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

Alexander Burcat
Faculty of Aerospace Engineering, Technion – Israel Institute of Technology

Branko Ruscic
Chemistry Division, Argonne National Laboratory

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Third Millennium Ideal Gas and Condensed Phase Thermochemical Database for Combustion

with updates from

Active Thermochemical Tables

Alexander Burcat[†]
and
Branko Ruscic[‡]

Chemistry Division, Argonne National Laboratory,
Argonne, Illinois

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 7th 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anticipation of the full coupling, which is under development, the database started incorporating the available (as yet unpublished) values from Active Thermochemical Tables.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.

[†] On sabbatical leave from the Faculty of Aerospace Engineering, Technion-Israel Institute of Technology, Haifa 32000, Israel; e-mail aer0201@tx.technion.ac.il
[‡] e-mail: ruscic@anl.gov

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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 ºC (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 (Cp), 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 thermo-chemical 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, *Thermo-dynamics 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 fist 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 thermo-chemical 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:

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

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

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

$$\frac{G_T^\circ}{RT} = \frac{H_T^\circ}{RT} - \frac{S_T^\circ}{R} = a_1(1 - \ln T) - \frac{a_2 T}{2} - \frac{a_3 T^2}{6} - \frac{a_4 T^3}{12} - \frac{a_5 T^4}{20} + \frac{a_6}{T} - a_7 \quad (4)$$

It should be noted that the value H_T° 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°/RT functions of the molecules in a reaction can be used directly to compute the reaction's equilibrium constant in terms of concentrations through

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

where the change in mole number is $\Delta\nu = \Sigma \nu_j$ and the coefficient changes are $\Delta a_1 = \Sigma \nu_j a_{ij}$. The summations are over all the reactant and product species j with the stoichiometric coefficients ν_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:

$$\frac{C_p^\circ}{R} = a_1T^{-2} + a_2T^{-1} + a_3 + a_4T + a_5T^2 + a_6T^3 + a_7T^4 \quad (7)$$

$$\frac{H^\circ_T}{RT} = -a_1T^{-2} + \frac{a_2 \ln T}{T} + a_3 + \frac{a_4T}{2} + \frac{a_5T^2}{3} + \frac{a_6T^3}{4} + \frac{a_7T^4}{5} + \frac{a_8}{T} \quad (8)$$

$$\frac{S_T^\circ}{R} = -\frac{a_1T^{-2}}{2} - a_2T^{-1} + a_3 \ln T + a_4T + \frac{a_5T^2}{2} + \frac{a_6T^3}{3} + \frac{a_7T^4}{4} + a_9 \quad (9)$$

$$\frac{G_T^\circ}{RT} = \frac{H_T^\circ}{RT} - \frac{S_T^\circ}{R} = -\frac{a_1T^{-2}}{2} + \frac{a_2(1+\ln T)}{T} + a_3(1-\ln T) - \frac{a_4T}{2} - \frac{a_5T^2}{6} - \frac{a_6T^3}{12} - \frac{a_7T^4}{20} + \frac{a_8}{T} - a_9 \quad (10)$$

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 (NRRAO) was used. In a very few cases both RRHO and NRRAO 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 (Frurip *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 it's variant G3B3 (Baboul *et al*., 1999) are able to achieve very high accuracy (with a 95% confidence limit that is generally around ± 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(*2df,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:

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

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 calorimetry 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 $\Delta_f H°_{298}$ 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 that 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_2O(g)	-241.815 ± 0.031
CO_2(g)	-393.472 ± 0.014
SO_2(g)	-296.84 ± 0.21
NO_2(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 ± 1 kJ/mol uncertainty in the enthalpy or Gibbs energy change of a reaction at 1000 K implies an uncertainty of ± 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_4	-74.85 ± 0.29	-74.48 ± 0.42
C_2H_6	-84.68 ± 0.50	-83.85 ± 0.29
C_3H_8	-103.89 ± 0.59	-104.68 ± 0.50
n-C_4H_{10}	-127.03 ± 0.67	-125.65 ± 0.67
i-C_4H_{10}	-135.60 ± 0.54	-134.18 ± 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 calorimetrical 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 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).

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 ± 0.04
CH(g)	596.30 ± 0.25
CN(g)	438.81 ± 0.52
NH(g)	358.76 ± 0.37
SH(g)	141.87 ± 0.52
CH_2OH(g)	-17.18 ± 0.37
CH_3O(g)	20.257 ± 0.42
HO_2(g)	12.296 ± 0.25
CHO(g)	42.296 ± 0.3
CH_2(g)	391.465 ± 0.27
CH_3(g)	146.582 ± 0.1
C_2O(g)	291.04 ± 63
C_2H(g)	568.06 ± 0.31
C_2H_3(g)	296.61 ± 0.92
C2H5(g)	118.66 ± 2
C_3H_3(g)	339 ± 4
C_3H_5(g)	171 ± 3
n-C_3H_7(g)	101.32 ± 1
i-C_3H_7(g)	90.19 ± 2
C_6H_5(g)	339.7 ± 2.5

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 ±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 ± 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 ± 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:

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

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

For example, $\Delta_f H_{298}(H^+)$ = 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, $\Delta_f H_{298}(H^-)$ = 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 thermo-chemical values calculated with the 1987 BAC/MP4 method are of low reliability.

C) For a solid or liquid species (not ideal gas) like $CaSO_4$ 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 cal = 4.184 J

R = 8.314472 J mol^{-1} K^{-1}

R = 1.987207 cal mol^{-1} K^{-1}

1 eV = 23.06055 kcal mol^{-1}

1 eV = 8065.537 cm^{-1}

1 kcal/mol = 349.7547 cm^{-1}

1 cm^{-1} = 2.859146 cal mol^{-1}

1 cm^{-1} = 29.9792458 GHz

1 Hartree = 627.5101 kcal mol^{-1}

1 Hartree = 2625.502 kJ mol^{-1}

1 Bohr = 0.5291772 Å

1×10^{-39} g cm^2 = 21.50545 amu Bohr^2

1×10^{-39} g cm^2 = 6.022137 amu Å^2

B/cm^{-1} = 60.19969/[I_B/(amu Bohr^2)]

B/cm^{-1} = 16.85763/[I_B/(amu Å^2)]

B/cm^{-1} = 2.799277/[I_B/(10^{-39} 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/aetdd/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.*

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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

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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This work has benefited from the from the support and effort of the team members of the Collaboratory 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 commitee 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)

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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     Sructure
for automatic formula calculation should be:
N   1.56O   0.42AR  0.01C   0.00     Max Lst Sq Error Cp @ 2500 K 0.19%
AIR               L 9/95   WARNING!       0.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    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    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
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Table 4 (continued)

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1344-28-1
Al2O3(G) HF298=-546.9 kJ REF=NASA (Glen) database Original data from Gurvich
1996. Max Lst Sq Error Cp @ 1200 K 0.19%
Al2O3             T 1/03AL 2.O  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
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Table 4 (continued)

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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
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Table 4 (continued)

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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   (OBCl)  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
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Table 4 (continued)

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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)  BE1.183086  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.O  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.O  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.O  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.O  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.O  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
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Table 4 (continued)

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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    0G   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
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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
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Table 4 (continued)

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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.O  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.O  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.O  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.O  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
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Table 4 (continued)

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10031-22-8
PbBr2  HF298=-104.39+/-6.3 kJ REF=JANAF 1973 {HF298=-103.9 REF=Gurvich 1991}
PbBr2             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
CBrClF2  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
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Table 4 (continued)

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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
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Table 4 (continued)

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1605-72-7
CCl2   DICHLOROMETHYLENE  SIGMA=2  T0(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
 0.80836736E+01-0.11686005E-02 0.47029320E-06-0.81695078E-10 0.51447645E-14    2
 0.25307376E+05-0.14232761E+02 0.96645165E+00 0.26370954E-01-0.34655778E-04    3
 0.14693679E-07-0.66489549E-13 0.26683995E+05 0.20047532E+02 0.27867073E+05    4

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
 8.43494631E+00 1.61095820E-03-6.32734606E-07 1.08218634E-10-6.73872264E-15    2
-1.55335532E+04-1.33240848E+01 2.48480800E+00 2.32678936E-02-3.17729264E-05    3
 2.09727276E-08-5.43785295E-12-1.41617230E+04 1.60941173E+01-1.26285253E+04    4

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
 1.06592482E+01 2.40830053E-03-9.45665269E-07 1.61716164E-10-1.00690307E-14    2
-6.27802926E+04-2.63364834E+01 1.43593509E+00 3.76738346E-02-5.53363470E-05    3
 3.99081002E-08-1.14079923E-11-6.07165307E+04 1.89063992E+01-5.90293355E+04    4

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
 7.86018378E+00 2.13271500E-03-8.22077158E-07 1.38951133E-10-8.58406653E-15    2
-2.91056423E+04-1.19011907E+01 1.70787910E+00 2.89369464E-02-4.93289116E-05    3
 4.16910139E-08-1.37057391E-11-2.78350932E+04 1.76202114E+01-2.63996315E+04    4

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
 8.86167674E+00 1.18055486E-03-4.65765318E-07 7.98915627E-11-4.98464418E-15    2
 5.60193095E+03-1.57461775E+01 2.66358332E+00 2.71296370E-02-4.42402957E-05    3
 3.46851463E-08-1.05866977E-11 6.88202237E+03 1.41172615E+01 8.55468332E+03    4

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
 1.11913531E+01 1.87182223E-03-7.37586831E-07 1.26418446E-10-7.88344911E-15    2
-3.79341138E+04-2.79829261E+01 1.78320835E+00 4.15078790E-02-6.83507494E-05    3
 5.43232731E-08-1.68194876E-11-3.59931694E+04 1.73140424E+01-3.41210727E+04    4
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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.O  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(2),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.O  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
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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   2O   1    0G   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    0G   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    0G   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    0G   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.   0.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
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Table 4 (continued)

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3889-75-6
CF  FLUOROMETHYLIDENE   SIGMA=1   Be=1.4172 cm-1  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-1  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
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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.O  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  CF3OO* 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%.
CF3OO  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
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Table 4 (continued)

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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  METHYLIDYNE 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
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Table 4 (continued)

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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
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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
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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
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Table 4 (continued)

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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
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Table 4 (continued)

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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    0G   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.   0.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.   0.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
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Table 4 (continued)

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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.O  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.O  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 o,oo5 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
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Table 4 (continued)

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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
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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    0G     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    0G   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.   0.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.   0.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
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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
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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    0G   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    0G   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    0G   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    0G   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
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Table 4 (continued)

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625-76-3
CH2(NO2)2 Di Nitro Methane  STATWT = 1 SYMNO = 2  IA = 13.497367 IB = 49.930024
IC = 50.708   (Ir(NO2) = 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%
CH2(NO2)2         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
CH2O  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
CH2O          L 8/88H   2C     1O   1    0G     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
CH2O2  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    0G   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
CH2S  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%.
H2CS              T05/97H  2.C  1.S  1.   0.G   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
CH3 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.   0.G   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
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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
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Table 4 (continued)

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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
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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
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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
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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= Janosheck 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
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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
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Table 4 (continued)

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67-56-1
CH3OH liquid METHANOL DATA TAKEN FROM TRC 12/84 HF298=-57.101 kcal
{HF298=-239.389+/-0.14 kJ  REF=ATcT A}
CH3OH(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    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
CH4O  METHANOL (CH3OH)  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%.
CH3OH 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
CH4O2 PEROXYMETHANE (CH3OOH) SIGMA=1  STATWT=1 A=1.434544 B=0.350826 C=0.301985
Ir(CH3)=0.4282  ROSYM(CH3)=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%
CH4O2             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
CH3SH 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%
CH4S              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
CH5N  METHYLAMINE (CH3NH2)  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%.
CH5N            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
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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    0G   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.   0.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.   0.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.   0.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.   0.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
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Table 4 (continued)

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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
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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.O  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   1O   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   1O   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   1O   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                tpis91C  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
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Table 4 (continued)

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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 Bromoacetynyl 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
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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    0G   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
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Table 4 (continued)

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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
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Table 4 (continued)

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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    0G   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    0G   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    0G   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.   0.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    0G   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
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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=SHIMANOUCHI  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    0G   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   2O   1    0G   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    0G   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   4O   1    0G   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
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Table 4 (continued)

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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    0G   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    0G   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    0G   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.   0.G   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.   0.G   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.   0.G   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
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Table 4 (continued)

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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   6O   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
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Table 4 (continued)

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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
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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=CFCl 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
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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
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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    0G   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.   0.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.   0.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.   0.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.   0.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
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Table 4 (continued)

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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
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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    0G   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, SCHAFER, 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    0G   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  2.H  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
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50663-45-1
C2H2Cl  CHCl=CH* 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-FCl   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
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Table 4 (continued)

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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
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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-1  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
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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    0G   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    0G   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
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42879-41-4
C2H2O2 Oxyranone  Ethylene-oxide-Ketone CH2(-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.O  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.O  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+  Vinylium 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+  Vinylium   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 CH2Br-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.O  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
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Table 4 (continued)

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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
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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    0G   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.   0.G   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-Deutherated 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.   0.G   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.   0.G   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.   0.G   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
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Table 4 (continued)

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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-Vayjooee,
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
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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%
CH3CO+  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            T04/83O   1H   3C   2    0G   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
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Table 4 (continued)

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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-1 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-1    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-1 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-1  V(3)(C-O)=2973. cm-1  V(3)(O-O)=1916.7 cm-1 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
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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=SHIMANOUCHI  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
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Table 4 (continued)

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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-11 1.28416330E+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
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Table 4 (continued)

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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
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Table 4 (continued)

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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 torrsion)
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+/-.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
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Table 4 (continued)

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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 DIMETHYLAZIDE 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
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Table 4 (continued)

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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
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Table 4 (continued)

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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 artificialy 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    0G   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    0G   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.   0.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.   0.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
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Table 4 (continued)

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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    0G   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 CH3-S-CH3  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 (CH3SCH3)   T 4/93C   2H   6S   1    0G   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
C2H6S2  DIMETHYL DISULFIDE CH3-S-S-CH3  DATA FROM STULL WESTRUM & SINKE EXTRAPO-
LATED TO 5000 K USING WILHOIT'S POLYNOMIALS. HF298=-5.77 KCAL  Max Lst Sq Error
H-Href @ 300 K *7.8%*
C2H6S2            T 4/93C   2H   6S   2    0G   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
C2H7N  DIMETHYLAMIN CH3-NH-CH3  SIGMA=2  STATWT=1  IA=2.4308  IB=9.0358
IC=10.2300 (IR=0.48178  ROSYM=3  V(3)=1253. cm-1)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%.
CH3-NH-CH3        A09/04C  2.H  7.N  1.   0.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
(CH3)2N-NH* UNSYMETRICAL DIMETHYL HYDRAZINE RADICAL    SIGMA=2  STATWT=2
Ia=8.5287  Ib=9.4466  Ic=16.6828  (Ir(CH3)=0.50137  V(3)=1049 cm-1 ROSYM=3)x2
Ir(NH)=0.162277  ROSYM=2  V(3)=3778 cm-1  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%.
(CH3)2N-NH*       A10/04C  2.H  7.N  2.   0.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
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Table 4 (continued)

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540-73-8
CH3NH-NHCH3 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-CH3 Rotation IR=0.488 Potential Barrier V(3)=1049 cm-1 ROSYM=3  N-N Rotation
IR=1.53152  Potential Barrier V(2)=3778 cm-1 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    0G   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
(CH3)2N-NH2 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(CH3)=0.503 IR(NH2)=0.303 ROT
INT BARRIER V3(CH3)=4.69 KCAL V3(NH2)=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    0G   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 CYANOOXOMETHYL 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.O  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
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Table 4 (continued)

