso-Butyl Radical	57.11426	73.785	97.92	$\pm 8.$	98.111	304.662	18.063	#
s-C4H <sub>9</sub> sec-Butyl Radical	57.11426	70.224	94.945	$\pm 8.$	86.395	327.417	17.538	#
C4H <sub>9</sub> ,t-Butyl Radical	57.11426	55.041	79.719	$\pm 8.$	82.410	323.393	17.010	#
C4H <sub>9</sub> N PYROLIDINE	71.1222	-3.59		$\pm 0.8$	82.112	309.206		
C4H <sub>9</sub> NO <sub>2</sub> Nitrobutane	103.121	-143.93	-109.63		115.119	369.874	21.040	
C4H <sub>9</sub> O n-BUTOXY RAD	73.11366	-56.350	-29.003	$\pm 8.$	101.894	337.600	19.314	#
C4H <sub>9</sub> O i-BUTOXY RAD	73.11366	-65.070	-36.703	$\pm 8.$	101.777	319.038	18.294	#
C4H <sub>9</sub> O s-BUTOXY RAD	73.11366	-69.84	-41.88	$\pm 8.$	102.025	327.058	18.700	#
C4H <sub>9</sub> O t-BUTOXY RAD	73.11366	-86.923	-58.899	$\pm 8.$	106.062	309.188	18.637	#
C4H <sub>10</sub> n-Butane	58.123	-125.790	-98.46	$\pm 0.67$	98.651	309.884	19.227	†
i-C4H <sub>10</sub> ISOBUTANE	58.123	-134.990	-106.37	$\pm 0.63$	96.643	295.493	17.936	†
C4H <sub>10</sub> FO <sub>2</sub> P SARIN	140.09437	-963.157	-927.62	$\pm 40$	161.667	412.013	29.468	#
C4H <sub>10</sub> N <sub>2</sub> 1,4-Piperazine	86.13568	32.058	70.65	$\pm 8.$	96.860	301.189	16.633	#
C4H <sub>10</sub> O-N 1-BUTANOL	74.1228	-274.68			108.168	361.616		
C4H <sub>10</sub> O-S 2-BUTANOL	74.1228	-292.629			111.134	363.877		
C4H <sub>10</sub> O-T 2-Methylpropanol	74.1228	-312.628			113.481	329.72		
C4H <sub>12</sub> Sn Sn(CH <sub>3</sub> ) <sub>4</sub>	178.84808	-20.502	+11.004	$\pm 4.2$	145.919	410.093	29.840	#
C4H <sub>12</sub> Sn H <sub>2</sub> Sn(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	178.84808	56.484	90.910	$\pm 4.2$	143.567	410.046	26.920	#
C4N <sub>2</sub> Carbon Subnitrid	76.0574	529.2	524.285	$\pm 0.8$	86.326	290.524	17.799	†
C <sub>5</sub>	60.05350	1050.924	1040.0	$\pm 60.$	75.507	271.676	16.192	†
C <sub>5</sub> F <sub>12</sub> FC 4-1-12	288.03584	-2543.311			229.036	555.108		
C <sub>5</sub> H	61.0629	778.276			65.158	260.415	12.013	*
C <sub>5</sub> H <sub>2</sub>	62.0709	691.412			82.981	266.639	14.674	*
C <sub>5</sub> H <sub>2</sub> CL <sub>2</sub> O CY	148.97418	-12.17	-5.59		111.295	349.650		#
C <sub>5</sub> H <sub>2</sub> CL <sub>3</sub> CY	168.42748	152.68	158.05		118.207	369.726		#
C <sub>5</sub> H <sub>3</sub> 1,3-Pentadiyne-5-yl Rad.	63.07882	602.58			87.499	295.196		
C <sub>5</sub> H <sub>3</sub> HCCCH*CCH	63.07882	564.61		$\pm 43$	93.241	306.147		
C <sub>5</sub> H <sub>3</sub> Cyclopentatriene-yl	63.07882	697.77		$\pm 75$	70.898	281.721		

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C5H3CL3O CY	185.43482	-104.72	-93.65	$\pm 8.$	139.671	397.902		#
C5H3N HCC-CH=CH-CN	77.08406	422.613	426.538	$\pm 8.$	93.766	318.598	18.380	#
C5H4 1,3-Pentadiyne	64.08526	411.835	416.818	$\pm 8.$	86.669	291.342	17.221	#
C5H4 1,4-Pentadiyne	64.08526	451.964	434.773	$\pm 8.$	89.940	305.243	17.191	#
C5H4 Pentane-Tetraene	64.08526	444.466	449.702	$\pm 8.$	86.132	287.480	16.968	#
H4C5 1,2-Pentadiene-4-yne	64.08526	433.354	438.929	$\pm 8.$	86.751	301.509	16.628	#
C5H4 1,2,4-Cyclo-Pentatriene.	64.08526	551.485		$\pm 9.$	73.235	279.6		
C5H4N *CH=CH-CH=CH-CN	78.09200	502.942	510.320	$\pm 8.$	97.601	341.652	19.160	#
C5H4N meta-Pyridyl Radical	78.09200	405.241	418.146	$\pm 8.$	74.123	292.227	13.634	#
C5H4O Cyclopentadiene-1-one	80.08616	55.229			80.941	289.977		
C5H4O2 3 ketene	96.08556	-105.834	-95.030	$\pm 8$	101.982	361.789	20.080	#
C5H5 1-Pentyne-3-ene-5-yl	65.09320	384.93	393.17	$\pm 8.$	94.137	324.558	18.196	#
C5H5 CY Cyclopentadienyl Rad.	65.09320	266.102			76.605	279.485		
C5H5N CH2=CH-CH=CH-CN	79.09994	238.944	250.471	$\pm 8.$	99.632	336.825	19.246	#
C5H5N PYRIDINE	79.10144	140.37		$\pm 0.54$	77.746	282.759		
C5H4OH CYCLO RAD	81.0941	66.526			95.625	310.007		
1,3C5H5O CY RADICAL	81.0941	59.8			90.023	307.695		
1,4C5H5O CY RADICAL	81.0941	103.3			90.479	307.805		
2,4-c-C5H5O CY RADICAL	81.0941	221.758			83.1	302.922		*
C5H5O2 2-pentenedialdehyde R	97.0935	-83.638			110.293	391.33		
C5H5O2 2-pentenedialdehyde R	97.0935	-72.76			113.89	387.94		
C5H6 1,2,4-Pentatriene	66.10264	252.295	264.571		93.878	318.687		
C5H6 1-ene-2-yne	66.10264	249.366			89.238	320.076		
C5H6 3-enE-1-yne	66.10264	256.479			94.424	314.637		
C5H6 CYCLOPENTADIENE	66.10264	134.3	151.43	$\pm 1.5$	75.368	274.152	13.535	†
C5H6N2 2-AMINOPYRIDINE	94.11612	118.616		$\pm 0.84$	103.84	309.401		
2,4-C5H5OH	82.10204	7.9			91.437	304.61		
1,3-C5H5OH	82.10204	-24.3			94.957	304.343		
1,4 C5H5OH	82.10204	-27.2			95.023	304.565		
C5H7 1,3-Pentadien-5-yl	67.10908	205.455	222.877	$\pm 8.$	92.672	325.606	17.484	#
C5H7 1,4-Pentadien-3-yl	67.10908	205.455	223.086	$\pm 8.$	93.92	323.195	17.275	#
C5H7 Cy 1-penten-1-yl	67.10908	172.623	192.745	$\pm 8.$	79.939	296.325	14.785	#
C5H7 Cy 1-penten-4-yl	67.10908	223.94	243.815	$\pm 8.$	80.499	290.579	15.031	#
C5H7CL	102.56178	58.091	76.235	$\pm 8$	110.072	374.067	21.352	#
C5H7CL2	138.01448	110.926	128.756	$\pm 8$	132.403	444.862	26.257	#
C5H7NO	97.11672	-108.7			120.7	387.6		
C5H7O 1-Cypenten-4-oxy Rad.	83.10848	95.04	117.53	$\pm 8.$	92.705	317.69		#
C5H8 1,3-Pentadiene	68.11702	84.157	105.770	$\pm 8.$	94.718	318.284	17.527	#
C5H8 ISOPRENE	68.11852	75.73			104.6	315.641		
C5H8 Cyclopentene	68.11852	33.9	58.183		81.275	291.379	14.857	†
C5H8CL CH2CICH=CHCH2CH2	103.56972	158.197	179.288	$\pm 8.$	119.551	399.520	22.640	#
PETN Solid	316.13828	-538.481		$\pm 0.84$	353.757	101.964		
C5H8N4O12 PETN	316.13828	-387.02	-332.00		294.758	614.706	53.542	
C5H8O Cyclopentanone	84.116420	-197.401	-171.29	$\pm 5.4$	97.436	309.296	17.366	#
C5H8O 1,5-Cyclopenten-2-ol	84.116420	-126.579	-99.582	$\pm 8.$	96.604	315.064	16.583	#
C5H9 CY	69.12496	111.131	138.404	$\pm 8.$	88.092	298.784	16.101	#
C5H9 2-PENTEN-5-YL	69.12496	174.615	196.937	$\pm 8.$	110.968	357.785	21.052	#
H9C5 2-PENTEN-1-YL	69.12496	116.700	140.617	$\pm 8.$	106.281	347.013	19.457	#
C5H9 3M-1-BUTEN3YL	69.12496	102.479	126.020	$\pm 8.$	107.506	333.972	19.833	#
C5H9 3M-1-BUTEN1YL	69.12496	219.091	243.190	$\pm 8.$	105.817	335.407	19.275	#
C5H9 3M-1-BUTEN4YL	69.12496	180.356	204.114	$\pm 8.$	108.450	348.534	19.616	#
C5H9N	83.1332	75.312		$\pm 8.4$	99.27	274.978		

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C5H10 1-PENTENE	70.13290	-21.28	+ 4.648		108.200	347.110	21.680	†
C5H10 2-PENTENE	70.1344	-31.757			108.449	340.41		
C5H10 2MB-1ene	70.1344	-36.317			109.956	339.532		