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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 DiNitroAcethylene  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
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83917-77-5
C2S2  Dicarbon Disulfide  S=C=C=S From original TRC(6/01) data to 2000 extrapo-
lated 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 & 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
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207602-05-9
C3F3  PerfluoroPropynyl radical CF3CC*   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 F2C=C=CF2  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-1  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  CF2=CF-CF3  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 CF3CF*CF3  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=Bauchlicher & Ricca JPC A 104,(2000),4581-85}
Max Lst Sq Error Cp @ 1300 K 0.40%
C3F7 CF3CF*CF3 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
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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
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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 adition 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-VINYLIDENE 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-VINYLIDENE 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
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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
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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
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Table 4 (continued)

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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=SHIMANOUCHI  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    0G   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 SHIMANOUCHI 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    0G     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
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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
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Table 4 (continued)

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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=3692,3268,3213,3178,1831,1715,1464,1380,1306,1180,1084,1031,1001,846,
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    0G   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
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15552-77-9
C3H5 TERTIARY NONSYMMETRIC RAD  (CH2=C*CH3) 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    0G   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 (CH3-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-1 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-CH3  SIGMA=1  STATWT=1  IA=2.0138 IB=34.8215
IC=36.3150  Ir=0.50042  ROSYM=3. [V(3)=752. cm-1 REF=CH3-C2H3 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 CH2=CH-CH2Cl  SIGMA=1  STATWT=1  IA=3.9170 IB=30.624
IC=31.5649  Ir=2.9602 ROSYM=1 [V(3)=1341.cm-1 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 CH2=CHCH2ClA 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
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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-1 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
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15843-24-0
C3H5O  PROPANAL RADICAL CH3CH2*CO  SIGMA=1 STATWT=2 IA=4.5640  IB=14.4953
IC=18.0265  Ir(CH3)=0.51267  ROSYM=3 V(3)=272 cm-1  Ir(CO)=0.35506  ROSYM=2
V(3)=200 cm-1 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  CH3CH2*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 *CH2COCH3 SIGMA=1  STATWT=2 SYMNO=1.  IA=7.7005  IB=9.3110
IC=16.4899  IR(CH3)=0.49327  ROSYM=3  V(3)=272 cm-1  Ir(CH2)=.28265  ROSYM=2
(V(3)=230 cm-1 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  CH3C(O)CH2 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  *CH2-CH(-O-)CH2 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-1 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  *CH2C2H3O  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-1  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=SHIMANOUCHI  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
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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 Hanbook
Military Pirotechnics 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 =Pepekin 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
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Table 4 (continued)

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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-1  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-1 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-1 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
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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=SHIMANOUCHI 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
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Table 4 (continued)

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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-1  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    0G   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    0G   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.   0.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
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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    0G   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  ROSIM=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 1propanol   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
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67-63-0
(CH3)2CHOH 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(CH3)=0.5036 ROSYM=3 V(3)=1399 cm-1)x2  Ir(OH)=0.1281 ROSYM=1 V(1)=30.4 cm-1
V(2)=-86.2 cm-1 V(3)=401.3 cm-1   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.O  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 CH3-O-CH2-O-CH3 DiMethoxyMethane  SIGMA=1 STATWT=1 IA=5.8896  IB=30.1703
IC=32.9248  Ir(CH3-1)=0.51501  Ir(CH3-2)=0.52847  Ir(CH3O-1)=4.03274
Ir(CH3O-2)=3.4016  ROSYM=3 and 2 V(3)=aprox 900.cm-1  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.]
CH3-O-CH2-O-CH3   A11/04C  3.H  8.O  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.O  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    0G     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    0G     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
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Table 4 (continued)

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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 &  Stedman J. Chem. Soc (1962), 512
MAX LST SQ ERROR @ 1300 K 0.44 % .
C4F6              T12/82C   4F   6    0    0G   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 & Stedmann J. Chem. Soc (1962), 512.   MAX LST SQ ERROR @ 1300 K
0.53%
F6C4              T12/82F   6C   4    0    0G   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
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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    0G   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    0G   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    0G   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.   0.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.   0.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
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Table 4 (continued)

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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  CH2=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    0G   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
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Table 4 (continued)

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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    0G   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    0G   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.   0.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.   0.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.   0.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
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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-1,3dien1yl 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
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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-1 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-1 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
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Table 4 (continued)

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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
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760-23-6
C4H6CL2  3,4-DICHLOROBUTENE-1 CH2=CH-CHCl-CH2Cl  SIGMA=1 STATWT=1  IA=24.4567
IB=63.7650  IC=84.7048  Ir(CH2Cl)=11.5823  ROSYM=1  [V3=1341. cm-1 REF=Ruscic
Burcat] Ir(CH2=CH-)=3.089  ROSYM=1  [V(3)=1420.cm-1 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 CH3-CO-O-O-CO-CH3  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=CHCH2CH3  SIGMA=1 STATWT=2  IA=3.4110  IB=19.5128
IC=20.1897  Ir(CH3)=0.511592  ROSYM=3  V(3)=1049.3 cm-1  Ir(C2H5)=2.0821
ROSYM=2  V(3)=524.6 cm-1  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
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Table 4 (continued)

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95045-33-3
C4H7  trans-1-Butene-2-yl  CH2=C*CH2CH3 SIGMA=1  STATWT=2  IA=3.1683  IB=20.4680
IC=21.5460  Ir=0.511592  ROSYM=3  V(3)=979.3 cm-1  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 CH3C*=CHCH3  SIGMA=1  STATWT=2  IA=1.9855  IB+23.2224
IC=24.1643  (Ir(CH3)=0.511592  ROSYM=3)x2 V(3)=489.7 cm-1 V(3)=454.8 cm-1
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 CH2=CHCH2CH2* RADICAL  SIGMA=1  STATWT=2  IA=3.3944
IB=19.4491  IC=19.9854   IR=2.105394  V(3)=384.7 cm-1 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  CH2*CHCHCH3 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-1  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      *CH2CH=CHCH3 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
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15157-95-6
C4H7   2-METHYL-ALLYL  *CH2C(CH3)=CH2 RADICAL  SIGMA=2  STATWT=2  IA=8.4666
IB=9.5538  IC=17.4983  IR=3.09356  ROSYM=3  V(3)=279.8cm-1  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 CH3-CH*CO-CH3   SIGMA=1  STATWT=2  IA=8.3576  IB=23.2184
IC=30.5369 Ir(CH3)=0.51535  ROSYM=3  V(3)=498. cm-1 REF=Bronstein 2002
Ir(CH3)=0.50717  ROSYM=3  V(3)=498 cm-1 Ir(CH3CH-)=3.06886  ROSYM=1  V(3)=1234
cm-1  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.O  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 H2C=C(CH3)CH2O*  SIGMA=1  STATWT=2  IA=10.5803
IB=20.5589  IC=28.7201 Ir(CH3)=0.51444 ROSYM=3 [V(3)=711. cm-1  REF=East Radom,
JCP 106,(1997),6655] Ir(CH2O*)=2.96655  ROSYM=1  [V(3)=1050. vm-1 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.O  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 CH2=CH-CH2-CH3 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    0G   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
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Table 4 (continued)

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115-11-7
CH2=C(CH3)2   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    0G   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
C4H8  2-BUTENE-TRANS  CH3-CH=CH-CH3  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 %*** .
C4H8TRANS         T 6/83C   4H   8    0    0G   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
C4H8  2-BUTENE-CIS  CH3-CH=CH-CH3   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 %***.
C4H8CIS           T 6/83C   4H   8    0    0G   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
C4H8  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 %.
C4H8 CY           T 1/90C   4H   8    0    0G   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
C4H8Cl2S  S(CH2CH2Cl)2  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(CH2CH2  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
C4H8N8O8 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    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
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Table 4 (continued)

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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
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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
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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)

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4630-45-9
C4H9  iso-BUTYL RADICAL CH3CH(CH3)CH2* STATWT=2  SIGMA=2  Ia=10.0033  Ib=10.6623
Ic=18.2551   FIRST ROTOR = SECOND ROTOR  ROSYM=3  V(3)=1254. cm-1  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  (CH3)3C*  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-1    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 (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    Ir(C3H7) = 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
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Table 4 (continued)

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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.O  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.O  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.O  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.O  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
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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 O.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
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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  10O   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  10O   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  10O   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
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Table 4 (continued)

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75-91-2
C4H10O2  tert-Butyl Hydroperoxy  (CH3)3COOH  SIGMA=3  STATWT=1  IA=18.7883288
IB=31.1526946  IC=31.4487605  (IR(CH3)=0.5172455  ROSYM=3  V(3)=1329.1 cm-1)x3
IR(OH)=0.147536  ROSYM=1  V(3)=314.8 cm-1  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(CH3)4  SIGMA(external)=12  STATWT=1
IA=IB=IC=35.1336  (IB=0.50857  ROSYM=3  V3=154. cm-1)x3  IB=0.50857   ROSYM=3
V3=147. cm-1  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(CH3)4          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 (C2H5)2SnH2  SIGMA(external)=2  STATWT=1
IA=18.0524  IB=56.3213  IC=68.6493  Ir(C2H5)=3.2144  ROSYM=1  V3=430.2 cm-1
Ir(C2H5)=3.02226  ROSYM=1  V3=447.7 cm-1  Ir(CH3)=0.4968  ROSYM=3  V3=1025 cm-1
Ir(CH3)=0.5069 ROSYM=3  V3=14002.5 cm-1   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(C2H5)2       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-1
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
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Table 4 (continued)

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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-CYLOPENTADIENE-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
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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 PENTADIYINE
C5H3              T 2/92C   5H   3    0    0G   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    0G   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    0G   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-hydroxyT06/03C  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.   0.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
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Table 4 (continued)

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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=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
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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-1
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
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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
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136936-20-4
1,3-C5H5O 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    0G   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-C5H5O 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    0G   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-C5H5O  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-C5H5O       D 9/97C   5H   5O   1   00G   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
C5H5O2 2-pentenedialdehyde-1-yl radical O=C*CH=CHCH2CHO    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.
C5H5O2 2-pentene  T 8/99C  5.H  5.O  2.   0.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
C5H5O2 2-pentenedialdehyde-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.
C5H5O2 2-pentene  T 8/99C  5.H  5.O  2.   0.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
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10563-01-6
C5H6 1,2,4 Pentatriene CH2=CH-CH=C=CH2 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-1
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
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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 POTTENTIAL 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    0G   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    0G   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    0G   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.   0.G   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.
```

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 (CH2=CHCH=CHCH2CL) SIGMA=1 STATWT=1 IA=6.8726
IB=90.6353 IC=92.1071 Ir(-CH2CL)=9.0981 ROSYM=1 V(3)=1341 cm-1 (From
CH3CH2CL) Ir(CH2=CH-)=3.2561 ROSYM=1 V(3)=1000. cm-1 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 ??
C5H7Cl2 1,5-DICHLOROPENTENE-1-YL-3 (*ClCHCH2CH=CHCH2Cl) SIGMA=1 STATWT=2
IA=15.2698 IB=161.6032 IC=172.2463 Ir(-CH2CL)=14.2488 ROSYM=1 V(3)=1341.
cm-1 Ir(*CLCH-)11.8413 ROSYM=1 V(3)=1500. cm-1 est. Ir(*CHCLCH2-)=21.9836
ROSYM=1 V(3)=1000. cm-1 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%
C5H7CL2 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

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N/A
C5H7NO 2-METHYL-3-OXO-BUTYRO-NITRYL 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
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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
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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.O  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
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Table 4 (continued)

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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 1buten3m1yl  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
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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    0G   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    0G   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    0G   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    0G   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
C5H10O 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%. .
C5H10O 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
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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
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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    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
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118-74-1
C6CL6 HEXACHLOROBENZENE DATA FROM STULL WESTRUM & 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    0G   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.   0.G   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=SHIMANOUCHI  HF298=58.18 kJ    REF=BURCAT, ZELEZNIK &
McBRIDE    MAX LST SQ ERROR CP @ 1300 K 0.86 %.
C6D6          L12/84C  6.D    6.   0.   0.G     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.   0.G   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    0G   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    0G   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
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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    0G   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
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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    0G   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 Thermochimica
Acta 58,(1982),11}    Max Lst Sq Error Cp @ 1300 K  0.43%.
TRICHLOROPHENOL   T 6/03C  6.H  3.O  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
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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
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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=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
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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.
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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
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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

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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    0G   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
```

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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    0G   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    0G   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
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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
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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=SHIMANOUCHI 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 scalled 0.8929  HF298=92+/-2 kcal REF=Wang & Law JPC 1001 (1997),3400.
Gausiann94 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
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Table 4 (continued)

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4447-21-6
C6H6 1,3-Hexadiyne HCC-CC-CH2CH3   SIGMA=1   STATWT=1  IA=3.8553  IB=63.3025
IC=66.1170  Ir(CH3)=0.52427  ROSYM=3  [V(3)=1162.cm-1 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  CH3-CC-CC-CH3  SIGMA=2  STATWT=1  IA=1.0501 IB+IC=75.8356
Ir(CH3)=0.26257 ROSYM=3  V(3)=25. cm-1 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-CH2CH2-CCH SIGMA=2  IA=3.3213  IB=58.0865  IC=60.3753
Ir=9.12833   ROSYM=2  V(3)=1140 cm-1   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  H2C=C=CH-CH=C=CH2  SIGMA=2   STATWT=1  IA=2.5855
IB=61.9688  IC=63.4654  Ir=7.2925  ROSYM=1  {V3=259.cm-1 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
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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    0G   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
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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=Sebbar & 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
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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 scalled 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
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Table 4 (continued)

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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    0G   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    0G   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
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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 atempts to use G3B3 ended up in transition species.
C6H9-1            S 8/01C   6H   9    0    0G   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
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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
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16183-00-9
C6H11 1-Hexene-6-yl CH2=CHCH2CH2CH2CH2* SIGMA=1 STATWT=2 IA=13.7894
IB=58.7630 IC=60.6715 Ir(CH2*)=0.2900 ROSYM=1 V(3)=257. est
Ir(CH2=CH-)=2.8357 ROSYM=1 V(3)=1200 cm-1 est. Ir(*CH2CH2-)=5.0872 ROSYM=1
V(3)=1049. cm-1 est Ir(CH2=CHCH2-)=6.62072 ROSYM=1 V(3)=1200. cm-1 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 1ene-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 CH3CH=CHCH2CH2CH2* SIGMA=1 STATWT=2 IA=5.3638 IB=67.8736
IC=68.8831 Ir(*CH2-)=0.288 ROSYM=1 V(3)=257. est Ir(CH3)=0.51556 ROSYM=3
V(3)=780. cm-1 est Ir(*C2H4-)=4.809 ROSYM=1 V(3)=1200. cm-1 est
Ir(CH3CH=CH_)=4.19524 ROSYM=1049. cm-1 V(3)=1049. cm-1 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 CH3CH2CH=CHCH2CH2* SIGMA=1 STATWT=2 IA=8.4509
IB=60.7525 IC=64.3746 Ir(CH3)=0.5226 ROSYM=3 V(3)=1773.cm-1 Ir(CH2*)=0.29068
ROSYM=1 V(3)=257. cm-1 Ir(*CH2-CH2-)=4.25007 ROSYM=1 V(3)=1049. cm-1
Ir(CH3CH2-)=4.62347 ROSYM=1 V(3)=1049. cm-1 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 CH2=C(CH2*)C3H7 SIGMA=1 STATWT=2 IA=11.4324
IB=45.6146 IC=51.6488 Ir(CH3)=0.51462 ROSYM=3 V(3)=1773. cm-1 Ir(CH2*)=
0.28542 ROSYM=1 V(3)=257. cm-1 Ir(C2H5-)=4.6966 ROSYM=1 V(3)=1049. cm-1
Ir(CH2=C(CH2*)-)=5.22857 ROSYM=1 V(3)=1049. cm-1 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

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N/A
C6H11  2-METHYL-1-PENTENE-5-YL RADICAL  CH2=C(CH3)C3H6*   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 CH3C(CH2*)=CHC2H5  SIGMA=1  STATWT=2
IA=12.1120  IB=44.4186  IC=50.9203  Ir(CH3)=0.51453  ROSYM=3  V(3)=18. cm-1
Ir(CH3)=0.5217  ROSYM=3  V(3)=1129 cm-1  Ir(CH2*)=0.28374  ROSYM=1 V(3)=257 cm-1
Ir(C2H5)=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  CH3C(CH3)=CHC2H4* 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  (CH3)2C=CHCH*CH3  SIGMA=1  STATWT=2
IA=11.2847  IB=46.9367  IC=56.6688  [Ir(CH3)=0.515754  ROSYM=3  V(3)=778 cm-1]x2
Ir(CH3)=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
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N/A
C6H11  2-METHYL-4-PENTENE-3-YL RADICAL  (CH3)2CHCH*CH=CH2  SIGMA=1  STATWT=2
IA=14.2398  IB=41.2367  IC=45.2456  [Ir(CH3)=0.5194  ROSYM=3 V(3)=1006. cm-1]x2
Ir(CH2=CH)=2.9734  ROSYM=1  V(3)=2000. cm-1  Ir(CH2=CH-CH*-)=7.729127  ROSYM=1
V(3)=1868. cm-1  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  CH2=C(CH3)CH2CH*CH3  SIGMA=1  STATWT=2
IA=11.9228  IB=45.0639  IC=52.0795  Ir(CH3)=0.51259  ROSYM=3  V(3)=318. cm-1
Ir(CH3)=0.52065  ROSYM=3  V(3)=879 cm-1  Ir(CH3CH*-)=4.53597   ROSYM=2
V(3)=1049. cm-1  Ir(CH2=C(CH3)-)=5.2778  ROSYM=1  V(3)=7320. cm-1  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
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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    0G   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    0G   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    0G   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    0G   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
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Table 4 (continued)

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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
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65596-90-9
C6H13  2-METHYL-PENTANE-5YL RADICAL CH3CH(CH3)C2H4CH2*  SIGMA=1  STATWT=2
IA=12.2796  IB=48.6781  IC=55.8408  [Ir(CH3)=0.5191  ROSYM=3  V(3)=780 cm-1 est]
x2  Ir(CH2*)=0.32193  ROSYM=1  V(3)=257. cm-1 est.  Ir(*CH2CH2-)=4.4635  ROSYM=1
V(3)=1200. cm-1 est.  Ir(*CH2CH2CH2-)=5.6854  ROSYM=1  V(3)=1200. cm-1 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   (CH3)2CHCH2CH*CH3  SIGMA=1
STATWT=2   IA=12.2796  IB=48.6781  IC=55.8408  [Ir(CH3)=0.5191  ROSYM=3
[V(3)=778. cm-1 est]]x3   Ir(CH3CH*-)=4.9974  ROSYM=1  V(3)=1200 cm-1 est.
Ir(CH3Ch*CH2-)=4.44475 ROSYM=1  V(3)=1200. cm-1 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  (CH3)2C*CH2CH2CH3  SIGMA(ext)=1
STATWT=2  IA=13.2158  IB=49.1410   IC=56.4702  [Ir(CH3)=0.51728  ROSYM=3
V(3)=780 cm-1 est]x3  Ir(C2H5-)=5.2773  ROSYM=1  V(3)=1200. cm-1
Ir((CH3)2C-)=5.32464  ROSYM=1  V(3)=1200. cm-1 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
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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 Chineese 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
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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
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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
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68364-31-8
C7H7 Quadricyclane Appex 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. Naturforshung 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
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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 Termody. 10,(1978),919 Max Lst Sq Error Cp @ 200 K **1.5%**
C7H8 BICY-DIEN    T 2/95C   7H   8    0    0G   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 oposite edges two cyclopropane & their
appex 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    0G   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    0G   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    0G     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
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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    0G     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    0G   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.   0.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 Pyrolidine 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
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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    0G   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    0G   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    0G   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
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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
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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 Poly-
nomials 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    0G   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    0G   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
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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    0G   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.   0.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.   0.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 Neguyen & Steele J. Chem. Thermodynamics 23 (1991), 759
HF298=39.74 KCAL REF= Pedley, Naylor & Kirby 1986
C8H6S             T12/93C   8H   6S   1    0G   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.   0.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
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Table 4 (continued)

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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    0G   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    0G   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.   0.G   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.   0.G   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
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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
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Table 4 (continued)

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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 ISOOCTANE  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
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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 AA0K  Max Lst Sq Error Cp @ 200 K 0.88 %.
C9H7 INDENYL      T 9/96C   9H   7    0    0G   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
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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    0G   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    0G   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 TETRAVINYLMETHANE  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
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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
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Table 4 (continued)

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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    0G     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.   0.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.   0.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.   0.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
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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 , GUNTHARD & 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
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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.
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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
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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-1  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-1  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
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Table 4 (continued)

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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
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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    0G   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-decenyl  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
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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
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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
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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
C12H4OCl4  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
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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

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

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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.CEData,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.CEData,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-09-1.11115340E-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
Cl2C6H2(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
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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
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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.O  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.Termodynam 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.O  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
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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
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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  Specto-
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
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Table 4 (continued)

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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
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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    0G   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    0G   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)

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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    0G   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
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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. EXTRAPO-
LATED 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
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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

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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=Fereira
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 - FOOTBALLENE  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
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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
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Table 4 (continued)

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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 & 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
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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  1O     2    0    0G     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
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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  2O   2    0    0G   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  CromiumMonochloride 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
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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
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12068-77-8
Cr2FeO4 Dichromium Ferrum Tetraoxide.   Data taken from I.Barin 1989.
HF298(S)=-1458.124 kJ
Cr2FeO4           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
Cr3C2  3-Chromium 2-Carbide Solid.  Data taken from I.Barin 1989
HF298(S)=-85.354 kJ
Cr3C2(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
Cr7C3  7-Chromium 3-Carbide Solid.  Data taken from I. Barin 1989.
CHF298(S)=-160.666 kJ.
Cr7C3(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
Cr23C6  23-Chromium 6-Carbide Solid.  Data taken from I. Barin 1989.
HF298(S)=-328.444 kJ.
C6Cr23            B  /89C  6.CR23.   0.   0.S   298.150  1793.000  C1267.97630 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    2
 2.59212596E+04 5.91714338E-01 2.50000000E+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+ 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+                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    2
 1.84512004E+05-1.01841452E-01 2.50000000E+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- DEUTERIUM ANION  REF=Hotop 1985 and Gordon 1999 HF298=142.753 kJ
D-                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    2
 1.64237667E+04-1.01023912E-01 2.50000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 1.64237667E+04-1.01023912E-01 1.71691417E+04    4
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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.OO24192  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  BROT1=30.573  BROT2=.551
BROT3=.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
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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 89O   1D   1    0    0G   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, Lineberer JCP 77,(1982),1153}
Max Lst Sq Error Cp @ 2500 K 0.11%
OD-               RUS 89O   1D   1E   1    0G   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.   0.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.   0.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.   0.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.   0.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
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11081-35-9
D2-   SIGMA=2  STATWT=2  We=1202  WeXe=17.5  Be=12.7  ALPHAE=0.141 REF=JANAF 77
estimeted   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%
D2O               g 6/99D  2.O  1.   0.   0.G   200.000  6000.000  A  20.02760 1
 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  BROT1=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 %.
D2O2              g 6/99D  2.O  2.   0.   0.G   200.000  6000.000  B  36.02700 1
 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
ALFAA1=0.0769  ALFAA2=-0.2164  ALFAA3=0.1239  ALFAB1=0.1308  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               g 6/01D  2.S  1.   0.   0.G   200.000  6000.000  A  36.09420 1
 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    0G     200.000  6000.000      0.00055 1
 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
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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.O  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.O  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.O  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
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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 TBBCC=-1.928D-06TAACC=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.O  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.O  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
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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    2
-4.11098210E+04-5.31930570E+01 1.22888630E+01 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
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7705-08-0
FeCl3  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
FeCL3             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)2 Ferric Hydroxide  HF298(S)=-574.04 +/- 2.9 kJ   REF=JANAF
Fe(OH)2(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)2  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)2           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)3  Ferrum Hydroxide HF298(S)=-832.62 +/-12.6 kJ   REF=JANAF
Fe(OH)3(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
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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 Soulfate  REF=JANAF  HF298(S)=-928.85 +/-8.4 kJ
FeSO4(s)          J 6/66FE 1.S  1.O  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
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1317-60-8
Fe2O3 HEMATITE  HF298(S)=-824.248 kJ  Data from I. Barin Database  1989
Fe2O3(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    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
Fe2O3(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
Fe3C  Triferrumcarbide   HF298(S)=25.104 kJ  Data from I. Barin database 1989.
Fe3C (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    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
Fe3C (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
Fe3C (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
Fe3O4  MAGNETITE  HF298(s)=-1118.383 kJ  Data from I. Barin database 1989
Fe3O4(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    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
Fe3O4(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
Fe3O4(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
GeBr2   Germanium DiBronide  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
0.21 %.
GeBr2             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
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57147-09-8
GeBr3   Germanium TriBomo  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
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10038-98-9
GeCl4 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%
GeCL4    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
GeH3Cl  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%
GeH3Cl            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
GeH4 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%
GeH4              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    0G   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    0G   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
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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    0G   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    0G   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    0G   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    0G   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    0G   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.   0.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
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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   1N   1O   2    0G   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
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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   1O   2    0    0G   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   1O   1    0G   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.   0.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   1O   1H   1    0G   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   1O   1    0G   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
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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   1O   2S   1    0G   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   1O   3    0G   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    0G     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
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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    0G   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    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    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    0G   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
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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    0G   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 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    0G   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    0G   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
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Table 4 (continued)

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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    0G   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    0G   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    0G   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    0G   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, Heimel, Ehlers & 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    2
-7.45375000E+02 9.28723974E-01 2.50000000E+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    2
 2.85323374E+05 1.62166556E+00 2.50000000E+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    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
```

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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
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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.O  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.O  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.O  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.O  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.O  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
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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    0G     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.O  1.   0.   0.G   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.O  1.   0.   0.G   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.   0.G   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.   0.G   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
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N/A
KNO3 (S,L) Potasium 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%
KNO3(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    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
KNO3(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    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
KNO3(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    2
-6.16499439E+04-8.01839G52E+01 1.69583829E+01 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
KNO3(G) Potasium 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%
KNO3              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
K2O(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%.
K20               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
K2O2(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%.
K2O2              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    2
-7.45375000E+02 5.49095651E+00 2.50000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-7.45375000E+02 5.49095651E+00 0.00000000E+00    4

16915-28-9
Kr+  HF298=1356.954 kJ  HF0=1350.756 kJ  REF=Sugar & 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
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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    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    2
-6.58934341E+02-1.93786894E+01 4.12531827E+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 &
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 & 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
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7789-48-2
MgBr2  Magnesium Dibromide HF298=-302.92+/-10.5 kJ  REF=JANAF
MgBr2             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
MgCO3 Solid  Magnesium Carbonate  HF298=-1111.69+/-8. kJ  REF=JANAF
MgCO3(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
MgCl2 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
MgCl2  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
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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
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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 & 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
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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
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13776-74-4
MgSiO3 Magnesium Silicate Condensed  HF298(S)=-1548.92+/-4.2 kJ
HF298(L)=-1494.86+/-20.9 kJ   REF=JANAF
MgSiO3(I)          J12/67MG 1.SI 1.O  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
MgSiO3(II)         J12/67MG 1.SI 1.O  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
MgSiO3(III)        J12/67MG 1.SI 1.O  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
MgSiO3(L)          J12/67MG 1.SI 1.O  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
MgTiO3  Magnesium Titanate Condensed  HF298(S)=-1572.56+/-6.3 kJ
HF298(L)=-1497.63+/-6.3 kJ   REF=JANAF
MgTiO3(s)          J 6/67MG 1.TI 1.O  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
MgTiO3(L)          J 6/67MG 1.TI 1.O  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
MgTi2O5 Magnesium Dititanium Pentoxide Condensed  HF298(S)=-2509.36+/-10.5 kJ
HF298(L)=-2382.31+/-8.4  kJ  REF=JANAF
MgTi2O5(s)         J 6/67MG 1.TI 2.O  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
MgTi2O5(L)         J 6/67MG 1.TI 2.O  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
Mg2                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
Mg2F4  Magnesium Fluoride  HF298=-1718.37+/-37.7 kJ  REF=JANAF
Mg2F4              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
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10034-94-3
Mg2SiO4  Condensed  HF298(S)=-2176.94+/-4.2 kJ  HF298(L)=-2113.88+/-20.9 kJ
REF=JANAF
Mg2SiO4(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
Mg2SiO4(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
Mg2TiO4  Magnesium Titanium Oxide Condensed  HF298(S)=-2164.38+/-6.3 kJ
HF298(L)=-2046.33 kJ   REF=JANAF
Mg2TiO4(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
Mg2TiO4(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
MnO2 Manganese Dioxide  Data from Barin Database 1989  HF298(S)=-520.029 kJ
MnO2(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
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12125-23-4
MnS2  Manganese Disulfide  Data fron 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    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    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.   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    2
 2.02140667E+03-2.28074752E+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

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
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18868-43-4
MoO2  Molibdenum 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  DiMolibdenum 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    0G     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
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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/mo
 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    0G   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
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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    0G   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    0G   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    0G   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
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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
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7790-98-9
NH4ClO4(I) and (II) Amonium Perchlorate crystal  REF=JANAF HF298=-70.69 kcal
NH4CLO4(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    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
NH4CLO4(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  HF0=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  {HF0=54.6+/-0.5 kJ
REF=Gurvich 89}  Max Lst Sq Error Cp @ 1300 0.66%.
NOCL              L 5/95N   1O   1CL  1    0G   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    0G   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
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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    0G   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    0G   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    0G   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    0G   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    0G   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)

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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.O  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.O  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   1O   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
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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    0G   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    0G   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    0G   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.   0.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.   0.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
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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    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    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    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    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    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    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    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
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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    0G     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    0G     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.   0.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  STATW=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    0G     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.   0.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.   0.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
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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, Heimel, 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.O  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.O  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
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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
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Table 4 (continued)

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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 1/90O  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 89O  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.
O2 REF ELEMENT    RUS 89O   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 89O  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.
O2-               L 4/89O  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
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 5/90O   3      0    0    0G     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
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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
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Table 4 (continued)

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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
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Table 4 (continued)

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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.O  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.O  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.O 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.O 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
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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    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 & 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
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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  TetraCloro 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
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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
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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.O  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.O  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
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Table 4 (continued)

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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
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Table 4 (continued)

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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
TO(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
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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.O  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.O  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.O  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.O  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.O  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.O  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
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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
S2Cl   (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
S2Cl2   (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
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Table 4 (continued)

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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.O  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+00-3.82444593E+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
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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  Tetafluorosilicon  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
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7803-62-5
SiH4  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}
SiH4              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
SiO2 Quarz  REF=JANAF  HF298(S)=-910.857 +/- 1.7 kJ
SiO2(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
SiO2(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
SiO2(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
SiS2  Silicon Disulfide  Data from Barin Database 1989  HF298(S)=-213.384 kJ.
SiS2  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
SiS2  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
Si2N2O  Silicon Oxynitride REF=Fegley Comm. Am. Ceram. Soc. 1981 C124-C126
HF298(S)=-947.71 kJ
Si2N2O(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
Si3N4  Silicon Nitride  REF=JANAF  HF298(S)=-744.752 +/- 29.3 kJ
Si3N4(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
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7646-78-8
SnCl4  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%.
SnCL4             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
SnH3  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%.
SnH3              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
SnH4  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%.
SnH4              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 ELEMENTcoda89ZN 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
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7646-85-7
ZnCl2(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%.
ZnCl2             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
ZnSO4 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%
ZnSO4(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
ZnSO4(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
ZnSO4(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 abreviated to kJ and kcal.

##!!##  - This CAS number was assigned to the species first described in the
A. Burcat paper cited as REF.
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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

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  1.00O   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  1.00O   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
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BrO2 STRUCTURE O-Br-O  M.W. Chase JPCRD 25 (1996),1069
 3 T02/97 BR  1.00O   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   JCPRD 25 (1996), 1069
 3 T02/97 BR  1.00O   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  2.00O   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  2.00O   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
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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   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  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  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 T04/04 C   1.00BR  4.00    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
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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  3.00O   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  0.0        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  0.0        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  0.0        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   1.00O   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  0.0        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  0.0        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  0.0        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   1.00O   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  0.0        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  0.0        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  0.0        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
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CD3OD Deuterated methyl alcohol Shimanouchi + Chem3D .
 3 T06/02 C   1.00D   4.00O   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   3.00O   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
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Table 5 (continued)

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CHBr2   DIBROMOMETHYL RADICAL  B97-1/Aug-VTZ calc
 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

CHBr3   TRIBROMOETHANE BROMOFORM HF298 B97-1/Aug-VTZ calc.
 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

CCL2OH RADICAL BOZZELLI JPC 105 (2001),4504 B3lyp/6-31G* scaled 0.9806
 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

CCl3OH TriChloroMethanol Bozzelli JPC 105 (2001), 4504 B3LYP/6-31G*scaled 0.9806
 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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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
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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         12400.452
-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         12400.452
-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         12400.452
 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         10000.000
 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         10000.000
-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         10000.000
 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         10008.000
 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         10008.000
-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         10008.000
-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          9939.626
 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          9939.626
-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          9939.626
 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
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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 & 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
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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
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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 & 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 & 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 & 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
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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
```