C5H10 2MB-2ene	70.1344	-42.551			105.018	338.569		
C5H10 2MB-3ene	70.1344	-28.953			118.616	333.465		
C5H10 Cyclopentane	70.1344	-77.1	-44.515		82.760	293.007	15.023	†
C5H10O TetraHydroPYRAN	86.1338	-224.283	-189.04	±0.84	96.359	301.959	16.710	#
N-C5H11 n-pentyl	71.14234	45.81	73.23		119.150	368.649	24.422	†
S-C5H11 1methyl-butyl	71.14234	45.564			119.653	369.949		
T-C5H11	71.14084	32.6	64.8	±8.	98.855	366.474	19.644	†
C5H11 neopentyl	71.14234	34.392			118.84	333.423		†
C5H11NO2 Nitropentane	117.14788	-164.431	-123.37	±2.1	137.100	390.905	23.792	
C5H12 PENTANE	72.14878	-146.76	-114.87		120.040	349.560	24.184	†
I-C5H12 Isopentane	72.14878	-153.70	-119.63		118.870	343.740	22.008	†
CH3C(CH3)2CH3 Neopentane	72.14878	-167.92	-135.02		120.830	306.000	23.179	†
C5H12O liquid MTBE	88.14968	-313.6	-293.85		187.510	265.650		
C5H12O Me-Tertiary Butyl Ether	88.14968	-283.7	-247.14	±0.8	138.010	355.489		#
C6 linear	72.0642	1313.	1302.33	±18.	84.585	300.600	17.770	#
C6CL6 Hexachlorobenzene	284.7822	-33.89			175.31	441.203		
C6D5 Deuterated phenyl radical	82.13651	315.700	327.525		94.997	300.504	15.919	†
C6D6 Deuterated Benzene	84.14881	58.157	73.86		100.398	282.629	16.325	†
C6F6 Hexafluorobenzene	186.05642	-956.63			157.938	384.457		
C6F14 FC 51-14Perfluorohexane	338.04364	-2949.201			269.551	629.592		
C6H	73.07394	1037.632			96.024	312.451		
C6H2	74.08188	700.82			104.103	299.19		†
C6H2CL3O Trichlorophenoxy ra	196.43758	-27.48	-20.29		140.508	398.583		#
C6H2CL3O Trichlorophenol Rad	196.43758	101.51	107.37		144.581	410.077		#
C6H2CL3O3 Peroxybiciclo Rad.	228.43638	131.42	142.99		174.462	429.942		#
C6H2CL3O3 Peroxybicyclo Rad	228.43638	28.95	40.414		171.330	433.035		#
C6H3	75.08802	682.016			100.896	319.344		
C6H3 Cy o-Benzyne-o-yl Rad.	75.08802	728.911	733.879	±8.	75.851	293.013	14.055	#
C6H3I Cy	201.99249	534.715	542.244	±12.	96.910	340.309	18.093	#
C6H3CL3O Trichlorophenol	197.44552	-189.07	-176.92		142.427	397.903		#
C6H3CL3O linear	197.44552	-19.83	+17.3		39.200	109.923		
C6H3CL3O2 CY	213.44492	-277.25	-263.99		162.216	420.242		#
C6H3(NO2)3 Trinitrobenzene	213.10464	62.342	82.617		205.633	485.335	37.794	
1,2-C6H4 o-BENZYNE	76.09596	461.135	470.128	±8.	78.406	283.240	14.265	#
1,3-C6H4 m-BENZYNE	76.09596	523.690	532.497	±8.	80.202	283.810	14.451	#
1,4-C6H4 p-BENZYNE	76.09596	574.254	582.364	±8.	85.476	282.239	15.147	#
C6H4 TRANS	76.09596	523.105	527.104	±8.	102.894	317.187	19.328	#
C6H4 CIS	76.09596	524.218	528.632	±8.	101.969	317.563	18.843	#
C6H4 HEXAPENTAENE	76.09596	568.263	572.160	±8.	99.977	309.859	19.359	#
C6H4 TRIENE-5YNE	76.09596	559.706	563.792	±8.	101.909	325.109	19.172	#
C6H4CL -ortho Radical	111.55046	303.173		±28.9	100.842	329.678		#
C6H4CL -metha Radical	111.55046	297.02		±28.0	101.165	329.135		#
C6H4CL -para Radical	111.55046	298.86		±28.0	101.264	329.476		#
C6H4CLO o-Chlorophenoxy Rad	127.54806	30.60	43.48		109.181	344.708		#
C6H4CLO Cy	127.54806	225.91	237.50		112.226	359.349		#
C6H4CL2O Dichlorophenol	163.00076	-167.01	-152.18		128.030	370.820		#
C6H4N4O2 4-Nitro-Phenyl-Azide	164.12172	389.7	410.723	±5.2	157.694	420.170	28.254	#
o-C6H4I Radical	203.00043	427.186	439.032		97.752	346.415	18.010	#
o-C6H4I2	329.90490	248.95	263.625	±5.9	113.052	386.892	21.778	#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
m-C6H4I2	329.90490	243.509	257.766		118.125	384.828	22.196	#
p-C6H4I2	329.90490	242.700	257.177		114.640	365.746	21.976	#
C6H4O2 O=C6H4=O	108.09656	-122.9			108.485	333.212		
C6H5 CHAIN	77.1057	531.368			109.472	339.195		
C6H5 PHENYL RAD	77.10390	339.740	353.657	$\pm 2.5$	76.656	286.072		#
C6H5 FULVENYL RAD	77.10390	467.315	479.324	$\pm 8.$	87.147	297.813	15.482	#
C6H5 FULVENYL Rad. Melius	77.1057	490.365		$\pm 52$	93.077	307.123		
C6H5Br Bromobenzen	157.0097	105.018			97.696	324.386		
C6H5BrO 2-Bromophenol	173.0073	-63.72	-39.09	$\pm 16.7$	115.957	352.602		#
C6H5Cl Chlorobenzen	112.5584	51.84			98.031	313.465		
C6H5ClO o-Chlorophenol	128.55600	-138.38	-121.06		113.660	343.513		#
C6H5ClO 2,4-Cy-hexadiene...	128.55600	-35.75	-19.81		113.199	352.445		#
C6H5ClO 2,5 Cy-hexadiene...	128.55600	-55.87	-39.79		113.969	346.868		#
C6H5F Fluorobenzen	96.1041	-116.566			94.433	302.629		
C6H5I Iodobenzen	204.00837	165.	181.038	$\pm 6.$	99.918	334.751	18.051	#
C6H5NO NITROSOBENZENE	107.11184	200.832			110.848	322.377		
C6H5NO2 NITRO-BENZENE	123.11124	68.534	88.137		120.38	348.800	20.903	
C6H5O PHENOXY RAD	93.10330	54.		$\pm 10.$	97.682	311.871		
C6H5O Cy-hexadiene-1one-2yl	93.10330	246.58	260.42		98.386	332.759		#
C6H5OO PEROXYPHENYL	109.1045	165.645			114.023	347.776		
C6H6(L)	78.11184	49.08	50.695		135.95	173.44	30.110	†
C6H6 BENZENE	78.11184	82.88	100.41		81.934	269.158	14.195	†
C6H6 FULVENE	78.11364	236.814		$\pm 10$	90.362	294.123		
C6H6 BENZVALENE	78.11364	384.9	403 ?	$\pm 8.3$	80.825	284.701		#
C6H6 1,5-Hexadiyne	78.11364	417.166	428.062	$\pm 8.$	111.036	336.936	20.829	#
C6H6 2,4-Hexadiyne	78.11364	369.100	379.830	$\pm 8.$	103.026	335.627	20.995	#
C6H6 1,3-Hexadiyne	78.11364	392.363	404.299	$\pm 8.$	107.021	328.174	19.790	#
C6H6 1,2,4,5 Hexatetraene	78.11364	396.229	407.942	$\pm 8.$	102.421	343.852	20.012	#
C6H6 1,2-Hexadiene-5-yne	78.11364	412.542			107.68	336.912		
C6H5OH PHENOL	94.11124	-96.399	-77.85		103.338	315.238	17.497	†
C6H6O 2,4-Cyclohexadiene1one	94.11124	-21.63	-3.31		99.188	322.935		#
C6H7 1,4 CYCLO Radical	79.11798	200.589		$\pm 35$	97.618	305.835		
C6H7 1,3,5-Hexatriene-6-yl	79.11798	431.387	446.410	$\pm 8.$	110.758	363.629	20.937	#
C6H7-1 CY C5H5-1-CH2*	79.11798	334.092	351.954	$\pm 6.3$	100.095	326.062	18.098	#
C6H7-3 CY C5H5-3-CH2*	79.11798	247.316	265.583	$\pm 19.2$	101.756	321.686	17.693	#
C6H7-1 CY C5H4-1*-CH3	79.11798	226.773	244.638	$\pm 12.5$	103.103	314.389	18.094	#
C6H5NH2(L) aniline	93.12832	31.50	37.774		191.92	191.060	34.020	†
C6H7N ANILINE	93.12832	87.04	--		108.385	319.27	--	
C6H8 DIHYDROBENZVALENE	80.12772	230.12	255.3	$\pm 8.3$	89.425	293.780		#
C6H8 CY 2,4-C5H5-1-CH3	80.12772	112.257	135.267	$\pm 8.$	95.574	310.854	17.183	#
C6H8 CY 2,4-C5H5-3-CH3	80.12772	102			116.8	310.3		
C6H8 1,3,5-HEXATRIENE	80.12772	152.214			107.911	330.388		
H8C6 (1,3-CYCLO)	80.12772	106.3			94.168	303.419		
C6H8 (1,4-CYCLO)	80.12772	109			94.053	296.34		
C6H9 1,3 hexadiene 5-yl Rad.	81.13566	173.49	195.692	$\pm 8.$	119.775	370.613	22.225	#
1,3-C6H9 hexadiene 6-yl Rad.	81.13566	265.533	286.651	$\pm 8.$	120.582	389.084	22.990	#
C6H9 Cyclohexenyl-3	81.13566	131.47	159.011	$\pm 8.$	97.860	313.685	16.886	#
C6H9 CY 1- C5H6-4-CH3-4-yl	81.13566	188.468	214.322	$\pm 8.$	103.489	321.009	18.574	#
C6H9 CY 1- C5H7-4-CH2*	81.13566	215.731	241.534	$\pm 8.$	106.551	323.588	18.625	#
C6H9 CY 1-C5H7-3-CH2*	81.13566	212.464	237.965	$\pm 8.$	104.037	333.573	18.926	#
C6H9 CY 1-C5H7-1-CH2*	81.13566	124.9			94.663	323.377		
C6H9I CY 1-C6H9-3-I	208.04013	69.036	99.331	$\pm 21.$	116.001	360.644	20.731	#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C6H10 1,3-HEXADIENE	82.14360	58.513	84.568	$\pm 8.$	120.575	372.675	22.606	#
C6H10 Cyclohexene	82.14360	-4.6	+26.79		101.464	310.632	17.271	†
C6H10 C5H7-CH3 Cypentene-4	82.14360	8.46	38.49	$\pm 8.$	101.249	309.518	17.208	#
C6H11 CH2=CHC3H6CH2*	86.15334	162.502	190.886	$\pm 8.$	127.963	417.768	24.512	#
C6H11 CH3CH=CHC2H4CH2*	86.15334	153.862	181.880	$\pm 8.$	129.760	404.206	24.878	#
C6H11 trans 3-hexene-6-yl Rad	83.15334	154.540	183.164	$\pm 8$	128.546	401.219	24.272	#
C6H11 CH2=C(CH2*)C3H7	83.15334	95.340	125.298	$\pm 8$	125.511	391.885	22.942	#
C6H11 CH2=C(CH3)C3H6*	83.15334	149.787			130.797	390.786		
C6H11 CH3C(CH2*)=CHC2H5	83.15154	90.847	121.134	$\pm 8.$	122.131	383.848	22.609	#
C6H11 CH3C(CH3)=CHC2H4*	83.15334	141.838			124.52	387.438		
C6H11 (CH3)2C=CHCH*CH3	83.15154	72.91	101.569	$\pm 8.$	128.105	375.530	24.237	#
C6H11 (CH3)CHCH*CH=CH2	83.15154	91.232	119.916	$\pm 8.$	135.913	384.042	24.212	#
C6H11 2-Methyl-1-pentene-4-yl	83.15154	136.913	165.834	$\pm 8.$	127.708	386.671	23.975	#
C6H11 Cyclohexy Radical	83.15154	75.839	110.421	$\pm 8.$	106.108	317.527	18.513	#
C6H11I Iodo-CycloHexane	210.05601	-50.0	-11.926	$\pm 4.7$	121.960	363.668	21.420	#
C6H12 TRANS-3-HEXENE	84.16128	-50.417	-17.218	$\pm 8.$	128.815	365.867	23.931	#
C6H12 1-HEXENE	84.16128	-41.95	-11.06		130.800	386.850	26.240	†
C6H12 2MP-1ene	84.16128	-59.371			135.603	382.167		
C6H12 2MP-2ene	84.16128	-66.86			126.608	378.443		
C6H12 4MP-2ene CIS	84.16128	-57.446			133.553	373.338		
C6H12 4MP-2ene TRANS	84.16128	-61.463			141.419	368.276		
C6H12 CYCLOHEXANE	84.15948	-123.3	-83.715		105.343	297.389	17.545	†
N-C6H13 n - HEXYL RAD.	85.16742	25.10	57.480		141.790	408.339	28.983	†
2-C6H13 2-HEXYL RAD.	85.16922	28.158	61.309	$\pm 8.$	147.533	428.452	28.213	#
C6H13 2MP-1YL	85.16922	35.635	70.799	$\pm 8$	140.892	399.411	26.200	#
C6H13 2MP-5YL	85.16922	32.367	67.427	$\pm 8.$	139.391	414.154	26.304	#
C6H13-S 2ME - 4PENTYL	85.16922	20.079	55.023	$\pm 8.$	141.737	402.960	26.420	#
C6H13-T 2ME 2PENTYL	85.16922	17.209	52.180	$\pm 8.$	139.289	404.566	26.392	#
C6H14(L) n-Hexan	86.17716	-198.660	-179.98		195.480	296.090	46.920	†
C6H14 n-Hexane	86.17716	-166.92	-130.02		142.59	388.85	28.702	†
H14C6 2-METHYLPENTANE	86.17716	-174.55			142.21	380.98		
C6H14 3MP	86.17716	-171.97			140.21	383.03		
C6H14 2,2-DMBUTANE	86.17716	-184.68			141.46	358.34		
C6H14 2,3-DMBUTANE	86.17716	-176.8			139.41	365.92		
C6N6O6 BENZOTRIFUROXAN	252.10284	N/A	N/A		200.972	416.395		
C7 linear	84.0749	1326.33	1313.33	$\pm 18.$	98.927	314.106	20.372	#
C7F16 Perfluoroheptane	388.05145	-3383.969			300.804	704.075		
C7H4	88.10666	676.13	682.585		100.798	312.080		#
C7H5N C6H5-CN Benzonitrile	103.12344	218.823			109.077	321.038		
TNT Solid	227.13122	-63.178		$\pm 5.0$	244.68	137.779		
C7H5N3O6 TNT	227.13122	24.1	53.992	$\pm 8.4$	215.417	481.936	37.698	#
C7H5N5O8 Tetryl Solid	287.1456	41.003			290.913	143.469		
C7H6O BENZALDEHYDE	106.12404	-36.8			111.673	336.019		
C7H7 2,4,6-Cycloheptatriene-1-yl	91.13048	280.696	298.308	$\pm 8.$	109.167	332.619	19.401	#
C7H7 BENZYL RADICAL	91.13048	208.0	226.8	$\pm 1.9$	109.700	318.229	18.178	#
C7H7 Quadricyclene Appex Rad.	91.13048	534.519	556.275	$\pm 2.2$	95.877	297.781		#
C7H7 Quadricyclene Basis Rad.	91.13048	581.346	603.316	$\pm 2.2$	90.683	299.778		#
C7H7 Quadricyclene Shoulder R	91.13048	588.94	611.424	$\pm 2.2$	90.774	299.687		#
TOLUENE(L)	92.13842	12.18	19.957		157.29	221.030	33.470	†
C7H8 TOLUENE	92.13842	50.17	73.476		103.279	320.187	17.940	†
C7H8 Norbornadiene	92.14052	247.6			96.748	295.226		
C7H8 (liq) Quadricyclene	92.13842	302.1		$\pm 2.2$	----	----		X



Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C7H8 Quadricyclene	92.13842	337.23	363.987	$\pm 2.2$	91.551	228.420		#
C7H8 1,3,5-Cycloheptatriene	92.14052	182.8			106.251	316.365		
C7H8 1,6-Heptadiyne	92.14052	395.8			134.202	379.7		
C7H8O CRESOL	108.13782	-132.298	-108.55		128.026	360.116	21.838	†
C7H8O BENZYL-ALCOHOL	108.13992	-100.416			115.529	330.58		
C7H10 3,5-dimethyl-CPD	94.1564	66.7			142.3	341.9		
C7H10 NORBORNENE	94.15640	90.	73.69	$\pm 30.$	103.136	306.087		
C7H10N2O2 Cyclo(Pro-Gly)	154.16658	-341.012	-301.25	$\pm 12.5$	158.210	401.299	27.301	#
C7H12 NORBORNANE	96.17228	-53.723		$\pm 8.4$	103.291	307.66		#
C7H12 CY-HEPTENE	96.17228	-9.4			120.422	324.001		
C7H13 1-Heptyl-4/5 ene	97.18022	132.2	194.632		148.532	435.136	--	
C7H14 n-HEPTENE	98.18816	-62.76	-26.9		153.500	425.600	30.790	†
C7H14 CY-HEPTANE	98.18816	-118.2			131.171	336.512		
C7H15 n-HEPTYL RAD.	99.1940	4.39	41.732		164.430	448.029	33.543	†
C7H15 NEOHEPTYL	99.1961	-4.853			163.769	414.969		
C7H15 NEOHEPTYL-2	99.1961	-15.941			160.737	405.848		
C7H15O 3,3dimethyl1-pentanoxy	115.1955	-142.256			171.86	328.026		
C7H16(L) n-Heptan	100.20194	-224.35	-201.87		224.980	328.560	52.640	†
C7H16 n-HEPTANE	100.20194	-187.78	-145.88		165.180	429.099	33.221	†
C7H16 i-Heptane	100.20194	-194.600	-150.40		164.500	420.500	30.920	†
C7H16 NEOHEPTAN	100.20194	-209.87			166.955	395.221		
C7H15OH n-Heptanol	116.20344	-339.741		$\pm 1.6$	178.605	480.449		
C7H15OH Neoheptanol	116.20344	-359.657			179.907	448.901		
C8H	97.09594	1162.06			132.416	358.74		
C8H2	98.10388	934.287			132.638	347.69		
C8H6 C6H5CCH	102.13564	328.151			115.734	327.918		
C8H6O BENZOFURANE	118.13264	17.0	37.048	$\pm 1.5$	111.964	326.193		#
C8H6O2 Benzodioxin	134.13204	-71.2	-49.95	$\pm 6.$	128.967	347.408		#
C8H6S BENZOTHIOPHENE	134.20164	166.272			131.558	337.481		
C8H7 STYRENE RADICAL	103.14358	389.112			127.45	344.397		
C8H7N INDOLE	117.15032	156.5		$\pm 1.25$	121.264	332.373		
C8H8 CUBANE	104.14912	651.7		$\pm 30$	98.47	271.426		
C8H8 STYRENE	104.14912	148.3	169.66	$\pm 2.$	120.190	344.770	20.940	†
C8H9 C6H5CH2CH2*	105.15706	237.714	262.114	$\pm 8.$	130.543	364.717		#