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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
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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   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 & 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
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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   1.00O   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
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Table 5 (continued)

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C2Br  Bromoacetynyl Radical   Martin & Burcat 2004
 3 T04/04 C   2.00BR  1.00    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 & 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 & 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 & 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
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C2Br5  Pentabromo ethyl Radical  Martin & Burcat 2004
 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

C2Br6 Hexabromoethane Martin & Burcat  2004
 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

C2Cl2F2 1,2-transDiflorodichloroEthylene Burcat G3B3 calc HF298=-81.617 kcal
 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

C2Cl2F2 1,2-cisDiflorodichloroEthylene Burcat G3B3 calc HF298=-81.154 kcal
 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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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  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  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  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 & Burcat 2004 W2
 3 T04/04 C   2.00BR  1.00H   1.00    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
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C2HBr2 Dibromovinyl Radical Martin & 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-TertraBromoethyl Radical CHBr2CBr2*  Martin & 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-TertraBromoethyl Radical CBr3CHBr*  Martin & 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
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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 TertraChloroethyl 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
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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
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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
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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-CFH2    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
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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
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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

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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CH2Br-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

CH3CBr3 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

C2H3+  Vinylium  FROM ORIGINAL ATcT A tables
 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

C2H3CL  ChloroEthylene          HF298 ATcT A 2005. Gurvich,1991
 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

CH2Cl-COOH  Chloroacetic acid    Dorofeeva JPCRD 30 (2001), 475
 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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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        12476.149
 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        12476.149
 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        12476.149
 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        12701.039
-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        12701.039
-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        12701.039
 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        12955.411
-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        12955.411
-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        12955.411
 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        18024.591
-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        18024.591
-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        18024.591
 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
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CH3CD3 1,1,1-Deutherated 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
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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
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CH3CO  ACETYL RADICAL    IUPAC Task Force on Selected Radicals
 3 IU3/03 C   2.00H   3.00O   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

CH3CO+  Acetylium Ion from B Ruscic ACTIVE TABLES generator. HF298=669.952 kJ.
 3 A12/04 C   2.00H   3.00O   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

C2H3O Ethylene Oxide (Oxyran) radical  Burcat G3B3 calc HF298=164.47 kJ
 3 A 1/05 C   2.00H   3.00O   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

CH2BrCH2Br 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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CH3CHBr2  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

C2H4Cl2  1,2-DiChloroETHANE CH2ClCH2Cl  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

C2H4CL2O2 CHCL2CH2OOH  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

C2H4F2 1,2-DiFLUOROETHANE CH2FCH2F 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
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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
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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        17852.976
-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        17852.976
-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        17852.976
 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        12887.523
-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        12887.523
-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        12887.523
 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  Iodooethane. 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        14575.140
-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        14575.140
-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        14575.140
 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        15760.911
 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        15760.911
-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        15760.911
 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
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CH3CH2O*   ETHOXY RADICAL    IUPAC Task Group on Selected Radicals
 3 IU2/03 C   2.00H   5.00O   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

C2H5O  CH3*CHOH RADICAL Janoshck & Rossi IJCK 36,(2004),661 HF298=-54.03+/-4. kJ
 3 T10/04 C   2.00H   5.00O   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

C2H5O   CH3-O-CH2  HF298=0.96 kJ  Janoschek Rossi Int. J. Chem. Kinet 36 (2004)
 3 A10/04 C   2.00H   5.00O   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