C8H10 C6H5C2H5	106.1650	29.790	58.81	$\pm 8.$	129.799	353.746		†#
C8H10 Di METHYLBENZENE	106.16699	17.994			125.745	352.115	21.974	*
C8H14 CH(-CH2-CH2-)3CH	110.19676	-99.035	-51.705	$\pm 1.$	125.174	327.572	20.374	#
C8H15 1-Octen-4-yl	111.20710	109.1			172.717	481.400		
1-C8H16 1-OCTENE	112.2144	-83.59	-42.768		176.100	464.840	35.350	†
C8H16 CycloOctane	112.21264	-124.4	-72.762	$\pm 1.$	146.194	366.725		#
N-C8H17 N-OCTYL RAD	113.2223	-16.32	+25.983		187.070	488.879	38.103	†
C8H18(L) n-Octane	114.22852	-250.260	-227.11		254.150	361.071	61.490	†
C8H18 OCTANE	114.22852	-208.75	-161.89		187.780	468.480	37.780	†
C8H18(L) isooctane	114.22852	-259.160	-224.71		239.000	328.110	50.190	†
C8H18 ISO-OCTANE	114.22852	-224.01	-171.54		188.410	423.090	32.170	†
C8H20Pb (C2H5)4Pb Liquid	323.4444	53.0		$\pm 5.$				X
C8H20Pb (C2H5)4Pb Gas	323.4444	109.6	169.315	$\pm 5.1$	233.217	477.890		#
C9H4 C(CCH)4	112.12806	913.78	918.435		126.858	330.747		#
C9H7 INDENYL	115.15458	285.6		$\pm 22$	128.21	342.843		
C9H7N QUINOLINE	129.16132	200.52			129.153	344.075		
C9H7N ISOQUINOLINE	129.16132	204.61			128.983	344.568		
C9H8 INDENE	116.16252	164.138		$\pm 1$	124.226	335.846		

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C9H10 METHYLSTYRENE	118.1784	112.968			146.858	383.673		
C9H12 C(CH=CH2)4	120.19158	250.6	279.18		174.032	417.887	31.734	#
C9H12 1,3,5-Trimethylbenzene	120.19158	-16.067	44.22 ?		147.800	385.300		
C9H12 1,2,4-Trimethylbenzene	120.19158	-13.933	46.36 ?		154.508	395.765		
C9H17 1-Nonenyl Radical	125.23398	88.400			195.709	520.900		
C9H18 1-Nonene	126.24192	-432.207			200.269	505.000		
C9H18O6 cyTriAcetoneTriPeroxy	222.23562	-395.472	-331.52	$\pm 22$	302.788	499.584	47.780	#
N-C9H19 n-NONYL RAD	127.2491	-37.03	+10.234		209.710	527.419	42.664	†
N-C9H20 liq. NONANE	128.2578	-275.475			284.386	393.673		
N-C9H20 NONANE	128.2578	-228.907	-177.09		210.413	506.431	42.342	
C10D8 NAPHTHALENE-D8	136.22281	118.111			156.96	350.669	23.646	*
C10H6 Naphtyne	126.15764	500.825	515.5		132.178	347.542	21.264	
C10H7 Naphtyl Radical	127.16558	396.225	415.418		132.216	352.133	20.980	
C6H4(C2H)CH=CH*	127.16558	617.140	634.110		144.841	367.587	23.203	
C10H7O* Naphthol Radical	143.15498	115.478	136.47		146.882	373.015	23.522	
H8C10 AZULENE	128.17352	279.932			128.868	338.065	20.368	*
C10H8 NAPHTHALENE	128.17352	150.582	174.276	$\pm 1.5$	131.920	333.267	20.713	†
C10H8O Naphtol	144.17292	-30.794	-6.37		154.318	368.709	24.318	#
C10H9 2-HydroNaphthalen Rad	129.17846	229.534	255.533		143.289	363.659	22.643	
C10H9 1-Methyl-1-Indenyl Rad	129.17846	262.337	287.549	$\pm 20$	144.004	369.098	23.429	#
C10H9 1-Methylene-Indene Rad	129.17846	337.649	363.520	$\pm 20$	144.045	364.065	22.771	#
C10H9 2-Methylene Indene Rad	129.17846	266.5		$\pm 20$	-	-		X
C10H10 1,2-DihydroNaphthalene	130.1864	117.152	147.213		143.955	359.383	22.797	
C10H10 1,1'-BiCyclo-Pentadiene	130.1864	291.625	320.336		143.016	385.011	24.164	#
C10H10 2,2''-BiCycloPentadiene	130.1864	291.056	318.773		150.301	386.504	25.159	#
C10H10 1-Methyl Indene	130.1864	184.933	214.695	$\pm 20$	144.346	360.391	23.113	#
C10H10 2-Methyl Indene	130.1864	173.636	202.811	$\pm 20$	146.240	364.509	23.701	#
C10H10 3-Methyl Indene	130.1864	173.218	202.400	$\pm 20$	146.056	364.755	23.694	#
C10H13 C5H7-C5H6*	133.21322	176.65			36.209	98.360		
C10H14 C5H7-C5H7	134.22116	66.52			154.175	405.346		
11-C10H15 JP-10 apex Radical	135.22910	105.650	157.726		142.526	359.233	21.970	#
6-C10H15 JP-10 Tert side Rad.	135.22910	96.32	149.14		138.190	355.345	21.225	#
C10H15 C5H8*-C5H7	135.22910	171.54	218.396	$\pm 125.5$	155.918	417.467		
C10H16 JP-10	136.23404	-86.856	-31.374		152.560	359.201	22.997	†
C10H19 1-Decenyl 4/5 Radical	139.26086	67.900			218.653	560.300		
C10H19 1-Decenyl 3 Radical	139.26086	2.600			221.077	567.300		
C10H20 1-Decene	140.26880	-123.900			223.362	544.500		
C10H20 2-Decene-trans	140.26880	-136.200			222.222	541.000		
C10H20 3-Decene-trans	140.26880	-135.500			220.659	542.600		
N-C10H21 n-DECYL 1-Radical	141.27374	-57.74	-5.514		232.350	567.109	47.224	†
C10H21 n-Decyl - 2-Radical	141.27674	-58.100			230.534	567.300		
C10H21 n-Decyl-3/4 Radical	141.27674	-58.200			230.534	567.300		
N-C10H22 liq DECANE	142.28468	-301.039			314.511	425.889		
N-C10H22 gas-DECANE	142.28468	-249.534	-192.75		233.049	545.677	46.903	
1-C10H7C*O Naphtaldehyde Rd.	155.17598	174.891	193.741		161.693	399.949	26.717	
1-C10H7CHO Naphtaldehyde	156.18392	30.543	54.59		162.397	383.881	25.754	
1-C10H7-CH2* Methyl-Naphthyl	141.19246	272.797	297.846		158.090	378.770	24.645	
1-C10H7-CH3 MethylNaphthalen	142.20040	116.106	145.0		157.922	381.348	25.026	
C11H24 N-UNDECANE	156.31156	-270.286	-208.54		255.684	584.923	51.463	
O-C12D9 O-BIOPHENYL R	162.25892	386.58			195.578	428.768		*
C12D10 BIPHENYL - D	164.27302	138.488	162.92		200.307	413.489		*
C12H4CL4O 2,3,6,7	305.97036	-50	-35.924	$\pm 10$	225.108	496.028	38.205	

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C12H4CL4O 2,4,6,8	305.97036	-58	-44.108	$\pm 10$	225.552	493.238	38.388	
C12H4CL4O2 2,3,7,8	321.97336	-136.1	-120.71	$\pm 10$	241.524	513.049	41.226	#
C12H4CL4O2 1,3,6,8	321.97336	-128.7	-113.55	$\pm 17$	241.759	521.354	41.467	#
C12H4CL4O3 1,3,6,8	337.97276	-295.37	-278.36		256.811	533.525	43.948	
C12H4CL5O2 6-2' ether radical	357.42606	-128.11	-115.13	$\pm 25.1$	265.216	609.381	48.225	
C12H4CL6O2 2-6' ether radical	392.87876	-146.44	-132.30		284.786	628.505	51.665	
C12H4CL6O2 Biphenyl-diol	392.87876	-321.92	-305.6	$\pm 33.5$	286.707	573.925	49.483	
C12H5CL3O3 2,4,7 trichloro	303.52800	-348.99	-329.03		241.279	505.020	40.642	
C12H5CL4O2 6-6' ether radical	322.98130	-85.52	-69.659	$\pm 25.1$	250.467	582.730	44.993	
C12H5CL4O3 radical	338.97710	-432.42	-412.55	$\pm 62.8$	265.578	551.043	45.331	
C12H5CL4O3 radical	338.97710	-321.79	-301.82	$\pm 62.8$	263.787	550.127	45.226	
C12H5CL5O2 6-6' ether	358.43400	-250.16	-232.43	$\pm 21.$	270.758	585.917	47.711	
C12H6CL2O DCDF	237.08084	5.2	25.245	$\pm 24.7$	192.255	439.242		#
C12H6CL2O2 DCDD	253.08024	-89.3	-67.92	$\pm 26.6$	209.088	461.386		#
C12H6CL4O2 6-2' ether	323.98564	-207.57	-187.21		256.821	561.466	44.729	
1-C10H7-C $\equiv$ C* EthynylNaphthyl	151.18758	694.962	710.644		162.077	397.847	26.598	
C12H8 Acenaphthylene	152.19552	259.7		$\pm 5.9$	154.775	358.632		
C10H7-C $\equiv$ CH EthynylNaphthalen	152.19552	379.070	398.592		169.895	391.974	26.992	
C12H8O Di-Benzo-Furan	168.19492	55.2	80.812	$\pm 4.8$	163.566	375.274	25.229	
C12H8O2 Di-Benzo-p-Dioxin	184.19432	-50.1	-23.24	$\pm 2.2$	180.004	396.647	28.336	#
1-C10H7-CH=CH* Vinyl-Naphthy	153.20346	469.863	492.963		172.891	404.234	27.649	
1-C10H7-C*=CH2	153.20346	412.208	434.879		175.034	407.260	28.077	
O-C12H9 O-BIPHENYL RAD	153.2031	427.73	451.889		163.048	405.110	26.589	†
C12H9CL	188.65616	148.55			178.868	433.51		
C12H9N CARBAZOLE	167.2102	200.7			176.877	388.305		
1-C10H7-CH=CH2	154.21140	215.058	242.302		173.671	400.851	27.738	
C12H10 BIPHENYL	154.21140	182.13	210.329		166.179	388.941	26.783	†
C12H10 1-C10H7-CH2CH2*	155.21934	292.88	322.861		185.266	418.370	29.235	
C12H10 1-C10H7-CH*-CH3	155.21934	220.497	250.340		184.272	426.717	29.373	
1-C10H7-C2H5 EthylNaphthalen	156.22728	96.901	131.723		181.943	406.323	28.829	
C12H12O 1-C10H7CH2CH2OH	172.22668	-52.718	-16.807		195.002	447.806	31.880	
C12H23 liquid JET-A(L)	167.31102	-303.469	--		350.336	448.112	--	†
C12H23 JET-A	167.31102	-211.46	--		293.494	612.539	--	†
C12H26 N-DODECANE	170.33844	-290.872	-224.17		278.32	624.253	56.024	
C13H9N ACRIDINE	179.2212	273.9			177.643	394.998		
C13H9N PHENANTHRIDINE	179.2212	240.5			184.131	391.6		
C14H6(NO2)6 solid HNS	450.23068	58.07		$\pm 10.$				X
C14H6(NO2)6 HexaNitroStilbene	450.23068	238.4	285.396		411.150	773.618	71.248	#
C14H10 ANTHRACENE	178.2334	230.1			184.993	392.693		
C14H10 PHENANTHRENE	178.2334	207.1			186.787	394.614		
C14H12 solid t-Stilbene	180.24508	136.73		$\pm 10.$				X
C14H12 trans-Stilbene	180.24508	223.3	255.957	$\pm 4.$	203.066	447.878	32.901	#
C14H14 BIBENZYL	182.26096	135.6	175.94	$\pm 1.3$	202.411	477.207	33.684	#
C16H10 PYRENE	202.2554	225.7	---		202.501	407.513	--	
C16H33 2-HEXADECYL Rad.	225.43802	-181.67	-25.09?		366.100	818.976	--	#
C16H34 n-HEXADECANE	226.44596	-374.51	-213.7?		370.284	780.943	--	#
C18H12 Naphthacene	228.29327	290.000			233.343	441.654		
C18H12 Triphenylene	228.29327	274.2			236.543	441.657		
C20H10 Corannulene	250.29340	463.712	495.843	$\pm 7.3$	216.018	412.967	31.264	#
C20H12 Perylene	252.30938	205.058	239.058	$\pm 20.5$	254.201	475.499	37.878	#
C22H14 Pentacene	278.35315	355.000			281.951	494.186		
C22H14 Pentafene	278.35315	345.000			282.920	501.187		

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
C24CL12 Perchloro-coronene	713.68920	146.6	146.7	$\pm 35.$	458.824	803.678	80.264	#
C24H12 Coronene	300.35208	307.5	345.262	$\pm 10.$	262.602	458.935	38.331	#
C24H17 Triphenylbenzene Rad.	305.39898	623.2			323.134	652.000		
C24H18 Triphenylbenzene	306.40692	373.05			327.478	621.65		
C60 Buckminster Fullerene	720.66	2585.7		$\pm 105.$	560.816	591.403		
C70 Footballene	840.77	2652.	2660.33	$\pm 34.$	558.171	589.537		#
JET-A(L)	167.31102	-303.469	-		350.336	448.112	-	†
JET-A(G) (C12H23)	167.31102	-211.46	-		293.494	612.539	-	†
Ca (S) REFERENCE ELEMENT	40.07800	0.	0.		25.75	42.536		‡
Ca (gas)	40.07800	177.8	177.386	$\pm 0.8$	20.786	154.887		†
Ca+	40.07740	773.2		$\pm 0.2$	20.786	160.650		
CL	35.4527	121.302	119.633	$\pm 0.008$	21.838	165.192		†
DCL	37.4668	-93.359	-93.333	$\pm 0.21$	29.170	192.773	8.661	*†
DOCL	53.4662	-78.539	-76.648	$\pm 2.1$	38.585	240.321	10.325	*†
CLF	54.4511	-50.293		$\pm 0.42$	32.082	217.939		*
CLF3	92.44791	-158.851		$\pm 2.9$	63.996	281.633		*
CLO	51.4521	101.218		$\pm 2.1$	31.558	226.646		*†
CLO2 (OCIO)	67.4515	104.599		$\pm 6.3$	42.003	257.213		*†
CLOO	67.4518	96.238			43.982	264.994		*
CLO3F	102.4493	-23.799	-15.076		64.927	278.989	13.299	†
CL2 REFERENCE ELEMENT	70.9054	0	0		33.949	223.082		*‡
CL2O	86.9048	87.868		$\pm 6.7$	47.884	267.976		*†
CL2O2	102.9042	138.976			65.034	295.883		
Cr(cr) REFERENCE ELEMENT	51.9961	0	0		23.434	23.618		*‡
Cr	51.9961	397.48		$\pm 4.2$	20.786	174.313		
CrCl	87.4488	129.9	129.159	$\pm 2.7$	34.684	249.790	9.389	#
CrClO		-117.9		$\pm 9.6$		301.01	13.574	X
CrClO2		-310.3		$\pm 21.6$		309.81	14.449	X
CrCl2	122.9015	-117.6	-120.00	$\pm 1.7$	59.00	319.36	15.638	X
CrCl2O		-336.5		$\pm 22.5$		333.03	16.784	X
CrCl2O2	154.90030	-519.2	-515.35	$\pm 4.2$	84.052	329.53	18.066	#
CrCl3		-283.		$\pm 6.1$		347.03	19.101	X
CrCl3O		-507.8		$\pm 3.0$		357.32	20.049	X
CrCl4		-396.5		$\pm 13.8$		371.92	22.480	X
CrCl5		-389.6				407.16	26.602	X
CrCl6	264.71230	-345.3	-344.58	$\pm 50. ?$	143.573	414.95	30.878	#
CrN(s)	66.00284	-117.294		$\pm 8.4$	51.093	37.215		*
CrN	66.00284	505.022		$\pm 20.9$	30.753	230.553		*
CrO	67.9955	188.285		$\pm 41.8$	31.33	239.27		*
CrO2	83.9949	-75.313		$\pm 41.8$	43.404	269.245		*
CrO3	99.9943	-292.88	-318.00	$\pm 41.8$	56.124	266.201	13.040	*
Cr2N(s)	117.99894	-125.532		$\pm 12.6$	66.318	64.921		*
Cr2O3(s)	151.9904	-1135.094		$\pm 8.4$	120.644	79.812		*
Cr2FeO4	223.8348	-1458.124			133.69	141.963		
Cr3C2(S)	180.0103	-85.354			99.326	85.437		
Cr7C3(S)	400.0057	-160.666			209.764	200.999		
C6Cr23	1267.9763	-328.444			628.117	612.119		
D	2.0141	221.717	219.804	$\pm 0.001$	20.786	123.352	6.197	†
D+	2.01355	1540.320	1532.210	$\pm 0.001$	20.786	117.585	6.197	†
D-	2.01465	142.753	147.037		20.786	117.592	6.197	†
DF	21.01251	-276.228	-276.17	$\pm 0.8$	29.139	179.704	8.638	*†
HD	3.02204	0.322	0.332		29.200	143.801	8.509	†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
HD+	3.02149	1496.793	1490.50		29.334	155.552	8.614	†
HDO	19.02144	-245.280	-242.35		33.798	199.517	9.926	†
HDO2	35.02084	-140.242	-134.38		43.779	243.581	11.335	†
OD	18.01350	37.226	36.852		29.939	189.666	8.999	†
OD-	18.01405	-145.378	-139.2		29.143	178.409	8.642	†
DO2	34.0129	6.487	9.387		35.845	232.883	10.065	†
SD	34.080102	140.14	140.17	±0.52	29.239	198.212	8.666	#
D2 REFERENCE ELEMENT	4.0282	0	0		29.195	144.96	8.569	±
D2+	4.02766	1498.586	1492.29		29.510	156.735	8.651	†
D2-	4.02875	235.161	241.213		30.315	158.261	8.714	†
D2O	20.0276	-249.209		±0.067	34.256	198.342	9.960	†
D2O2	36.027	-144.3	-138.61		45.252	242.085	11.563	†
D2S	36.0942	-24.047	-21.114	±0.8	35.795	215.316	10.089	†
ELECTRON GAS e-	0.00055	0	0		20.786	20.979	6.197	*±
F	18.9984	79.39	77.274	±0.3	22.747	158.752	6.518	†
FO	34.9978	111.267	110.632	±0.69	31.995	216.396	9.388	†
FO2 O-F-O	50.9972	378.6	381.154	±20	41.126	251.289	10.538	†
FO2 F-O-O	50.9972	25.4		±2	44.453	259.511	11.256	†
F2 REFERENCE ELEMENT	37.99681	0	0		31.304	202.792	8.825	†
F2O F-O-F	53.99621	24.5	26.754	±2	43.495	247.508	10.912	†