C2H5OO PEROXYETHYL RADICAL  MELIUS  A40
 3 T08/00 C   2.00H   5.00O   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
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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
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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 tpis91 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   1.00O   1.00    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
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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
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C3F3  PerfluoroPropaynyl Radical CF3-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 CF2=CF-CF3  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 CF3CF*CF3 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
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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   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
```

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C3H2F3   CF3-C*=CH2 Radical  Burcat G3B3 calc  HF298=-89.613 kcal
 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

C3H2N Cyano-Ethylene Radical CH=CHCN Burcat B3G3 calc. HF298=105.84 kcal
 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

C3H3Cl 1 Chloro 1 propyne ClCC-CH3     Burcat G3B3 calc   HF298=184.7 kJ
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

C3H3F2  *CF2-CH=CH2 Radical  Burcat G3B3 calc  HF298=-53.642 kcal
 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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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        17481.219
-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        17481.219
-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        17481.219
 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        15179.741
 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        15179.741
 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        15179.741
 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. Sivaramakrrishnan 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        14450.542
 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        14450.542
 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        14450.542
 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 (Acrilonitrile) 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        13274.933
-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        13274.933
-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        13274.933
 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
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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        14131.563
 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
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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        14925.139
 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        14925.139
-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        14925.139
 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        14284.139
 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        14284.139
-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        14284.139
 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        15243.180
 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        15243.180
-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        15243.180
 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        13576.765
 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        13576.765
-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        13576.765
 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
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C3H5 Cyclopropyl radical Melius H4
 3 T02/03 C   3.00H   5.00    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  CH2=CH-CH2Cl  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-CH3  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  Propionitryle  C2H5CN  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
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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
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C3H6O Acetone CH3-O-CH3  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 CH3-C2H3O  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  -CH2CH2CH2O-  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 C2H3-O-CH3 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
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C3H6O  CyC3H5-OH   CycloPropanol Burcat  G3B3 Calc.  HF298=-101.50 kJ
 3 A01/05 C   3.00H   6.00O   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        13307.565
-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        13307.565
-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        13307.565
 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        14970.083
-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        14970.083
-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        14970.083
 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        14751.796
-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        14751.796
-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        14751.796
 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   8.00O   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        20879.540
-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        20879.540
-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        20879.540
 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
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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
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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
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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         13562.362
-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         13562.362
-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         13562.362
 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         13604.723
-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         13604.723
-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         13604.723
 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         18348.806
 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         18348.806
-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         18348.806
 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         16229.239
 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         16229.239
-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         16229.239
 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
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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        15339.409
 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        15339.409
-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        15339.409
 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        15362.378
-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        15362.378
-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        15362.378
 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        15188.157
 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        15188.157
-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        15188.157
 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        15308.163
 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        15308.163
-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        15308.163
 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
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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   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   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   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   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
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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  1.0  2.0  3.0  4.0  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  1.0  2.0  3.0  4.0  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  1.0  2.0  3.0  4.0  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  1.0  2.0  3.0  4.0  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  1.0  2.0  3.0  4.0  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  1.0  2.0  3.0  4.0  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  1.0  2.0  3.0  4.0  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
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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 5.164440450D+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
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C4H7  2-methylallyl CH2C*(CH3)CH2  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         16229.425
 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 CH3-CO-CH*CH3  HF298=-18.163 kcal Burcat G3B3 calc
 3 A 8/05 C   4.00H   7.00O   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 H2C=C(CH3)CH2O* Burcat G3B3  HF298=13.324 kcal
 3 A 2/05 C   4.00H   7.00O   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
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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
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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
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C4H9O n-butoxy radical  CH3CH2CH2CH2O*  HF298=-56.350 kJ  Burcat  G3B3 calc
 3 A08/04 C   4.00H   9.00O   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   9.00O   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   9.00O   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   9.00O   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
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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

C4H10FO2P  SARIN CH(CH3)2OP(O)FCH3  Melius BACMP4 Q2U
 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

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

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
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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
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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
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C5H4 Pentane Tetraene H2C=C=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   64.0852600     444466.320
     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   64.0852600     433353.616
     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   78.0920000     502941.904
     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   78.0920000     405241.320
     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
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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
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C5H7  1,4-Pentadiene-3yl Radical  G3B3 calc HF298=49.105 kcal HF0=53.151 k
 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         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   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   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  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
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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
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C5H8O CYCLOPENTANONE   IR +B3PW91/6-31G* NIST HF298 Wiberg JACS 113 (1991),3447.
 3 T 7/01 C   5.00H   8.00O   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        17365.925
 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        17365.925
-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        17365.925
 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   8.00O   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        16583.000
-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        16583.000
-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        16583.000
 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        16101.337
-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        16101.337
-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        16101.337
 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        21051.831
-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        21051.831
-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        21051.831
 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
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Table 5 (continued)

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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   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         19457.491
-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         19457.491
-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         19457.491
 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   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         19832.991
-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         19832.991
-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         19832.991
 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   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         19274.833
-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         19274.833
-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         19274.833
 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   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         19615.853
-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         19615.853
-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         19615.853
 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
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C5H10O CYCLO   TerahydroPyran  Burcat  G3B3 calc  HF298=-53.605 kcal
 3 A 4/05 C   5.00H  10.00O   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  12.00O   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 Cumulenic 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   2.00O   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
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C6H2OCl3 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         25386.281
-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         25386.281
-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         25386.281
 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         30007.626
 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         30007.626
 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         30007.626
 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         30116.917
-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         30116.917
-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         30116.917
 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         14055.431
 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         14055.431
-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         14055.431
 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
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C6H3OCl3 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
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1,3-C6H4 m-Benzyne Burcat G3B3 calc HF298=125.16 kcal;
 3 A02/05 C   6.00H   4.00    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  0.0         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  0.0         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  0.0         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-C6H4 p-Benzyne   Burcat G3B3 calc HF298=137.25 kcal
 3 A02/05 C   6.00H   4.00    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  0.0         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  0.0         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  0.0         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-C6H4  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   76.0959600     523104.600
     50.000   200.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         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  0.0         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  0.0         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-C6H4 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   76.0959600     524217.544
     50.000   200.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         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  0.0         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  0.0         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
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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
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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
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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
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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
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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

C6H5O  2,4-cyclohexadiene-1-one-2-yl Janoschek G3MP2B3 Calc J. Mol. Struct. 2003
 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

C6H6   Benzvalene  Gaussian 94 HF/6-31G(d) scal. 0.8929 Wang & Law JPC 1997 3400
 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
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C6H6 2,4-Hexadiyne  CH3-CC-CC-CH3  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-CH2-CH2-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  H2C=C=CH-CH=C=CH2   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   6.00O   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
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C6H7 1,3,5 Hexatriene-6-yl CH2=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

C6H7 2,4-Cyclopentadiene-1-Methynyl  2,4-C5H5-1-CH2*  Melius P72JB
 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

C6H7 2,4-Cyclopentadiene-3-Methynyl  2,4-C5H5-3-CH2*.  Melius  P72JA
 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

C6H7 2,4-Cyclopentadienyl-1-Methyl  2,4-C5H4*-1-CH3.  Melius P72JC
 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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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   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   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   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   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
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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   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   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   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   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
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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  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
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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
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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  4.0  0.0        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  4.0  0.0        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  4.0  0.0        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  4.0  0.0        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  4.0  0.0        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  4.0  0.0        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  4.0  0.0        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  4.0  0.0        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  4.0  0.0        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  4.0  0.0        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  4.0  0.0        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  4.0  0.0        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
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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
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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
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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   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

C7 Cumulenic 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  1.0  2.0  3.0  4.0  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  1.0  2.0  3.0  4.0  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  1.0  2.0  3.0  4.0  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  1.0  2.0  3.0  4.0  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  1.0  2.0  3.0  4.0  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
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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   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         19400.968
 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         19400.968
-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         19400.968
 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     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         18178.294
-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         18178.294
-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         18178.294
 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   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         15256.036
 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         15256.036
-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         15256.036
 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   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         14543.211
 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         14543.211
-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         14543.211
 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
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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        14528.576
 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        14528.576
-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        14528.576
 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        14490.751
 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        14490.751
-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        14490.751
 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        16310.491
-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        16310.491
-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        16310.491
 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        27122.418
 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        27122.418
-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        27122.418
 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
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C8H6O  2,3-Benzofuran Zhu & 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 & 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
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C8H14 Bicyclo[2,2,2]octane CH(-CH2-CH2-)3CH B3LYP vibs PM3 Moments
 3 T08/04 C   8.00H  14.00    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  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  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  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
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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  120.1915800     250621.600
     50.000   200.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         31734.238
-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  0.0         31734.238
-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  0.0         31734.238
 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  18.00O   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  4.0  0.0         47779.648
-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  4.0  0.0         47779.648
-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  4.0  0.0         47779.648
 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  4.0  0.0         42342.080
-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  4.0  0.0         42342.080
 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   8.00O   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  4.0  0.0         24318.233
-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  4.0  0.0         24318.233
-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  4.0  0.0         24318.233
 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  4.0  0.0         23429.478
 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  4.0  0.0         23429.478
-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  4.0  0.0         23429.478
 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
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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 kc
 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
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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  130.1864000     173636.000
     50.000   200.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23700.742
 1.003688111D+03 1.718212211D+01 5.047925370D-01 7.486384360D-02-2.308957539D-04
 9.146137620D-07-1.130975767D-09 0.000000000D+00 1.808033552D+04 2.313589380D+01
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23700.742
-4.732341770D+05 9.064807680D+03-6.426474980D+01 2.702028660D-01-3.243457540D-04
 2.063656754D-07-5.376239420D-11 0.000000000D+00-2.271735983D+04 3.698746110D+02
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23700.742
 7.528527480D+06-3.744765400D+04 7.805523970D+01-6.386713430D-03 1.143166096D-06
-1.097172061D-10 4.368142520D-15 0.000000000D+00 2.349250937D+05-4.865200690D+02

C10H10 3-methyl-indene   Lifshitz Dubnikova JPC A 108,(2004),3430  HF298=41.4 kc
 3 A03/05 C  10.00H  10.00    0.00    0.00    0.00 0  130.1864000     173217.600
     50.000   200.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23693.604
 4.121674680D+03-1.511103108D+02 3.495474250D+00 5.731265920D-02-2.397825419D-04
 1.277863205D-06-1.946336503D-09 0.000000000D+00 1.862383934D+04 9.575702530D+00
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23693.604
-4.539804490D+05 8.819608700D+03-6.318994310D+01 2.678982127D-01-3.217018550D-04
 2.047739215D-07-5.336682720D-11 0.000000000D+00-2.154447805D+04 3.636491850D+02
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         23693.604
 7.541562560D+06-3.745623590D+04 7.802914550D+01-6.368773430D-03 1.138168422D-06
-1.090654728D-10 4.335388010D-15 0.000000000D+00 2.349608522D+05-4.863372800D+02

C10H15 JP-10 RADICAL AM1 unscaled calc apex position
 3 S 4/01 C  10.00H  15.00    0.00    0.00    0.00 0  135.2261000     105650.184
     50.000   200.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21970.002
-3.332408930D+03 2.986120501D+02-6.337313420D+00 1.561535636D-01-8.186248850D-04
 2.731731555D-06-2.968971731D-09 0.000000000D+00 9.184951160D+03 5.188220230D+01
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21970.002
-1.104811531D+06 2.034385152D+04-1.388103590D+02 4.798872480D-01-5.865175610D-04
 3.767602990D-07-9.861766970D-11 0.000000000D+00-8.236921640D+04 7.759670470D+02
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21970.002
 1.083397728D+07-5.331905390D+04 1.018129921D+02-8.788665370D-03 1.540686696D-06
-1.445586275D-10 5.618818920D-15 0.000000000D+00 3.206116430D+05-6.582677680D+02

C10H15  JP-10 RADICAL AM1 unscaled calc Tertiary rad. side position
 3 S 4/01 C  10.00H  15.00    0.00    0.00    0.00 0  135.2261000      96319.864
     50.000   200.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21224.621
-6.879164980D+02 1.241446582D+02-2.027091799D+00 1.082761304D-01-5.943875370D-04
 2.218412324D-06-2.507974232D-09 0.000000000D+00 8.723448110D+03 3.421507720D+01
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21224.621
-1.103770024D+06 2.040448949D+04-1.396167445D+02 4.793142930D-01-5.827874750D-04
 3.729624160D-07-9.738330370D-11 0.000000000D+00-8.359352970D+04 7.803392510D+02
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         21224.621
 1.086373123D+07-5.393049090D+04 1.025035975D+02-9.120480680D-03 1.621955531D-06
-1.545086670D-10 6.101331200D-15 0.000000000D+00 3.229570760D+05-6.642650340D+02

C10H22  N-DECANE D.W.Scott buletin 666 Bartlesville 1974
 2 T 5/99 C  10.00H  22.00    0.00    0.00    0.00 0  142.2816800    -249533.760
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         46902.640
-1.183018848D+06 2.127103844D+04-1.313401133D+02 4.822989070D-01-5.786556750D-04
 3.671450740D-07-9.557529820D-11 0.000000000D+00-1.330191669D+05 7.575089670D+02
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         46902.640
 9.077387930D+06-4.826984880D+04 1.080580594D+02-6.266355700D-03 1.547275132D-06
-1.954174423D-10 9.814021840D-15 0.000000000D+00 2.418142466D+05-6.635913680D+02
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C11H24  N-UNDECANE  TRC 10/1975
 2 T 5/99 C  11.00H  24.00    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   4.00O   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   4.00O   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 & Bozzelli JPCRD 32 (2003),1713-1735.
 3 T03/04 C  12.00H   6.00CL  2.00O   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 & Bozzelli JPCRD 32 (2003),1713-1735.
 3 T02/04 C  12.00H   6.00CL  2.00O   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
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C12H8O p-dibenzo-dioxine hf298  Dorofeeva JPC 107 (2003), 2848.
 3 T 8/03 C  12.00H   8.00O   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

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

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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C16H33 Hexadecyl secondry radical  Bozzelli-THERM  Rough Approximation
 2 S05/01 C  16.00H  33.00    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  0.0            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  0.0            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  0.0            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  0.0            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  0.0         31267.815
 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  0.0         31267.815
-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  0.0         31267.815
 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  252.3092800     205057.840
     50.000   200.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         37877.283
 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  0.0         37877.283
-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  0.0         37877.283
 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  0.0         80263.828
-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  0.0         80263.828
-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  0.0         80263.828
-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
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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
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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 & 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 & 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 & 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
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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        21149.662
 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        21149.662
 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        21149.662
-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        11995.393
 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        11995.393
 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        11995.393
 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        10747.508
-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        10747.508
 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        10747.508
 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        11866.000
 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        11866.000
 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        11866.000
-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   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         8813.000
-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         8813.000
 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
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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
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NHD Amidogen-D   Hf:est. from NH2,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          9912.414
-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          9912.414
-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          9912.414
 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 NH2,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          9962.325
 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          9962.325
 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          9962.325
 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 NH3,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         10234.000
 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         10234.000
 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          9911.000
-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          9911.000
-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         10074.137
-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         10074.137
-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         10074.137
 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
```

```
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,&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
```

```
N3 Azide Radical  HF298=453.54+/-3.5 kJ  REF=Ruscic ATcT A
 3 tpis89 N   3.00    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   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   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   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
```

```
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   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   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  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   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
```

```
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   Stanumtetrahidride 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	± 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	± 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	±40	48.873	288.83	12.851	#
BrO2 O-Br-O	111.9028	152	161.545	±25	45.364	271.112	11.395	#
BrO3	127.9022	221	233.180	±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	±0.11	36.057	245.469	9.725	†
Br2O BrBrO	175.8074	168	183.722	±20	51.385	312.704	13.137	†#
Br2O Br-O-Br	175.8074	107.6	124.061	±3.5	50.168	290.823	12.399	†#
Br2Pb Br-Pb-Br	3 67.008	-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	±0.45	20.839	158.102	6.536	†
C+	12.01045	1809.444	1797.65	±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	±15	74.650	318.724	15.528	†
CBrF3 Freon 1301	148.90991	-650.59	-638.48	±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	±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	±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	±30.	42.962	259.150	10.902	†
COCLF	82.4615	-426.779		±33	52.402	277.019		*
CCLF2	85.460206	-275.	-272.96	±25.	55.172	287.353	12.432	†
CCLF3 FC-13	104.45861	-710.02	-704.93	±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		±42	45.103	265.974		*
CCL2	82.91670	231.7	230.5	±1.7	51.028	266.112	11.728	#
CCL2F	101.91450	-105.	-103.57	±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	±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		±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	±0.7	30.056	213.034	9.065	†
CF+	31.008554	1131.292	1121.86	±0.92	29.642	201.509	8.697	†
FCN	45.01614	35.987		±16.7	42.359	225.416		*
COF	47.0088	-171.539		±63	38.943	248.48		*
CF2	50.007506	-191.26	-191.73	±1.35	38.915	240.831	10.351	†
CF2+	50.006958	917.03	910.37	±1.6	38.541	246.731	10.342	†
COF2	66.00721	-640	-636.92	±5.	47.365	258.971	11.134	†
CF3	69.00591	-467.4	-464.6	±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	± 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	±1.96	49.339	254.540	11.541	†
CF3I	195.91068	-589.11		±3.3	70.941	307.633		
CF3O Radical	85.005309	-630.696	-625.69	±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	±0.53	61.052	261.459	12.730	†
CH	13.01894	595.8	592.5	±0.6	29.175	183.037	8.625	#
CHBr	92.92264	377.857	384.99	±2.	39.789	252.872	10.416	#
CHBrClF	137.37374	-230.000	-217.24	±15	62.869	304.928	13.787	#
CHBrF2 HBFC-22B1	130.91975	-425.46	-412.26	±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	±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_2OH	99.92374	-94.977	-91.0		69.410	307.164		#
CHCL3 liquid Chloroform	119.3779	-133.784		±0.72				X
CHCL3 CHLOROFORM	119.3779	-102.928			65.5	295.666		†
CHCL3O CCl_3OH	135.37644	-275.977	-270.06.	±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	±4.2	75.072	355.672	17.157	†
HCN anharmonic	27.02568	129.799	180.136	±0.38	35.857	201.824	9.235	†
HNC	27.02568	191.908	191.530	±0.69	40.271	205.511	10.001	†
HNCO Isocyanic acid	43.02478	-118.600	-115.60	±4.2	45.078	238.265	10.966	†
HOCN Cyanic acid	43.02478	-15.456	-12.76	±20.	46.047	241.244	11.268	#
HCNO Fulminic acid	43.02478	167.603	171.042	±12	48.395	225.025	10.623	#
HONC	43.02478	234.164	235.73	±17.	49.654	248.364	12.400	#
CHN2	41.03242	319.796		±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	±0.3	34.680	224.28	10.000	#
CHO+	29.0178	833.059			36.015	203.32		*
COH	29.01804	218.10	217.72	±0.83	34.970	225.030	10.008	#
COOH equilibrium	45.01744	-181.32	-178.16	±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	±1.6	35.130	194.436	10.032	#
CH2 Methylene SINGLET	14.02658	428.8	428.3	±1.6	33.781	189.220	9.940	#
CH2 Methylene Triplet only	14.02658	391.2	390.7	±1.6	35.014	194.418	10.027	#
CH2BrCL HALON101	129.38358	-45		±15	52.726	287.29		
CH2Br2	173.83458	4.937	26.329	±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	±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	±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	± 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		±9.9	52.926	256.458		
CH2NO CH_2=N-O*	44.03302	173.427		±21	49.153	249.913		
H2CNO H_2C*N=O	44.03302	223.928		±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		±20	51.505	247.641		
H2CN2 HN=C=NH	42.04036	149.005		±15	50.223	247.113		
CH2N2 H_2C=N=N	42.04036	286.382		±25	51.144	240.982		
H2CN2 CY DIAZIRENE	42.04036	320.143		±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	±0.3	38.417	194.008	10.366	#
CH3+	15.03397	1101.792	1099.37	±0.097	34.749	186.827	9.983	#
CH3BR	94.93852	-36.443	-21.034	±2.	42.312	245.954	10.607	#
CH3CL	50.48722	-81.87	-73.94	±0.6	40.741	234.396	10.416	†
CH3F FC-41	34.032923	-239.55	-231.52	±2.65	37.504	222.826	10.135	†
CH3Hg Methyl Mercury	215.62452	188.28	200.21	±8.4	46.073	260.58	11.165	#
CH3I Methyl Iodide	141.93899	14.30	23.838	±1.4	44.084	253.007	10.816	†#
CH3N (H_2C=NH) Methanelmine	29.04126	84.015	91.93	±4.5	38.084	221.567	10.176	#
CH3N Methyl-N Radical	29.04126	319.950	327.711	±4.5	39.990	226.694	10.330	#
CH3NO NITROSOMETHYL	45.04096	79.002		±7.3	50.77	260.833		
OCHNH2 FORMAMIDE	45.04096	-195.263		±10.5	48.473	253.646		