F2O2 F-O-O-F	69.99561	32.87	36.597	±1.3	62.073	277.214	13.778	†
Fe(a) REFERENCE ELEMENT	55.847	0	0		25.094	27.321		*±
Fe	55.847	415.5		±1.3	25.675	180.49		
Fe+	55.84645	1181.144			26.068	181.859		
Fe-	55.84755	393.338			25.023	180.2		
FeCL	91.2997	251.036		±84.	38.245	257.577		*
FeCL2(s)	126.7524	-341.841		±0.42	76.707	117.954		*
FeCL2	126.7524	-141		±2.1	57.624	299.297		*
FeCL3(s)	162.2051	-399.405		±0.84	96.651	142.338		
FeCL3	162.2051	-253.12		±5	77.78	344.226		*
FeO(s)	71.8464	-272.037			49.972	60.754		*
FeO	71.8464	251.047		±20.9	31.415	241.926		*
Fe(OH)2(s)	89.86168	-574.059		±2.9	97.079	87.875		*
Fe(OH)2	89.86168	-330.536		±2.1	71.505	283.092		
Fe(OH)3(s)	106.86902	-832.627		±12.6	101.928	104.627		*
FeS(a)	87.913	-101.818		±0.8	50.214	59.883		*
FeS(G)	87.911	370.767			34.002	252.344		
FeSO4(s)	151.9106	-928.877		±8.4	100.666	120.949		*
FeS2(s)	119.979	-171.549		±2.1	62.18	52.926		*
Fe2CL4	253.5048	-431.374		±4.2	125.966	464.528		*
Fe2CL6	324.4102	-654.378		±8.4	173.665	536.945		
Fe2O3(S) Solid-A Hematite	159.6882	-824.248			103.866	87.404		
Fe3C (S) Solid-A	179.546	25.104			105.868	104.6		
Fe3O4(S) Solid-A Magnetite	231.5326	-1118.383			150.73	146.147		
GeBr	152.5140	137.438	144.470	>±4.2	37.250	257.225	9.864	†
GeBr2	232.4180	-60.963	-46.00	±5.	55.757	319.172	14.193	†
GeBr3	312.3220	-119.031	-96.164	>±50.	78.139	363.175	18.549	†
GeBr4	392.2260	-291.	-261.29	±6.	101.687	396.195	23.963	†
GeCl	108.0627	69.030	68.66	±18.	36.990	245.904	9.599	†
GeCl2 singlet	143.5154	-166.9	-166.39	±5.	53.806	296.332	13.307	†#
GeCl2 triplet	143.5154	102.3	102.525	±5.	54.217	307.835	13.593	#
GeCl3	178.9681	-234.4	-233.69	±5.	76.149	338.232	17.700	†#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
GeCl <sub>4</sub>	214.4208	-500.9	-498.55	±5.	95.975	348.572	21.150	†#
GeH <sub>3</sub> Cl	111.08652	57.70	67.63	±5.	54.795	273.113	11.995	#
GeH <sub>4</sub>	76.64176	90.3	101.125	±5.	45.011	217.303	10.748	†#
H	1.00794	217.998	216.034	±0.001	20.786	114.718	6.197	†
H+	1.00739	1536.244	1528.084	±0.001	20.786	108.948	6.197	†
H-	1.00849	139.031	143.246	±0.001	20.786	108.961	6.197	†
HBr	80.91194	-36.29	-28.45	±0.16	29.141	198.699		
HCL	36.46094	-92.31	-92.125	±0.10	29.136	186.901		
HOCL	52.46004	-75.741	-72.8		37.285	236.587		
HF	20.00634	-273.3	-273.25	±0.7	29.137	173.778		
HOF	36.00574	-96.898	-94.		35.94	226.757		
HI	127.91241	26.5	28.676	±0.1	29.153	206.589		*
HNO	31.01408	106.842	109.809	±0.125	33.880	220.920	9.942	†
HNO <sub>2</sub>	47.01348	-78.452	-72.8	±0.6	46.320	254.071	11.597	†
HNO <sub>3</sub>	63.01288	-134.3	-124.58	±0.5	54.092	266.816	11.876	#
OH	17.00734	37.3	37.1	±0.3	29.886	183.737	8.813	#
OH+	17.00679	1290.204			29.196	182.746		
OH-	17.00789	-143.199	-150.81		29.141	172.433		
HO <sub>2</sub>	33.00674	12.552			34.893	229.106		†
HPO	47.9811	-56.869			35.81	235.685		
SH	33.07394	141.87	141.212	±0.52	32.446	195.751	9.274	#
SOH	49.07334	-20.895		±42	36.707	239.818		
HSO	49.07334	-4.782		±7.3	37.659	242.486		
HO <sub>2</sub> S	65.07274	-255.88		±6	50.708	276.742		
HSO <sub>3</sub>	81.07214	-385			67.209	294.061		
HS <sub>2</sub> Hydrothiosulpheno Radical	65.13994	104.60	107.145	±10.46	39.703	253.304	10.484	#
H <sub>2</sub> REFERENCE ELEMENT	2.01588	0	0		28.836	130.679		*‡
H <sub>2</sub> F <sub>2</sub>	40.01269	-569.924	-566.5		58.132	260.905		
H <sub>2</sub> O(L)	18.01528	-285.83			75.351	69.939		†
H <sub>2</sub> O	18.01528	-241.826		±0.04	33.588	188.829		†
H <sub>2</sub> O <sub>2</sub> (L)	34.01468	-187.778	-193.58		89.328	109.604	22.949	†
H <sub>2</sub> O <sub>2</sub>	34.01468	-135.88	-129.89	±0.2	42.416	234.542	11.162	#
H <sub>2</sub> S	34.08188	-20.6			34.248	205.803		
H <sub>2</sub> SO <sub>4</sub> (L)	98.07948	-814.01			138.594	156.907		*†
H <sub>2</sub> SO <sub>4</sub>	98.07948	-732.7	-720.85	±2.0	90.235	311.333	18.391	#
H <sub>2</sub> S <sub>2</sub>	66.14788	15.500	21.243		48.745	251.070	11.549	
H <sub>3</sub> F <sub>3</sub>	60.01903	-883.677	-873.		73.884	280.947		
H <sub>3</sub> O+	19.02267	598			35.485	193.139		
H <sub>4</sub> F <sub>4</sub>	80.02537	-1186.932	-1174.		104.022	350.016		
H <sub>5</sub> F <sub>5</sub>	100.03172	-1490.188	-1475.		134.161	417.286		
H <sub>6</sub> F <sub>6</sub>	120.03806	-1805.545	-1788.		163.735	486.619		
H <sub>7</sub> F <sub>7</sub>	140.0444	-2099.699	-2080.		194.438	548.654		
He REFERENCE ELEMENT	4.0026	0	0		20.786	126.154	6.197	*‡
He+	4.00205	2378.519	2372.322	±0.001	20.786	131.915	6.197	†
Hg(L) REFERENCE ELEMENT	200.5900	0	0		27.978	76.028		
Hg (gas)	200.5900	-61.38	-64.53	0.04	20.786	174.972		†
HgBr <sub>2</sub> (solid)	360.398	-169.457			75.312	170.778		†
HgBr <sub>2</sub> (gas)	360.398	-85.452			60.319	320.239		†
HgCl (gas) Calomel	236.0427	78.45			36.34	260.0		
HgCl <sub>2</sub> (solid)	236.0427	-230.12						
HgCl <sub>2</sub> (liquid)	236.0427	-213.22						
HgCl <sub>2</sub> (gas) from 1500 K and up	271.4954	-146.29			----	-----		

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
HgO (solid)	216.5894	-90.789	-86.208	0.1	44.132	70.282		†
I	126.90447	106.76		$\pm 0.04$	20.786	180.789		
INO2 NITRO-IODINE	172.91001	60.25			59.366	294.432		
IO	142.90387	126		$\pm 18$	33.117	239.835		
IO2 O-O-I	158.90327	116.5		$\pm 40$	48.727	296.374		
IO2 O-I-O	158.90327	159.3		$\pm 25$	46.697	281.231		
IO3	174.90267	241.9		$\pm 50$	61.56	292.975		
I2	253.8089	62.444			36.889	260.584		*
I2O I-I-O	269.80834	106.7		$\pm 40$	52.359	330.647		
I2O I-O-I	269.80834	119.5		$\pm 25$	51.874	308.111		
K(S) REFERENCE ELEMENT	39.09830	0	0		29.6	64.680		‡
K (gas)	39.09830	89.0	89.82	$\pm 0.4$	20.786	160.470		†
K+	39.09775	514.0		$\pm 0.4$	20.786	154.578		
KNO3(S)	101.10320	494.0	-488.31	$\pm 0.5$	95.060	132.900		†
KNO3	101.10320	-315.833	-307.31		68.358	311.473	15.917	†
K2O	94.19600	-74.09	-87.945		54.180	286.548		†
K2O2	110.19540	-191.566	-207.86		70.589	306.461		†
Kr REF ELEMENT	83.8	0	0		20.786	164.086	6.197	*‡
Kr+	83.79945	1356.954	1350.76	$\pm 0.001$	20.786	175.613	6.197	†
Mg (S) REFERENCE ELEMENT	24.30500	0	0		24.775	32.535-		‡†
Mg(L)	24.30500	4.79		?	---	---		
Mg (G)	24.30500	-147.10	145.90	$\pm 0.8$	20.786	148.649		†
Mg+	24.30445	891.047	883.65	$\pm 1.3$	20.786	154.412	6.197	†
MgAl2O4 (S)	142.26568	-2299.11			116.163	88.781		†
MgAl2O4 (L)	142.26568	-2106.53			---	---		†
MgBr	104.2090	-35.34	-27.7	$\pm 41.8$	35.645	244.952		†
MgBr2(S)	184.1130	-524.6		$\pm 2.1$	73.298	117.143		†
MgBr2(L)	184.1130	-490.41			----	---		†
MgBr2	184.1130	-302.92		$\pm 10.5$	58.720	301.048		†
MgCO3(S) Magnesium Carbonat	84.31420	-1111.69		$\pm 8.$	76.262	65.863		†
MgCl	59.75770	-43.51		$\pm 42.$	34.858	233.423		†
MgCl+	59.75715	652.7		$\pm 84.$	35.476	228.566		
MgClF	78.75610	-569.02		$\pm 21.$	49.912	265.994		
MgCl2 (S)	95.21040	-641.62		$\pm 0.46$	71.509	89.660		†
MgCl2(L)	95.21040	-601.58			---	---		†
MgCl2	95.21040	-392.46		$\pm 2.1$	57.146	277.041		†
MgF	43.30340	-236.81		$\pm 8.4$	32.570	221.089		†
MgF+	43.30285	512.29		$\pm 46.$	32.644	215.348		
MgF2(S)	62.301810	-1124.2		$\pm 1.3$	61.546	57.243		†
MgF2(L)	62.301810	-1072.35			---	---		†
MgF2	62.301810	-726.76		$\pm 16.7$	48.264	256.514		†
MgF2+	62.30126	592.		$\pm 20.9$	52.459	258.152		
MgH	25.31294	169.03			29.557	193.199		†
MgI	151.20947	24.61		$\pm 41.8$	36.816	252.650		†
MgI2(S)	278.11394	-366.94		$\pm 6.3$	74.907	129.698		†
MgI2(L)	278.11394	-342.25			---	---		†
MgI2	278.11394	-160.25		$\pm 10.5$	59.631	317.496		†
MgN	38.31174	288.70	289.04	$\pm 25.1$	32.761	224.845		†
MgO(S)	40.30440	-601.24		$\pm 0.63$	37.146	36.938		†
MgO(L)	40.30440	-532.61			---	---		†
MgO	40.30440	58.16		$\pm 25.1$	32.241	213.299		†
MgOH	41.31234	58.16		$\pm 37.7$	43.049	226.467		†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
MgOH+	41.31179	584.42		$\pm 62.8$	43.229	220.834		
Mg(OH)2(S)	58.31968	-924.66		$\pm 2.1$	77.264	63.236		†
Mg(OH)2	58.31968	-572.37		$\pm 33.5$	69.505	267.295		†
MgS(S)	56.37100	-345.72		$\pm 4.2$	45.605	50.329		†
MgS	56.37100	-145.23		$\pm 66.9$	34.664	225.518		†
MgSO4(S)	120.36860	-1261.79		$\pm 20.9$	96.209	91.393		†
MgSO4(L)	120.36860	-1246.59			---	---		†
MgSiO3 (S)	100.38870	-1548.92		$\pm 4.2$	82.198	67.839		†
MgSiO3 (L)	100.38870	-1494.86		$\pm 20.9$	---	---		†
MgTiO3(S)	120.18320	-1572.56		$\pm 6.3$	91.953	74.583		†
MgTiO3(L)	120.18320	-1497.63		$\pm 6.3$	---	---		†
MgTi2O5(S)	200.06200	-2509.36		$\pm 10.5$	147.009	135.655		†
MgTi2O5 (L)	200.06200	-2382.31		$\pm 8.4$	---	---		†
Mg2	48.61000	287.63		$\pm 08$	24.293	240.189		†
Mg2F4	124.60361	-1718.37		$\pm 37.7$	107.553	337.041		†
Mg2SiO4(S)	140.69310	-2176.94		$\pm 4.2$	119.151	95.239		†
Mg2SiO4(L)	140.69310	-2113.88		$\pm 20.9$	---	---		†
Mg2TiO4(S)	160.48760	-2164.38		$\pm 6.3$	128.724	115.153		†
Mg2TiO4(L)	160.48760	-2046.33			---	---		†
MnO (S)	70.93745	-385.221			44.102	59.71		
MnO2(S)	86.93685	-520.029			54.415	53.049		
Mn2O3 (S)	157.8743	-959.002			99.034	110.499		
Mn3O4 Solid-A	228.81175	-1387.799			140.515	155.599		
Mn5N2(S)	302.70373	-204.2			175.724	187.443		
MnS Solid	87.00405	-214.2			49.943	78.199		
MnS2 (S)	119.07005	-223.844			70.075	99.914		
Mo(cr) REFERENCE ELEMENT	95.94	0	0		23.933	28.605		*‡
MoC Solid-C	107.951	-28.451			30.878	36.652		
MoO2 Solid	127.9388	-588.94			55.982	46.275		
MoO2	127.9388	-8.314			34.002	252.344		
Mo2C(S)	203.891	-53.137			60.207	65.814		
N	14.00674	472.68		$\pm 0.4$	20.786	153.302		†
ND	16.0208	355.309	355.710	$\pm 8.$	29.159	187.234	8.648	†
NHD Radical	17.028782	178.165	181.106	$\pm 8.$	33.703	205.600	9.912	#
ND2	18.0349	181.937	184.878	$\pm 8.$	34.415	204.335	9.962	†
ND2H	19.04288	-52.748	-45.684		35.976	209.279	10.074	#
ND3	20.04901	-54.501	-47.546	$\pm 0.4$	38.225	203.931	10.234	†#
NF	33.00514	232.99	233.	$\pm 3.$	30.228	212.908	8.738	†
NF2	52.00355	34.421	37.000	$\pm 5.$	41.058	249.638	10.582	†
NF3	71.00195	-131.7	-125.98	$\pm 1.$	53.497	260.812	11.855	†
NH	15.01468	358.792	358.76	$\pm 0.37$	29.193	181.227	8.601	†
NH+	15.01413	1665.795	1656.29		32.775	187.651	9.495	†
NHF	34.01308	112.0	114.952	$\pm 15$	35.234	230.806	10.030	†
NHF2	53.01149	-103			43.384	252.814		†
NH2 AMIDOGEN RADICAL	16.02258	186.2	189.1	$\pm 1.0$	33.663	194.868	9.911	#
NH2D	18.03672	-48.697	-41.627		35.157	205.591	10.018	#
NH2F	35.02102	-75			36.474	229.534		†
NH3 AMONIA RRHO calc	17.03056	-45.567	-38.513	$\pm 0.03$	34.597	192.475	9.984	#
NH3 AMONIA Anharmonic calc	17.03056	-45.567	-38.946	$\pm 0.03$	35.630	192.770	10.043	†
NH2OH Hydroxyl Amine	33.02996	-50		$\pm 10$	46.472	236.181		†
NH4+ AMONIUM ION	18.03795	644.905			34.764	186.095		†
NH4CLO4(l)	117.4888	-295.767	-277.78		128.072	184.18	25.238	†



Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
NO	30.00614	91.271	90.767		29.862	210.748	9.179	†
NO+	30.00559	990.807	982.137		29.123	198.234		†
NOCL	65.45884	52.524	54.425	±0.5	44.623	261.590	11.364	†
NOF	49.00454	-65	-62.633	±2.0	41.530	248.224	10.720	†
NOF3	87.00135	-187	-178.78	±7.	68.067	277.731	13.698	†
NO2	46.00554	34.193	37.0	±0.5	37.177	240.171	10.208	†
NO2-	46.00609	-200.036			37.215	236.241		†
NO2CL	81.45824	12.5	17.901	±1.	53.246	272.128	12.205	†
NO2F	65.00394	-109	-102.92	±20	48.999	259.287	11.347	†
NO3	62.00494	74.628	81.024	±0.69	46.935	252.623	10.959	†
NO3-	62.00549	-310.78	-298.0		44.724	245.638		†
NO3F	81.00334	15			66.958	293.171		†
N2 REFERENCE ELEMENT	28.01348	0	0		29.124	191.607	8.670	††
N2D2 Cis	32.0416	202.857	209.788		39.025	224.095	10.308	†#
N2F2	66.01029	62.374	67.	±10	56.569	268.216	12.869	†
N2F4	104.00709	-22	-13.491	±10	88.384	317.531	17.812	†
N2H	29.02142	249.517		±13.6	34.662	224.505		†
N2H2	30.02936	211.859.	219.	±10	35.045	218.333	9.997	†
NH2NO2 NITRAMIDE	62.02816	-26.000	-12.346	±10	56.672	268.548	12.164	†
H3N2 HYDRAZINE RAD	31.0373	220.659	209.946	±8.	42.496	236.791	10.634	#
N2H4(L) Hydrazin	32.04524	50.38	--		98.839	121.545	--	†
N2H4 HYDRAZIN	32.04524	95.18	109.337	±0.5	48.43	238.466	11.449	†
NH4NO3 (solid)	80.04344	-365.6	--	1	139.080	150.810	--	†
N2O (NNO)	44.01288	81.6(82.6)		0.1	38.628	220.01		†
N2O+	44.01233	1333.399		±0.63	42.263	233.859		†
N2O3	76.01168	86.631	91.2		72.733	314.736		†
N2O4	92.01108	11.111	20.4		79.168	304.451		†
N2O5	108.01048	13.3			95.332	355.717		†
N3 AZIDE RADICAL	42.02022	453.54	456.97	±3.5	36.175	223.072	9.571	†#
N3H (s) Azidic Acid	43.02816	261.59		±0.77				X
N3H AZIDIC ACID	43.02816	291.713	298.005	±0.65	44.219	239.330	10.947	†#
N4H4 NH3N3 (cr)		114.14		± 0.94				X
N4H4 NH4N3 (g) ??		179.7 ?						X
Ne REFERENCE ELEMENT	20.1797	0	0		20.786	146.33	6.197	*†
Ne+	20.17915	2086.966	2080.66	±0.001	22.120	158.310	6.304	†
Ni(cr) REFERENCE ELEMENT	58.6934	0	0		25.987	29.87	4.786	*†
NiO Solid-A	74.689	-8.314			44.309	37.991		
NiS(b) Crystal	90.7594	-87.869		±6.3	47.121	52.986		*
NiS2(s)	122.8254	-131.381		±16.7	70.627	71.966		*