CH2NOH	45.04096	29.288			53.359	248.547		
NCH3O FORMIMIDIC ACID	45.04096	-148.436		±10.9	43.477	254.079		
H3CNO CH_2-NH=O	45.04096	59.032		±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	±1.	64.891	302.910	15.345	#
CH3NO3 METHYL-NITRATE	77.03976	-122.005	-107.13	±4.2	76.597	305.793	16.234	
CH3N2 CH_3N=N*	43.0483	247.651		±12	53.694	257.186		
CH3N3 CH_3-N=N=N MethylAzide	57.05474	297.29	309.93	±8.	63.015	279.531	14.118	#
CH3O	31.03392	21.0	28.4	±2.1	42.541	234.278	10.719	#
CH2OH	31.03392	-17.0	-10.7	±0.7	47.401	244.170	11.781	†
CH2OH+	31.03337	716.400	718.149	±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		±5.1	52.257	268.762		
CH3S Thiomethoxy Radical	47.10082	124.6		±1.7	46.64	242.040		#
CH4 RRHO	16.04276	-74.6	-66.633	±0.3	35.613	186.314	10.023	
CH4 ANHARMONIC	16.04276	-74.6	-66.626	±0.3	35.691	186.371	10.016	†
CH4N CH_3NH*	30.0492	187.569		±4.8	47.372	235.967		
CH4N *CH_2NH_2	30.0492	153.49	164.62	±8.	48.597	244.694		#
(NH2)2C=O Urea	60.05564	-235.5			79.088	282.953		
CH4N4O2 Nitroguanidine, Picrite	104.06852	1.		±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_3OOH)	48.04126	-126.733	-114.22	±4.2	66.753	275.904	14.160	#
CH4S (CH_3SH)	48.10876	-22.525			50.415	258.382		
CH5N CH_3-NH_2	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	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
CH5N2 CH_3N*NH_2	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 CH3SnH3	136.76834	118.407	136.091	±4.2	73.750	285.712	15.907	#
CI4 TetraIodoMethane	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(NO2)4 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		*†
CO2	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	†
CS2 Anharmonic	76.143	116.70	115.913	±1.	45.482	237.889	10.664	†
C2	24.0214	824.35	816.288	±1.6	43.549	197.097	10.169	†
C2Br	103.9260	623.667	626.39	±2.	45.103	295.017	11.648	#
C2Br2	183.8300	335.31	346.51	±2.	68.067	294.448	15.427	#
C2Br2F4 HALON 2402	259.82361	-790.776		±4.2	120.019	252.529		
C2Br3	263.7340	385.388	405.674		83.269	369.892	18.602	#
C2Br4	343.638	215.584	218.816		102.196	387.413	22.410	#
C2Br5	423.54200	283.257	318.915		126.162	444.694	27.749	#
C2Br6	503.44600	165.480	209.480		146.665	459.134	31.667	#
C2CL	59.4747	494.09			45.046	241.948		†
C2CL2	94.9274	226.6		±14	65.668	271.942		*†
C2CL2F2 CCLF=CFCL E(trans)	132.92361	-341.486	-339.3	±8.	87.333	327.192	17.925	#
C2CL2F2 CCLF=CCLF Z(cis)	132.92361	-339.548	-337.37	±8.	87.632	327.213	17.934	#
C2CL2F4 FC-114	170.92101	-900.4			116.6	364.2		
C2CL3	130.3801	190.28			76.033	328.166		†
CCl2F-CCLF2 FC-113	187.37531	-705.8			121	386.9		
C2CL3F3 FC-113A	187.37531	-740.6			120.3	369.3		
C2CL4	165.834	-24.2	-23.336	±8.0	94.92	340.925	19.606	†
C2CL5	201.2855	39			118.832	397.906		
C2CL6	236.7376	-162.110	-159.69	±8	136.326	407.696	27.235	†#
C2D2	28.0502	222.194	222.675		49.556	208.92		*
C2D2O	44.0496	39.932			55.669	249.614	12.388	*
C2D4	32.0784	30.279			52.064	230.672		*
C2OD4	48.0778	-180.582			64.697	275.315	14.042	*
C2D6	36.1066	-110.676			64.743	244.479	13.228	*
C2D6N2 Azomethane-D6	64.12001	119.248			92.1	312.346		*
C2D6O DimethylEther-D6	52.10601	-209.49	-192.04		77.528	283.259	15.875	*
C2F	43.019803	353.847	350.00	±50.	42.6	231.036	10.367	†
C2F2	62.018206	-144.666	-147.	±20	60.114	249.570	13.266	†
C2F3	81.01661	-228.175	-227.0	±20.	66.178	297.643	14.164	†
C2F4 FC-1114	100.01501	-675.34	-671.91	±2.0	80.459	300.128	16.331	†#
C2F5	119.01402	-891.192			94.111	341.49		
C2F6 FC-116	138.01182	-1347.38	-1339.0	±0.31	106.294	341.033	20.229	†#
CF3-O-O-CF3	170.01122	-1507.077		±12.5	137.807	433.17		
C2H ETHYNYL	25.02994	568.522		±4	41.999	213.304		†
C2HBr	104.93394	282.43	289.073	±2	55.087	252.719	11.948	#
C2HBr2	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	± 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	±8.4	107.701	425.045	23.519	#
C2HBr4 1,1,1,2-CBr3CHBr	344.64534	243.634	274.593	±8.4	113.967	417.090	24.422	#
C2HBr5	424.54994	113.09	153.50		126.586	439.181		#
C2HCL	60.48264	226.4		±10.	54.32	241.999		†
C2HCLF 1,1-CLF Radical	79.48074	101.87	103.90	±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	±3.0	80.016	324.941	16.605	†
C2HCL4	166.84014	21.824	26.108	±8.	100.608	375.159	20.419	#
C2HCL5	202.29284	-160.410	-153.83	±8.	113.348	379.920	22.716	#
C2HF	44.027743	41.692	41.	±25	52.268	231.573	11.446	†
C2HF2	63.02615	-42.5	-40.52	±17.9	59.249	279.393		#
C2HF3	82.02455	-490.78	-485.53	±8.24	69.191	292.665	14.328	†
C2HF5 FC-125	120.02136	-1120.00	-1110.4	±8.	95.808	334.635	18.776	#
HCCN	39.03668	610.431		±100	54.238	240.596		
C2HNO NC-CHO	55.03548	44.120	46.152	±8.	55.793	270.935		#
C2HNO2 HCC-NO2	71.03488	278.654	283.597	±8.	69.580	289.604	14.414	#
HCCO Ketyl Radical	41.02934	177.402		±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	±0.8	44.001	200.917	10.006	†
C2H2Br2 1,2-DiBromoEthylene	185.84528	101.9	121.55	±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	±8	53.700	270.153	11.996	#
C2H2CLF	80.48868	-165.393	-159.0	±15	64.216	283.339		†
C2H2CL2 CCL2=CH2	96.94328	2.2	8.084	±1.4	67.722	288.285		#
C2H2CL3 CH2-CCL3	132.39538	82.81	88.908	±5.	94.764	329.695		#
C2H2F2-1,1+cis+trans equilib.	64.03409	-336.4	-329.48	±4.	60.237	266.054	12.480	†
C2H2F2-1,1 FC-1132A	64.03409	-336.4	-329.48	±4.	60.123	266.041	12.476	#
H2C2F2 *cis*	64.03409	-306.5	-299.80	±5.	58.349	268.723	12.701	#
F2C2H2 *trans* FC-1132	64.03409	-303.73	-297.15	±5.	60.074	267.847	12.955	#
C2F3H2	83.03309	-517.142			79.499	303.093		
CF3-CFH2	102.03089	-913.3	-902.01	±17.5	86.273	315.752	16.937	#
CHF2-CHF2 HFC-134	102.03089	-883.3	-872.21	±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 Isocyana	40.04402	358.23	360.59	±8.	53.971	256.71	12.550	#
C2H2NO NC-CH2-O*	56.04342	175.619	181.426	±8.	61.512	281.028	13.444	#
C2H2NO2 NC-CH2-O-O*	72.04282	177.987	185.371	±8.	74.150	312.514	16.207	#
1,2-C2H2(NO2)2 trans	118.04896	40.953	56.131	±8.	108.234	360.962	21.428	#
CH2CO Ketene	42.03728	-47.698		±1.7	51.744	241.896		†
HCCOH ETHYNOL	42.03728	93.186		±18.3	57.403	249.142		
C2H2O2 trans & cis GLYOXAL	58.03608	-212.082	-206.51	±0.8	60.409	272.483	13.682	†
C2H2O2 CIS GLYOXAL	58.03668	-193.35		±0.8				X
C2H2O2 Oxyranone	58.03608	-177.916	-170.37	±8.	53.635	263.960	11.713	#
C2H2O4 Oxalic Acid	90.03488	- 731.8	-721.2	±2.0	86.149	320.662		#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± 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	±0.92	42.071	233.663	10.522	†#
C2H3+ Vinylium Ion	27.04467	1122.34	1119.2	±1.17	50.714	225.350	11.780	#
C2H3BrO2 Bromoacetic Acid	138.94802	-383.5	-364.61	±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	±8.	53.681	264.024	11.820	#
C2H3CLO3	94.49672	-427.6	-416.0	±1.0	78.839	325.918		#
C2H3CL3 CH3-CCL3	133.40332	-144.6	-133.98	±2.0	92.410	320.413	18.025	#
C2H3F	46.043623	-140.1	-132.21	±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	±1.0	78.074	287.652	15.298	#
CH3CD3 1,1,1-Ethane-D3	33.087526	-107.57	-92.313	±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	±0.37	52.249	243.267	12.094	#
C2H3N CH3NC Methylcyanate	41.05196	163.5	169.982	±7.2	52.947	246.658	12.660	#
C2H3NO NCCH2OH	57.05136	-49.910	-39.97	±8.	64.965	280.796		#
C2H3NO2 NCCH2-O-OH	73.05136	29.476	39.641	±8.	82.503	323.081	17.659	#
C2H3NO2 Nitroethylene	73.05136	33.284	46.001	±8.6	73.68	300.503	15.108	
C2H3O (CH3CO) RADICAL	43.04522	-10.3	-3.6	±1.8	50.785	267.448	12.385	#
C2H3O+ (CH3CO+) ion	43.044714	669.952	670.921	±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	±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	±0.6	72.544	303.542	15.531	#
C2H4CL2 CH3-CHCL2	98.95856	-127.6		±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	±8.0	87.266	282.502		#
C2H4O VINYL-ALCOHOL	44.05316	-124.683			61	289.996		
C2H4O OXYRANE	44.05316	-52.635	-40.082	±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		±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	±2	50.484	247.118	12.185	†
C2H5Br BROMOETHANE	108.9651	-61.60	-39.65	±1.01	64.206	287.668	13.584	#†
C2H5CL CHLOROETHANE	64.5138	-106.827	-92.25	±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	±4.9	59.575	270.530	12.888	#
C2H5I IODOETHANE	155.96557	-7.047	8.253	±0.56	71.670	298.362	14.575	#
C2H5NO2 NITROETHANE	75.06724	-103.784	-83.506	±5.	79.018	320.512	16.015	
C2H5ONO2 ETHYLNITRATE	91.06664	-154.975	-132.82	±8.	95.103	328.863	18.480	
C2H5N3 Ethyl Azide	71.081320	266.872	287.394	±8.	80.026	303.042	15.761	#
C2H5O* ETHOXY RADICAL	45.0609	-13.6	-0.2	±8.0	66.321	277.642	14.325	#
CH2CH2OH RADICAL	45.0609	-23.849	-11.640	±8.0	68.668	291.708	15.564	
CH3CH*OH RADICAL	45.0609	-54.030	-40.776	±8.0	64.038	288.991	14.263	#
C2H5O Dimethylether Radical	45.0609	0.960	14.079	±8.0	66.124	281.519		#
C2H5O2 EthylPeroxy Radical	61.06050	-28.70	-12.450	±8.4	73.721	299.991		#
C2H6 ETHANE	30.0694	-83.852	-68.232	±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	± 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	±8.	66.912	270.641.		#
C2H6N *CH2-NH-CH3	44.07578	156.58	174.07	±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	±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	±8.	68.541	267.185		#
C2H7N2 (CH3)2N-NH*	59.09046	207.685	232.276	±8.	81.384	284.772		#
C2H8N2 SYM Dimethylhydrazine	60.099	94.491		±7.5	82.347	287.346		
C2H8N2 UNSYM	60.099	53.22			91.524	302.186		
CCN	38.02814	679.07	674.474	±6.23	44.231	237.159	11.089	#†
CNC	38.02814	675.85	670.935	±5.89	45.042	233.804	11.357	#†
C2NO	54.02754	210.00	207.188	±10.	56.145	278.187	13.594	#†
C2N2	52.03488	309.28	307.342	±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	±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		±5.9	273.376	667.098		
C2O	40.02080	291.039	287.000	±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	±8	55.612	277.062	13.479	#
C3F3 FCC-CF2*	93.02731	-134.419	-135.23	±8	81.990	326.463	17.210	#
C3F3 *CC-CF3	93.02731	-79.078	-79.609	±8	80.749	313.306	16.929	#
C3F4 PerFluoroAllene	112.02571	-553.685	-551.89	±8	92.135	336.733	19.021	#
C3F6 Hexafluoropropene	150.02252	-1157.253	-1150.95	±8	121.759	373.675	23.337	#
C3F7 RADICAL	169.02182	-1347.122	-1339.5	±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	±8	53.430	247.795	12.696	#
C3HF7 FC-227EA	169.02092	-1564.816	-1552.4	±8	136.690	399.058	25.901	#
C3HN CyanoAcetylene	51.04678	368.414	367.225	±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	±62.7	67.953	260.782	15.215	
C3H2(1) HC-C≡CH*	38.04888	817.972	816.374	±62.7	58.770	251.691	13.227	
C3H2F3 CF3-CH=CH*	95.04319	-376.895	-369.47	±8	90.727	323.105	17.442	#
C3H2F3 CF3-C*=CH2	95.04319	-374.941	-367.82	±8	91.100	125.439	17.741	#
C3H2N HC*=CH-CN	52.05472	442.855	445.486	±8	59.531	272.030	13.333	#
C3H3 PROPARGYL RADICAL	39.05682	346—349		±8	64.891	256.659		†
CLC3H3 1-Chloro-1-propyne	74.50862	184.711	189.553	±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	±8	89.452	316.769		#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
C3H3F3 CF3-CH=CH2	96.051130	-631.131	-619.51	±6.	90.704	319.468		#
C3H3I CH2ICCH Propargyl Iod.	163.96039	269.072	276.353	±12.5	74.028	354.081	15.180	#
C3H3I CH2=C=CHI Allenyl Iod.	163.96039	264.117	272.127	±12.5	70.463	305.857	14.451	#
C3H3N CH2=CHCN	53.06266	184.037	190.874	±8	59.387	263.290	13.361	#
C3H3O CH2=CHC*=O	55.05532	88.530	94.601	±8	61.410	300.654		#
C3H3O *CH2-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-CH2CL	75.51656	250.253	259.680	±8.	73.850	303.749	15.261	#
CLC3H4 *CH2-CH=CHCL	75.51656	137.444	147.12	±8.	71.705	303.390	15.012	#
C3H4N CH3-CH*-CN	54.07060	222.706	232.213	±8.	72.044	298.672	14.925	#
C3H4N2 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		#
C3H4O2 CH2=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 CH3C*=CH2 " "	41.0727	237.651			61.663	266.064		
S-C3H5 CH3CH=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	#
CH3CH=CHNO2 Nitropropylene	87.07824	9.987	29.046	±8.9	93.59	330.004	18.288	
C3H5NO2 NitroCycloPropane	87.07824	21.033	41.466	±8.	90.786	311.278	16.913	#
C3H5N3O9 NITROGLYCERINE	227.08752	-279.073	-246.14	±2.7	234.24	545.865	43.458	
C2H5CO Propanal	57.0712	-32.83	-19.862	±8.	67.859	314.290		#
CH2COCH3 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	†
C3H6N2O2 N-NITRO-AZETIDIN	102.09292	114.123	141.198		100.656	328.954	18.840	
C3H6N6O6 RDX Solid	222.11748	79.078	--		284.884	146.189	--	
C3H6N6O6 RDX 135 Triazine	222.11748	192.000	233.285		230.174	482.441	39.331	
C2H5CHO Propionaldehyde	58.08004	-192.046			80.73	304.51		
CH3COCH3 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		
C3H5NH2 CY-PROPYLAMINE	57.09499	77.389			89.045	285.464	16.956	*
C3H7N AZETIDINE	57.09532	98.198			67.14	267.274		
C3H7NO2 Nitropropane	89.09412	-124.265	-97.795	±0.4	104.085	350.046	19.344	
C3H7NO3 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	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
(CH3)2CHOH 2-Propanol	60.09592	-272.7	-248.59		89.594	309.226	17.265	†
C3H8O2 CH3-O-CH2-O-CH3	76.0953	-346.967	-321.13	±8.	100.842	347.098		#
C3N2O NC-CO-CN	80.0449	247.5	246.523	±6.4	80.854	310.032	17.148	#
C3O2	68.0318	-93.64			67.37	276.816		†
C4	48.044	1033.904	1025.0		57.272	252.862	13.118	†
C4Cl2 Cl-CC-CCCl	118.94820	453.592	447.208	±8.	93.858	319.209	19.779	#
C4CL6 Perchloro-1,3-Butadiene	162.0343	-96.65	-97.33		38.364	110.307		
C4F2 FCC-CCF	86.03961	215.309	210.191	±8.	88.863	294.682	18.157	#
C4F6 Perfluoro 1,3-Butadiene	162.0343	-1004.122			137.272	388.442	24.949	*
F6C4 Perfluorocyclobutene	162.03439	-1210.843			131.589	379.256	25.135	*
C4F8 Perfluorocyclobutane	200.03123	-1513.6			145.483	405.3		
C4F10 FC-3110 Perfluorobutane	238.02803	-2137.417			189.038	480.624		
C4H	49.05194	803.328			66.759	265.569		
C4H2 Butadiyne	50.05988	458.299	456.653	±8	73.738	249.613	14.328	#†
C4H2N2 Fumaronitrile	78.072160	330.996	334.8	±8..	85.445	308.998	17.549	#
C4H3 E,1-butene-3-yne-1-yl	51.06662	543.104	545.65	±8	71.773	281.767	14.371	#
C4H3 i,1-butene-3-yne-2-yl	51.06662	501.829	502.00	±8..	77.383	305.368	16.739	#
C4H4 1-Butene 3-yne	52.07456	287.859	294.717	±8.	71612	277.319	14.292	#
C4H4 Cyclobutadiene	52.07456	385.000	394.047		60.969	251.442	12.104	†
C4H4N2 PYRAZINE	80.08804	195.811	212.069	±1.3	73.945	280.378	13.562	#
C4H4N2 PYRIMIDINE	80.08804	196.648	212.864	±1.	73.69	280.677	13.645	#
C4H4N2 SUCCINONITRILE	80.08804	209.7	221.172	±0.9	92.458	325.114	18.349	#
C4H4O FURAN	68.07516	-34.685			65.407	267.251		
C4H4O VINYL-KETENE	68.07516	22.719	31.98	±8.	81.797	309.171	16.229	#
C4H4O2 1,4-DIOXIN	84.07456	-86.0	-71.5	±7.	81.291	284.693		#
C4H4S Thiophene	84.14176	114.9			72.818	278.778		
E-C4H5 1,3-butadiene 1-yl	53.08250	363.339	373.360	±8.	74.144	303.589	15.362	#
I-C4H5 1,3-butadiene-2-yl	53.08250	315.223	325.419	±8.	77.138	290.119	15.188	#
T-C4H5 1,2,butadiene-4-yl	53.08250	315.223	325.299	±8.	78.273	293.833	15.308	#
C4H5 1-butyne-3-yl	53.08250	316.530	325.987	±8.	81.528	293.864	15.928	#
C4H5N PYRROLE	67.09044	108.18		±0.81	71.6	270.722		
C4H5N Cyclopropanecarbonitrile	67.09044	184.096		±0.84	78.734	321.389		
C4H6 1-Butayn Ethylacetylen	67.09044	165.2	178.798	±0.88	81.820	291210	16.020	†
C4H6 2-ButaynDimethylacetylen	54.09044	146.314	159.388	±8.	77.886	291.909	16.544	†#
1,3-C4H6 Butadiene	54.09044	110.834	125.118	±8.	74.219	293.330	15.335	†#
1,2-C4H6 Butadiene	54.09044	161.314	175.436	±2.	78.663	290.993	15.496	#
C4H6 Cyclobutene	54.09164	156.7	173.761		64.414	262.076	12.558	†
C4H6CL2 1,4-Dichlorobutene	124.99584	-51.882	-34.587	±8.	108.341	386.083	21.505	#
CL2C4H6 3,4-Dichlorobutene	124.99584	-53.572	-36.121	±8.	109.803	379.398	21.349	#
C4H6O 2,5 Di-Hydro FURAN	70.09104	-108.78			75.6	284.25		
C4H6O4 CH3-CO-OO-CO-CH3	118.08804	-500.	-477.02	±10	122.291	390.682	23.944	#
2,5 C4H6S Dihydrothiophene	86.15764	86.9			83.306	297.089		
C4H7 tt-1-Butene-1-yl	55.09838	245.871	262.755	±8.	83.705	311.281	16.968	#
C4H7 cc-1-Butene-1-yl	55.09838		264.85	±8.	-	-		X
C4H7 trans 1-Butene-2-yl	55.09838	231.162	248.45	±8.	83.973	300.371	16.425	#
C4H7 cis 1-Butne-2-yl	55.09838		248.11	±8.	-	-		X
C4H7 *trans*-2-Butene-2-yl	55.09838	223.853	239.743	±8.	83.237	313.256	17.962	#
C4H7 *cis*-2-Butene-2-yl	55.09838		243.09	±8.	-	-		X
C4H7 *trans* 3-Butene 1-yl Rad.	55.09838	204.595	220.915	±8.	84.719	317.348*	17.533	#
C4H7 cis 3-Butene-1-yl Radical	55.09838		223.01	±8.	-	-		X
C4H7 *trans* (CH2=CH*CHCH3)	55.09838	136.111	153.553	±8	80.787	306.087*	16.411	#
C4H7 *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	± 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	±5.	82.196	300.803	16.229	#
C4H7 Cyclobutyl Radical	55.09838	230.306	249.366	±8.	73.070	286.490	14.792	#
C4H7O 2-Butanone Radical	71.09778	-75.994	-57.670	±8.	97.420	344.655	19.868	#
C4H7O CH2=C(CH3)CH2O*	71.09778	55.748	75.378	±8.	96.143	334.259	18.562	#
C4H8 CH2=CH-CH2-CH3	56.107	-0.544			85.362	307.923	16.929	*
H8C4 CH2=C(CH3)2	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		†
C4H8CL2S Mustard	159.07772	-124.77	-100.66		136.283	420.586	27.569	#
beta HMX solid	296.15664	74.894	--		307.302	145.101	--	
C4H8N8O8 HMX	296.15664	187.862	245.304	±25.1	275.455	568.833	50.045	
C4H8O 2-Methyl-Allyl Alcohol	72.10572	-161.143	-137.34	±2	100.007	316.183	18.622	#
C4H8O 2-BUTANONE	72.10572	-238.362			102.432	339.991		
H8C4O 2,3-Dimethyloxyrane	72.10572	-137.658	-113.00	±8.	95.471	303.780	17.777	#
OC4H8 ETHYL-OXYRANE	72.10572	-115.960	-91.115	±8	91.134	316.499	17.582	#
C4H8O Tetrahydrofuran, Oxolan	72.10572	-184.18			76.25	302.41		
C4H8O2 1,4 DIOXANE	88.10632	-314.428		±7.	92.568	294.582		
(CH3COOH)2 Acetic Acid dimer	120.1048	-929.015	-901.62		137.254	414.396	28.053	†
C4H8O4 Tetraoxocan	120.10512	-620.2			116.255	340.343		
C4H8S Tetrahydrothiophen	88.17352	-34.1			92.55	309.627		
1,4-C4H8S2 Dithiane	120.23952	0			109.655	326.252		*
1,3-C4H8S2 Dithiane	120.23952	-10			110.434	333.542		
C4H9,n-Butyl Radical	57.11426	81.80	105.91	±8.	94.555	307.628		#†
i-C4H9 iso-Butyl Radical	57.11426	73.785	97.92	±8.	98.111	304.662	18.063	#
s-C4H9 *sec*-Butyl Radical	57.11426	70.224	94.945	±8.	86.395	327.417	17.538	#
C4H9,t-Butyl Radical	57.11426	55.041	79.719	±8.	82.410	323.393	17.010	#
C4H9N PYROLIDINE	71.1222	-3.59		±0.8	82.112	309.206		
C4H9NO2 Nitrobutane	103.121	-143.93	-109.63		115.119	369.874	21.040	
C4H9O n-BUTOXY RAD	73.11366	-56.350	-29.003	±8.	101.894	337.600	19.314	#
C4H9O I-BUTOXY RAD	73.11366	-65.070	-36.703	±8.	101.777	319.038	18.294	#
C4H9O S-BUTOXY RAD	73.11366	-69.84	-41.88	±8.	102.025	327.058	18.700	#
C4H9O T-BUTOXY RAD	73.11366	-86.923	-58.899	±8.	106.062	309.188	18.637	#
C4H10 n-Butane	58.123	-125.790	-98.46	±0.67	98.651	309.884	19.227	†
I-C4H10 ISOBUTANE	58.123	-134.990	-106.37	±0.63	96.643	295.493	17.936	†
C4H10FO2P SARIN	140.09437	-963.157	-927.62	±40	161.667	412.013	29.468	#
C4H10N2 1,4-Piperazine	86.13568	32.058	70.65	±8.	96.860	301.189	16.633	#
C4H10O-N 1-BUTANOL	74.1228	-274.68			108.168	361.616		
C4H10O-S 2-BUTANOL	74.1228	-292.629			111.134	363.877		
C4H10O-T 2-Methylpropanol	74.1228	-312.628			113.481	329.72		
C4H12Sn Sn(CH3)4	178.84808	-20.502	+11.004	±4.2	145.919	410.093	29.840	#
C4H12Sn H2Sn(C2H5)2	178.84808	56.484	90.910	±4.2	143.567	410.046	26.920	#
C4N2 Carbon Subnitrid	76.0574	529.2	524.285	±0.8	86.326	290.524	17.799	†
C5	60.05350	1050.924	1040.0	±60.	75.507	271.676	16.192	†
C5F12 FC 4-1-12	288.03584	-2543.311			229.036	555.108		
C5H	61.0629	778.276			65.158	260.415	12.013	*
C5H2	62.0709	691.412			82.981	266.639	14.674	*
C5H2CL2O CY	148.97418	-12.17	-5.59		111.295	349.650		#
C5H2CL3 CY	168.42748	152.68	158.05		118,207	369.726		#
C5H3 1,3-Pentadiyne-5-yl Rad.	63.07882	602.58			87.499	295.196		
C5H3 HCCCH*CCH	63.07882	564.61		±43	93.241	306.147		
C5H3 Cyclopentatriene-yl	63.07882	697.77		±75	70.898	281.721		

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± 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	±8.	139.671	397.902		#
C5H3N HCC-CH=CH-CN	77.08406	422.613	426.538	±8.	93.766	318.598	18.380	#
C5H4 1,3-Pentadiyne	64.08526	411.835	416.818	±8.	86.669	291.342	17.221	#
C5H4 1,4-Pentadiyne	64.08526	451.964	434.773	±8.	89.940	305.243	17.191	#
C5H4 Pentane-Tetraene	64.08526	444.466	449.702	±8.	86.132	287.480	16.968	#
H4C5 1,2-Pentadiene-4-yne	64.08526	433.354	438.929	±8.	86.751	301.509	16.628	#
C5H4 1,2,4-Cyclo-Pentatriene.	64.08526	551.485		±9.	73.235	279.6		
C5H4N *CH=CH-CH=CH-CN	78.09200	502.942	510.320	±8.	97.601	341.652	19.160	#
C5H4N meta-Pyridyl Radical	78.09200	405.241	418.146	±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	±8	101.982	361.789	20.080	#
C5H5 1-Pentyne-3-ene-5-yl	65.09320	384.93	393.17	±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	±8.	99.632	336.825	19.246	#