Ni3S2(l)	240.2122	-216.325		±5	117.75	133.871		*
Ni3S4(s)	304.3442	-301.121		±25.1	164.813	186.484		*
O	15.9994	249.175	246.79	±0.1	21.912	161.06	6.725	†
O-	15.99995	101.846	105.813		21.685	157.797	6.571	†
O2 REFERENCE ELEMENT	31.9988	0	0		29.378	205.149	8.680	*†
O2+	31.99825	1171.828	1165.		30.67	205.393	9.311	†
O2-	31.99935	-48.028	-42.5		31.422	209.336	9.350	†
O3 OZONE	47.9982	141.8	144.454		39.378	239.011	10.366	†
P	30.97376	316.39		±1	20.786	163.2		†
PCL3	137.33186	-288.58		±5.4	71.706	311.715		*†
PF	49.97217	-52.377		±20.9	31.616	224.968		*†
PF2	68.97057	-488.269		±20.9	44.716	262.958		*†
PF3	87.96897	-958.457		±3.8	58.801	273.073		*†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
PF5	125.96578	-1594.433		$\pm 2.9$	85.05	300.855		*†
PH	31.9817	230.752	231.698	$\pm 33.5$	29.175	196.381	8.648	†
PH2 Phosphonium Radical	32.989641	135.474	139.333	$\pm 8.$	34.272	212.710	9.969	#†
PH2-	32.990190	-9.265	+0.800	$\pm 10.$	34.124	205.247	9.960	†
PH3 PHOSPHINE RRHO	33.997581	11.786	19.712	$\pm 8.$	37.102	210.245	10.137	#†
PN	44.9805	104.776			29.667	211.126		*
PO	46.97316	-29.597		$\pm 4.2$	31.725	222.768		*
PO2	62.97256	-314.533			41.397	253.682		*
P2	61.94752	143.651		$\pm 2.1$	32.057	218.135		*
P4	123.89505	58.917		$\pm 2.1$	67.326	280.022		*
P4O6	219.89145	-2144.519		$\pm 33.5$	143.998	345.664		*
P4O10(s)	283.88905	-3010.022		$\pm 8.9$	211.82	228.786		*
P4O10	283.88905	-2904.154		$\pm 8.9$	188.827	403.974		*
Pb (cr) REFERENCE RLEMENT	207.2	0.	0.		24.430	36.899	6.870	†
Pb (gas)	207.2	195.2	195.88	$\pm 0.8$	20.786	175.377		†
PbBr	287.1040	64.821	73.805	$\pm 20$	36.916	272.744	10.146	†
PbBr2	367.0080	-103.908	-87.54	$\pm 7.$	56.966	339.673	15.022	†
PbBr3	446.9120	-104.011	-80.330	$\pm 80.$	80.540	385.255	19.969	†
PbBr4	526.8260	-182.436	-152.4	$\pm 80.$	104.468	427.724	25.871	†
PbCl	242.65270	8.819	10.493	$\pm 12.$	36.215	261.306	9.787	†
PbCl2	278.10540	-175.046	-173.5	$\pm 5.$	55.299	315.621	14.003	†
PbCl3	313.55810	-177.654	-175.27	$\pm 80.$	77.918	351.604	18.256	†
PbCl4	349.0108	-327.43	-325.65	$\pm 80.$	100.537	381.682	23.449	†
PbF	226.19840	-98.072	-96.853	$\pm 10.$	34.401	249.962	9.268	†
PbF2	245.19681	-443.427	-440.30	$\pm 11.$	50.981	291.532	12.573	†
PbF3	264.19521	-489.573	-485.0	$\pm 60.$	70.582	316.287	15.535	†
PbF4	283.1936	-799.925	-795.03	$\pm 60.$	90.232	331.825	19.626	†
PbI	344.10447	108.904	112.033	$\pm 4.$	37.152	280.413	10.339	†
PbI2	461.00894	-10.253	-5434	$\pm 5.$	57.182	352.613	15.247	†
PbI3	587.91341	21.755	27.35	$\pm 80.$	81.624	411.532	21.065	†
PbI4	714.81788	-41.281	-35.485	$\pm 80.$	106.276	463.806	27.521	†
PbO(S)	223.19940	-218.6	-216.61	$\pm 0.5$	46.414	67.840	9.225	†
PbO	223.19940	68.187	70.385	$\pm 4.5$	32.513	240.045	8.962	†
PbO2(S)	239.19880	-276.0	-271.41	$\pm 1.5$	60.997	71.920	10.962	†
PbO2	239.19880	136.153	139.452	$\pm 100.$	51.721	261.093	12.251	†
PbS(S)	239.2660	-99.475	-99.703	$\pm$	49.499	91.200	11.510	†
PbS	239.2660	127.945	129.797	$\pm 1.5$	35.085	251.414	9.430	†
PbS2	271.3320	244.049	245.722	$\pm 10.$	57.511	286.141	14.021	†
PbN6(S) Lead Azide	291.3	469.						X
S(S) REFERENCE ELEMENT	32.066	0	0		22.690	33.070	4.412	††
S	32.066	277.17	274.925	$\pm 0.25$	23.674	167.832	6.657	†
SCL	67.5187	156.47		$\pm 16.7$	37.555	237.334		*†
SCL2	102.9714	-17.572		$\pm 3.3$	50.909	281.641		*†
SF	51.0644	12.971		$\pm 6.3$	35.157	225.282		*†
SF2	70.06281	-296.653		$\pm 16.7$	44.906	257.708		*†
SF3	89.06121	-503.041		$\pm 33.5$	62.998	286.186		*†
SF4	108.05961	-763.18		$\pm 20.9$	77.62	299.657		*†
SF5	127.05802	-908.467		$\pm 15.1$	89.687	304.774		*†
SF5Br	206.96202	-972.8		$\pm 59$	107.075	333.654		
SF5CL	162.51072	-1038.9		$\pm 10.5$	104.344	319.936		
SF6	146.05642	-1220.502		$\pm 0.8$	96.994	291.551		*†
SN	46.07274	263.583		$\pm 105$	31.758	222.081		*

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	$\pm$ kJ/mol	$C_{p298}$ J/mol/K	$S_{298}$ J/mol/K	$H_{298}-H_0$ kJ/mol	
SO	48.0654	5.008		$\pm 1.3$	30.164	221.944		*
SOF2	86.06221	-543.926		$\pm 105$	57.202	279.156		*
SO2	64.0648	-296.835		$\pm 0.21$	39.867	248.206		*
SO2CLF	118.5159	-556.476		$\pm 21$	71.719	302.879		*
SO2CL2	134.9702	-354.802		$\pm 2.1$	77.218	311.127		*
SO2F2	102.06161	-758.569		$\pm 8.4$	65.946	283.651		*
SO3	80.0642	-395.753		$\pm 0.71$	50.692	256.775		*
S2	64.132	128.404		$\pm 0.3$	32.481	228.313		*
S2CL	99.5847	78.562		$\pm 8.4$	50.968	292.162		*
S2CL2	135.0374	-16.736			72.776	327.237		
S2F2 (SSF2)	102.11681	-401.422		$\pm 41.8$	63.146	292.729		*
FS2F	102.11681	-336.443		$\pm 41.6$	66.061	293.985		*
S2F10	254.11603	-2064.386		$\pm 29.3$	176.702	397.041		
S2O	80.1314	-56.486		$\pm 33.5$	44.112	267.029		*
S8	256.528	100.42		$\pm 0.63$	156.046	430.319		
Si(cr) REFERENCE ELEMENT	28.0855	0	0		19.789	18.81		*†
SiC(b)	40.0965	-73.22			26.867	16.617		*
SIF2 DifluoroSilylene	66.082306	-627.014	-626.2	$\pm 16.8$	44.707	256.710	11.228	#
SiF3 TrifluoroSilyl Radical	85.080710	-993.365	-990.4	$\pm 8.$	59.613	282.433	13.398	#
SiF4 TetrafluoroSilane	104.07911	-1614.98	-1609.4	$\pm 4.2$	73.534	282.615	15.325	#
SiHF3 TriFluoroSilane	86.088650	-1207.67	-1200.5	$\pm 5.4$	63.486	277.351	13.545	#
SiO2(Lqz) Quarz	60.0843	-910.857			44.59	41.463		
Si2N2O(s) Silicon Oxynitride	100.18388	-947.711			67.46	46.06		
Si3N4(a) Silicon Nitride	140.28346	-744.77			99.579	112.968		*
SiS2 Solid	92.2175	-213.384			77.482	80.333		#
SnCl4 TetraChloroStanum	260.52080	-478.650	-476.30	$\pm 4.2$	98.459	364.549	22.340	†#
SnH3 TriHydroStanum Radical	121.73382	258.153	266.252	$\pm 4.2$	44.818	240.204	10.926	#
SnH4 TetraHydroStanum	122.74176	162.758	174.594	$\pm 4.2$	51.108	228.991	11.423	#
Xe REFERENCE ELEMENT	131.29	0	0		20.786	169.686	6.197	*†
Xe+	131.28945	1176.552	1170.35		20.786	181.212	6.197	†
Zn(cr) REFERENCE ELEMENT	65.39	0	0		25.390	41.630	5.657	‡
ZnCL2	136.29540	-265.684	-		56.902	276.672	-	
ZnSO4 (cr)	161.4536	-980.144	-969.95	$\pm 4.2$	99.035	110.541	17.238	†

- \* The polynomials are pinned at 1000 K, therefore the property values are not exact at 298 K. All other polynomials are pinned at 298 K, therefore the property values are exact.
- # 9 term NASA polynomials are available in the NEWNASA.TXT file for this species.
- † 9-term NASA polynomials are available in <http://cea.grc.nasa.gov>
- ‡ 9-term NASA polynomials for all Reference Elements are available in the ELEMENTS.DAT file.
- X Polynomials not available