C5H5N PYRIDINE	79.10144	140.37		±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	±1.5	75.368	274.152	13.535	†
C5H6N2 2-AMINOPYRIDINE	94.11612	118.616		±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	±8.	92.672	325.606	17.484	#
C5H7 1,4-Pentadien-3-yl	67.10908	205.455	223.086	±8.	93.92	323.195	17.275	#
C5H7 Cy 1-penten-1-yl	67.10908	172.623	192.745	±8.	79.939	296.325	14.785	#
C5H7 Cy 1-penten-4-yl	67.10908	223.94	243.815	±8.	80.499	290.579	15.031	#
C5H7CL	102.56178	58.091	76.235	±8	110.072	374.067	21.352	#
C5H7CL2	138.01448	110.926	128.756	±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	±8.	92.705	317.69		#
C5H8 1,3-Pentadiene	68.11702	84.157	105.770	±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 CH2ClCH=CHCH2CH2	103.56972	158.197	179.288	±8.	119.551	399.520	22.640	#
PETN Solid	316.13828	-538.481		±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	±5.4	97.436	309.296	17.366	#
C5H8O 1,5-Cyclopenten-2-ol	84.116420	-126.579	-99.582	±8.	96.604	315.064	16.583	#
C5H9 CY	69.12496	111.131	138.404	±8.	88.092	298.784	16.101	#
C5H9 2-PENTEN-5-YL	69.12496	174.615	196.937	±8.	110.968	357.785	21.052	#
H9C5 2-PENTEN-1-YL	69.12496	116.700	140.617	±8.	106.281	347.013	19.457	#
C5H9 3M-1-BUTEN3YL	69.12496	102.479	126.020	±8.	107.506	333.972	19.833	#
C5H9 3M-1-BUTEN1YL	69.12496	219.091	243.190	±8.	105.817	335.407	19.275	#
C5H9 3M-1-BUTEN4YL	69.12496	180.356	204.114	±8.	108.450	348.534	19.616	#
C5H9N	83.1332	75.312		±8.4	99.27	274.978		

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± 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	± 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	±2.5	76.656	286.072		#
C6H5 FULVENYL RAD	77.10390	467.315	479.324	±8.	87.147	297.813	15.482	#
C6H5 FULVENYL Rad. Melius	77.1057	490.365		±52	93.077	307.123		
C6H5Br Bromobenzen	157.0097	105.018			97.696	324.386		
C6H5BrO 2-Bromophenol	173.0073	-63.72	-39.09	±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	±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.		±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		±10	90.362	294.123		
C6H6 BENZVALENE	78.11364	384.9	403 ?	±8.3	80.825	284.701		#
C6H6 1,5-Hexadiyine	78.11364	417.166	428.062	±8.	111.036	336.936	20.829	#
C6H6 2,4-Hexadiyne	78.11364	369.100	379.830	±8.	103.026	335.627	20.995	#
C6H6 1,3-Hexadiyne	78.11364	392.363	404.299	±8.	107.021	328.174	19.790	#
C6H6 1,2,4,5 Hexatetraene	78.11364	396.229	407.942	±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		±35	97.618	305.835		
C6H7 1,3,5-Hexatriene-6-yl	79.11798	431.387	446.410	±8.	110.758	363.629	20.937	#
C6H7-1 CY C5H5-1-CH2*	79.11798	334.092	351.954	±6.3	100.095	326.062	18.098	#
C6H7-3 CY C5H5-3-CH2*	79.11798	247.316	265.583	±19.2	101.756	321.686	17.693	#
C6H7-1 CY C5H4-1-*-CH3	79.11798	226.773	244.638	±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	±8.3	89.425	293.780		#
C6H8 CY 2,4-C5H5-1-CH3	80.12772	112.257	135.267	±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	± 8.	119.775	370.613	22.225	#
1,3-C6H9 hexadiene 6-yl Rad.	81.13566	265.533	286.651	± 8.	120.582	389.084	22.990	#
C6H9 Cyclohexenyl-3	81.13566	131.47	159.011	± 8.	97.860	313.685	16.886	#
C6H9 CY 1- C5H6-4-CH3-4-yl	81.13566	188.468	214.322	± 8.	103.489	321.009	18.574	#
C6H9 CY 1- C5H7-4-CH2*	81.13566	215.731	241.534	± 8.	106.551	323.588	18.625	#
C6H9 CY 1-C5H7-3-CH2*	81.13566	212.464	237.965	± 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	±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	± 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	±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	±8.	101.249	309.518	17.208	#
C6H11 CH2=CHC3H6CH2*	86.15334	162.502	190.886	±8.	127.963	417.768	24.512	#
C6H11 CH3CH=CHC2H4CH2*	86.15334	153.862	181.880	±8.	129.760	404.206	24.878	#
C6H11 trans 3-hexene-6-yl Rad	83.15334	154.540	183.164	±8	128.546	401.219	24.272	#
C6H11 CH2=C(CH2*)C3H7	83.15334	95.340	125.298	±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	±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	±8.	128.105	375.530	24.237	#
C6H11 (CH3)CHCH*CH=CH2	83.15154	91.232	119.916	±8.	135.913	384.042	24.212	#
C6H11 2-Methyl-1-pentene-4-yl	83.15154	136.913	165.834	±8.	127.708	386.671	23.975	#
C6H11 Cyclohexy Radical	83.15154	75.839	110.421	±8.	106.108	317.527	18.513	#
C6H11I Iodo-CycloHexane	210.05601	-50.0	-11.926	±4.7	121.960	363.668	21.420	#
C6H12 TRANS-3-HEXENE	84.16128	-50.417	-17.218	±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	±8.	147.533	428.452	28.213	#
C6H13 2MP-1YL	85.16922	35.635	70.799	±8	140.892	399.411	26.200	#
C6H13 2MP-5YL	85.16922	32.367	67.427	±8.	139.391	414.154	26.304	#
C6H13-S 2ME - 4PENTYL	85.16922	20.079	55.023	±8.	141.737	402.960	26.420	#
C6H13-T 2ME 2PENTYL	85.16922	17.209	52.180	±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	±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		±5.0	244.68	137.779		
C7H5N3O6 TNT	227.13122	24.1	53.992	±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	±8.	109.167	332.619	19.401	#
C7H7 BENZYL RADICAL	91.13048	208.0	226.8	±1.9	109.700	318.229	18.178	#
C7H7 Quadricyclene Appex Rad.	91.13048	534.519	556.275	±2.2	95.877	297.781		#
C7H7 Quadricyclene Basis Rad.	91.13048	581.346	603.316	±2.2	90.683	299.778		#
C7H7 Quadricyclene Shoulder R	91.13048	588.94	611.424	±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		±2.2	----	----		X

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± 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	±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	±30.	103.136	306.087		
C7H10N2O2 Cyclo(Pro-Gly)	154.16658	-341.012	-301.25	±12.5	158.210	401.299	27.301	#
C7H12 NORBORNANE	96.17228	-53.723		±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		±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	±1.5	111.964	326.193		#
C8H6O2 Benzodioxin	134.13204	-71.2	-49.95	±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		±1.25	121.264	332.373		
C8H8 CUBANE	104.14912	651.7		±30	98.47	271.426		
C8H8 STYRENE	104.14912	148.3	169.66	±2.	120.190	344.770	20.940	†
C8H9 C6H5CH2CH2*	105.15706	237.714	262.114	±8.	130.543	364.717		#
C8H10 C6H5C2H5	106.1650	29.790	58.81	±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	± 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	± 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		±5.				X
C8H20Pb (C2H5)4Pb Gas	323.4444	109.6	169.315	±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		±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		±1	124.226	335.846		

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± 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	±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	±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	±20	144.004	369.098	23.429	#
C10H9 !-Methylene-Indene Rad	129.17846	337.649	363.520	±20	144.045	364.065	22.771	#
C10H9 2-Methylene Indene Rad	129.17846	266.5		±20	-	-		X
C10H10 1,2-DihydroNapthalene	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	±20	144.346	360.391	23.113	#
C10H10 2-Methyl Indene	130.1864	173.636	202.811	±20	146.240	364.509	23.701	#
C10H10 3-Methyl Indene	130.1864	173.218	202.400	±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	±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	±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	± 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	±10	225.552	493.238	38.388	
C12H4CL4O2 2,3,7,8	321.97336	-136.1	-120.71	±10	241.524	513.049	41.226	#
C12H4CL4O2 1,3,6,8	321.97336	-128.7	-113.55	±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	±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	±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	±25.1	250.467	582.730	44.993	
C12H5CL4O3 radical	338.97710	-432.42	-412.55	±62.8	265.578	551.043	45.331	
C12H5CL4O3 radical	338.97710	-321.79	-301.82	±62.8	263.787	550.127	45.226	
C12H5CL5O2 6-6' ether	358.43400	-250.16	-232.43	±21.	270.758	585.917	47.711	
C12H6CL2O DCDF	237.08084	5.2	25.245	±24.7	192.255	439.242		#
C12H6CL2O2 DCDD	253.08024	-89.3	-67.92	±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≡C* EthynylNaphthyl	151.18758	694.962	710.644		162.077	397.847	26.598	
C12H8 Acenaphthylene	152.19552	259.7		±5.9	154.775	358.632		
C10H7-C≡CH EthynylNaphthalen	152.19552	379.070	398.592		169.895	391.974	26.992	
C12H8O Di-Benzo-Furan	168.19492	55.2	80.812	±4.8	163.566	375.274	25.229	
C12H8O2 Di-Benzo-p-Dioxin	184.19432	-50.1	-23.24	±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		±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		±10.				X
C14H12 trans-Stilbene	180.24508	223.3	255.957	±4.	203.066	447.878	32.901	#
C14H14 BIBENZYL	182.26096	135.6	175.94	±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	±7.3	216.018	412.967	31.264	#
C20H12 Perylene	252.30938	205.058	239.058	±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	± 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	±35.	458.824	803.678	80.264	#
C24H12 Coronene	300.35208	307.5	345.262	±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		±105.	560.816	591.403		
C70 Footballene	840.77	2652.	2660.33	±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	±0.8	20.786	154.887		†
Ca+	40.07740	773.2		±0.2	20.786	160.650		
CL	35.4527	121.302	119.633	±0.008	21.838	165.192		†
DCL	37.4668	-93.359	-93.333	±0.21	29.170	192.773	8.661	*†
DOCL	53.4662	-78.539	-76.648	±2.1	38.585	240.321	10.325	*†
CLF	54.4511	-50.293		±0.42	32.082	217.939		*
CLF3	92.44791	-158.851		±2.9	63.996	281.633		*
CLO	51.4521	101.218		±2.1	31.558	226.646		*†
CLO2 (OClO)	67.4515	104.599		±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		±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		±4.2	20.786	174.313		
CrCl	87.4488	129.9	129.159	±2.7	34.684	249.790	9.389	#
CrClO		-117.9		±9.6		301.01	13.574	X
CrClO2		-310.3		±21.6		309.81	14.449	X
CrCl2	122.9015	-117.6	-120.00	±1.7	59.00	319.36	15.638	X
CrCl2O		-336.5		±22.5		333.03	16.784	X
CrCl2O2	154.90030	-519.2	-515.35	±4.2	84.052	329.53	18.066	#
CrCl3		-283.		±6.1		347.03	19.101	X
CrCl3O		-507.8		±3.0		357.32	20.049	X
CrCl4		-396.5		±13.8		371.92	22.480	X
CrCl5		-389.6				407.16	26.602	X
CrCl6	264.71230	-345.3	-344.58	+50. ?	143.573	414.95	30.878	#
CrN(s)	66.00284	-117.294		±8.4	51.093	37.215		*
CrN	66.00284	505.022		±20.9	30.753	230.553		*
CrO	67.9955	188.285		±41.8	31.33	239.27		*
CrO2	83.9949	-75.313		±41.8	43.404	269.245		*
CrO3	99.9943	-292.88	-318.00	±41.8	56.124	266.201	13.040	*
Cr2N(s)	117.99894	-125.532		±12.6	66.318	64.921		*
Cr2O3(s)	151.9904	-1135.094		±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	±0.001	20.786	123.352	6.197	†
D+	2.01355	1540.320	1532.210	±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	±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	± 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	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
GeCl4	214.4208	-500.9	-498.55	±5.	95.975	348.572	21.150	†#
GeH3Cl	111.08652	57.70	67.63	±5.	54.795	273.113	11.995	#
GeH4	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	†
HNO2	47.01348	-78.452	-72.8	±0.6	46.320	254.071	11.597	†
HNO3	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		
HO2	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		
HO2S	65.07274	-255.88		±6	50.708	276.742		
HSO3	81.07214	-385			67.209	294.061		
HS2 Hydrothiosulpheno Radical	65.13994	104.60	107.145	±10.46	39.703	253.304	10.484	#
H2 REFERENCE ELEMENT	2.01588	0	0		28.836	130.679		*‡
H2F2	40.01269	-569.924	-566.5		58.132	260.905		
H2O(L)	18.01528	-285.83			75.351	69.939		†
H2O	18.01528	-241.826		±0.04	33.588	188.829		†
H2O2(L)	34.01468	-187.778	-193.58		89.328	109.604	22.949	†
H2O2	34.01468	-135.88	-129.89	±0.2	42.416	234.542	11.162	#
H2S	34.08188	-20.6			34.248	205.803		
H2SO4(L)	98.07948	-814.01			138.594	156.907		*†
H2SO4	98.07948	-732.7	-720.85	±2.0	90.235	311.333.	18.391	#
H2S2	66.14788	15.500	21.243		48.745	251.070	11.549	
H3F3	60.01903	-883.677	-873.		73.884	280.947		
H3O+	19.02267	598			35.485	193.139		
H4F4	80.02537	-1186.932	-1174.		104.022	350.016		
H5F5	100.03172	-1490.188	-1475.		134.161	417.286		
H6F6	120.03806	-1805.545	-1788.		163.735	486.619		
H7F7	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		†
HgBr2 (solid)	360.398	-169.457			75.312	170.778		†
HgBr2 (gas)	360.398	-85.452			60.319	320.239		†
HgCl (gas) Calomel	236.0427	78.45			36.34	260.0		
HgCl2 (solid)	236.0427	-230.12						
HgCl2 (liquid)	236.0427	-213.22						
HgCl2 (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	± 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		±0.04	20.786	180.789		
INO2 NITRO-IODINE	172.91001	60.25			59.366	294.432		
IO	142.90387	126		±18	33.117	239.835		
IO2 O-O-I	158.90327	116.5		±40	48.727	296.374		
IO2 O-I-O	158.90327	159.3		±25	46.697	281.231		
IO3	174.90267	241.9		±50	61.56	292.975		
I2	253.8089	62.444			36.889	260.584		*
I2O I-I-O	269.80834	106.7		±40	52.359	330.647		
I2O I-O-I	269.80834	119.5		±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	±0.4	20.786	160.470		†
K+	39.09775	514.0		±0.4	20.786	154.578		
KNO3(S)	101.10320	494.0	-488.31	±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	±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	±0.8	20.786	148.649		†
Mg+	24.30445	891.047	883.65	±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	±41.8	35.645	244.952		†
MgBr2(S)	184.1130	-524.6		±2.1	73.298	117.143		†
MgBr2(L)	184.1130	-490.41			----	---		†
MgBr2	184.1130	-302.92		±10.5	58.720	301.048		†
MgCO3(S) Magnesium Carbonat	84.31420	-1111.69		±8.	76.262	65.863		†
MgCl	59.75770	-43.51		±42.	34.858	233.423		†
MgCl+	59.75715	652.7		±84.	35.476	228.566		
MgClF	78.75610	-569.02		±21.	49.912	265.994		
MgCl2 (S)	95.21040	-641.62		±0.46	71.509	89.660		†
MgCl2(L)	95.21040	-601.58			---	---		†
MgCl2	95.21040	-392.46		±2.1	57.146	277.041		†
MgF	43.30340	-236.81		±8.4	32.570	221.089		†
MgF+	43.30285	512.29		±46.	32.644	215.348		
MgF2(S)	62.301810	-1124.2		±1.3	61.546	57.243		†
MgF2(L)	62.301810	-1072.35			---	---		†
MgF2	62.301810	-726.76		±16.7	48.264	256.514		†
MgF2+	62.30126	592.		±20.9	52.459	258.152		
MgH	25.31294	169.03			29.557	193.199		†
MgI	151.20947	24.61		±41.8	36.816	252.650		†
MgI2(S)	278,11394	-366.94		±6.3	74.907	129.698		†
MgI2(L)	278.11394	-342.25			---	---		†
MgI2	278.11394	-160.25		±10.5	59.631	317.496		†
MgN	38.31174	288.70	289.04	±25.1	32.761	224.845		†
MgO(S)	40.30440	-601.24		±0.63	37.146	36.938		†
MgO(L)	40.30440	-532.61			---	---		†
MgO	40.30440	58.16		±25.1	32.241	213.299		†
MgOH	41.31234	58.16		±37.7	43.049	226.467		†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
MgOH+	41.31179	584.42		±62.8	43.229	220.834		
Mg(OH)2(S)	58.31968	-924.66		±2.1	77.264	63.236		†
Mg(OH)2	58.31968	-572.37		±33.5	69.505	267.295		†
MgS(S)	56.37100	-345.72		±4.2	45.605	50.329		†
MgS	56.37100	-145.23		±66.9	34.664	225.518		†
MgSO4(S)	120.36860	-1261.79		±20.9	96.209	91.393		†
MgSO4(L)	120.36860	-1246.59			---	---		†
MgSiO3 (S)	100.38870	-1548.92		±4.2	82.198	67.839		†
MgSiO3 (L)	100.38870	-1494.86		±20.9	---	---		†
MgTiO3(S)	120.18320	-1572.56		±6.3	91.953	74.583		†
MgTiO3(L)	120.18320	-1497.63		±6.3	---	---		†
MgTi2O5(S)	200.06200	-2509.36		±10.5	147.009	135.655		†
MgTi2O5 (L)	200.06200	-2382.31		±8.4	---	---		†
Mg2	48.61000	287.63		±08	24.293	240.189		†
Mg2F4	124.60361	-1718.37		±37.7	107.553	337.041		†
Mg2SiO4(S)	140.69310	-2176.94		±4.2	119.151	95.239		†
Mg2SiO4(L)	140.69310	-2113.88		±20.9	---	---		†
Mg2TiO4(S)	160.48760	-2164.38		±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		±0.4	20.786	153.302		†
ND	16.0208	355.309	355.710	±8.	29.159	187.234	8.648	†
NHD Radical	17.028782	178.165	181.106	±8.	33.703	205.600	9.912	#
ND2	18.0349	181.937	184.878	±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	±0.4	38.225	203.931	10.234	†#
NF	33.00514	232.99	233.	±3.	30.228	212.908	8.738	†
NF2	52.00355	34.421	37.000	±5.	41.058	249.638	10.582	†
NF3	71.00195	-131.7	-125.98	±1.	53.497	260.812	11.855	†
NH	15.01468	358.792	358.76	±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	±15	35.234	230.806	10.030	†
NHF2	53.01149	-103			43.384	252.814		†
NH2 AMIDOGEN RADICAL	16.02258	186.2	189.1	±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	±0.03	34.597	192.475	9.984	#
NH3 AMONIA Anharmonic calc	17.03056	-45.567	-38.946	±0.03	35.630	192.770	10.043	†
NH2OH Hydroxyl Amine	33.02996	-50		±10	46.472	236.181		†
NH4+ AMONIUM ION	18.03795	644.905			34.764	186.095		†
NH4CLO4(I)	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	± 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	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
PF5	125.96578	-1594.433		±2.9	85.05	300.855		*†
PH	31.9817	230.752	231.698	±33.5	29.175	196.381	8.648	†
PH2 Phosphonium Radical	32.989641	135.474	139.333	±8.	34.272	212.710	9.969	#†
PH2-	32.990190	-9.265	+0.800	±10.	34.124	205.247	9.960	†
PH3 PHOSPHINE RRHO	33.997581	11.786	19.712	±8.	37.102	210.245	10.137	#†
PN	44.9805	104.776			29.667	211.126		*
PO	46.97316	-29.597		±4.2	31.725	222.768		*
PO2	62.97256	-314.533			41.397	253.682		*
P2	61.94752	143.651		±2.1	32.057	218.135		*
P4	123.89505	58.917		±2.1	67.326	280.022		*
P4O6	219.89145	-2144.519		±33.5	143.998	345.664		*
P4O10(s)	283.88905	-3010.022		±8.9	211.82	228.786		*
P4O10	283.88905	-2904.154		±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	±0.8	20.786	175.377		†
PbBr	287.1040	64.821	73.805	±20	36.916	272.744	10.146	†
PbBr2	367.0080	-103.908	-87.54	±7.	56.966	339.673	15.022	†
PbBr3	446.9120	-104.011	-80.330	±80.	80.540	385.255	19.969	†
PbBr4	526.8260	-182.436	-152.4	±80.	104.468	427.724	25.871	†
PbCl	242.65270	8.819	10.493	±12.	36.215	261.306	9.787	†
PbCl2	278.10540	-175.046	-173.5	±5.	55.299	315.621	14.003	†
PbCl3	313.55810	-177.654	-175.27	±80.	77.918	351.604	18.256	†
PbCl4	349.0108	-327.43	-325.65	±80.	100.537	381.682	23.449	†
PbF	226.19840	-98..072	-96.853	±10.	34.401	249.962	9.268	†
PbF2	245.19681	-443.427	-440.30	±11.	50.981	291.532	12.573	†
PbF3	264.19521	-489.573	-485.0	±60.	70.582	316.287	15.535	†
PbF4	283.1936	-799.925	-795.03	±60.	90.232	331.825	19.626	†
PbI	344.10447	108.904	112.033	±4.	37.152	280.413	10.339	†
PbI2	461.00894	-10.253	-5434	±5.	57.182	352.613	15.247	†
PbI3	587.91341	21.755	27.35	±80.	81.624	411.532	21.065	†
PbI4	714.81788	-41.281	-35.485	±80.	106.276	463.806	27.521	†
PbO(S)	223.19940	-218.6	-216.61	±0.5	46.414	67.840	9.225	†
PbO	223.19940	68.187	70.385	±4.5	32.513	240.045	8.962	†
PbO2(S)	239.19880	-276.0	-271.41	±1.5	60.997	71.920	10.962	†
PbO2	239.19880	136.153	139.452	±100.	51.721	261.093	12.251	†
PbS(S)	239.2660	-99.475	-99.703	±	49.499	91.200	11.510	†
PbS	239.2660	127.945	129.797	±1.5	35.085	251.414	9.430	†
PbS2	271.3320	244.049	245.722	±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	±0.25	23.674	167.832	6.657	†
SCL	67.5187	156.47		±16.7	37.555	237.334		*†
SCL2	102.9714	-17.572		±3.3	50.909	281.641		*†
SF	51.0644	12.971		±6.3	35.157	225.282		*†
SF2	70.06281	-296.653		±16.7	44.906	257.708		*†
SF3	89.06121	-503.041		±33.5	62.998	286.186		*†
SF4	108.05961	-763.18		±20.9	77.62	299.657		*†
SF5	127.05802	-908.467		±15.1	89.687	304.774		*†
SF5Br	206.96202	-972.8		±59	107.075	333.654		
SF5CL	162.51072	-1038.9		±10.5	104.344	319.936		
SF6	146.05642	-1220.502		±0.8	96.994	291.551		*†
SN	46.07274	263.583		±105	31.758	222.081		*

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
SO	48.0654	5.008		±1.3	30.164	221.944		*
SOF2	86.06221	-543.926		±105	57.202	279.156		*
SO2	64.0648	-296.835		±0.21	39.867	248.206		*
SO2CLF	118.5159	-556.476		±21	71.719	302.879		*
SO2CL2	134.9702	-354.802		±2.1	77.218	311.127		*
SO2F2	102.06161	-758.569		±8.4	65.946	283.651		*
SO3	80.0642	-395.753		±0.71	50.692	256.775		*
S2	64.132	128.404		±.0.3	32.481	228.313		*
S2CL	99.5847	78.562		±8.4	50.968	292.162		*
S2CL2	135.0374	-16.736			72.776	327.237		
S2F2 (SSF2)	102.11681	-401.422		±41.8	63.146	292.729		*
FS2F	102.11681	-336.443		±41.6	66.061	293.985		*
S2F10	254.11603	-2064.386		±29.3	176.702	397.041		
S2O	80.1314	-56.486		±33.5	44.112	267.029		*
S8	256.528	100.42		±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	±16.8	44.707	256.710	11.228	#
SiF3 TrifluoroSilyl Radical	85.080710	-993.365	-990.4	± 8.	59.613	282.433	13.398	#
SiF4 TetrafluoroSilane	104.07911	-1614.98	-1609.4	± 4.2	73.534	282.615	15.325	#
SiHF3 TriFluoroSilane	86.088650	-1207.67	-1200.5	± 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	±4.2	98.459	364.549	22.340	†#
SnH3 TriHydroStanum Radical	121.73382	258.153	266.252	±4.2	44.818	240.204	10.926	#
SnH4 TetraHydroStanum	122.74176	162.758	174.594	±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	± 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