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Third Millennium Ideal Gas and Condensed Phase Thermochemical Database for Combustion
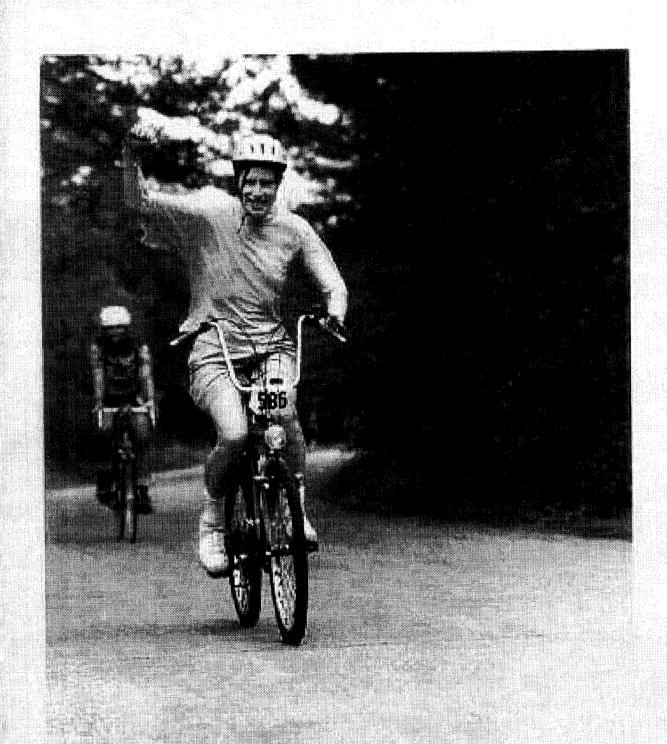
Alexander Burcat

Dedication

This database is dedicated to the memory of Professor William C. Gardiner (Bill) of the Chemistry Department at The University of Texas in Austin. Because of Professor Gardiner's initiative and encouragement this database was started 20 years ago, and he was the first to publish it in 1984. Since then and untill the day of his tragic accident, he showed continuous interest in the development of this project.

May He Rest in Peace.

Dr. William C. Gardiner, Jr.

January 14, 1933-November 17, 2000

MS-150 BIKE TOUR
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The database is available at:

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

Third Millennium Ideal Gas and Condensed Phase Thermochemical Database for Combustion

Alexander Burcat

Faculty of Aerospace Engineering,
Technion - Israel Institute of Technology, Haifa, 32000, Israel

Abstract

A database of Thermodynamic data for substances important in combustion research is available for free use over the Internet. The database is presented in a polynomial form suitable for use in computer programs. This is an update and enlargement of an earlier printed database. It includes now more than 850 species as compared to 215 in the first database version (1984), of which about two thirds were recalculated for updating purposes. This database is explained and discussed.

Introduction

There are two widespread misconceptions about thermochemical data. The first is the wrong belief that thermochemical data are always available and that there are no outstanding problems in this domain. In fact, thermochemical data of any kind are available for at most 10-15 thousand chemical species out of the several million ones known, i.e., less than 1%.

The second misconception is that whatever thermochemical data may not be available from experiments reported in the literature can be estimated readily with sufficient accuracy by group additivity methods (Benson 1976; Pedley *et al.*, 1986; Ritter and Bozzelli

1990, 1991; Stein *et al.*, 1991; Stein 1994, Cohen and Benson 1992; Lay *et al.*, 1995; Muller *et al.*, 1995; Cohen 1996). The truth about group additivity is that it cannot be used for many species, or can be used with very high uncertainty, for lack of group and bond data.

On the other hand, molecular quantum mechanics has reached a point where molecular fundamentals such as vibrational frequencies, bond lengths and configurations can be calculated with reasonable accuracy, and only the standard enthalpies of formation cannot be calculated with enough confidence, if the molecule is big.

The science of combustion routinely uses calculations for evaluation and estimation of properties of combustion processes such as flames, ignition, detonation and so on. The performance of experiments and routine operation of combustion processes depend on calculation of various properties. In these calculations the understanding of chemical detail, i.e., elementary chemical reactions and knowledge of chemical composition may be crucial. The most important properties of the chemical substances that are of interest in combustion research and applications are the thermochemical ones.

Various thermodynamic and thermochemical properties are used in the domain of combustion. The enthalpy of formation $\Delta_f H_T^\circ$,

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is very useful in order to compute the heat of reaction $\Delta_r H_T$ from which the heat of the system can be computed and also the adiabatic flame temperature can be calculated. As these have to be calculated at different temperatures, the enthalpy of formation has to be available as a function of T. The heat content C_p or enthalpy are used to calculate the properties of shock and detonation.

The equilibrium conditions are usually computed using the gibbs function or the equilibrium constant. Again these functions should be known as a function of T, and they can be calculated from the other thermodynamic and thermochemical properties, if the entropy and the enthalpy of formation are known.

Since all calculations and evaluations are computerized nowadays, the thermodynamic and thermochemical data have to be provided in a form suitable for computer access. A polynomial form of representing thermochemical data has been found to be the most suitable, as discussed in detail previously (Burcat 1984). An alternate representation preferred by some authors is to tabulate standard molar $\Delta_f H_{298}$ (or $\Delta_f H_{300}$) and S_{298} (or S_{300}) values together with a list of standard molar $C_p(T)$ values from $T = 300$ to $T = 1000$ or 1500 K. It is based on the idea that S_T°, $H_T^\circ - H_{298}^\circ$ and $G_T^\circ - H_{298}^\circ$ values can be calculated by apropriately integrating the C_p° function for interpolation. Extrapolation of the functions to higher temperatures is necessary and must be done in a suitable way.

The problems of extrapolating thermochemical values was discussed before (Burcat 1984). The Wilhoit (1975) method for extrapolating thermochemical properties has become a standard procedure (McBride and Gordon 1992). Other extrapolations procedures were introduced by Ritter and Bozzelli (1990) for use in special circumstances.

Such tabulations for thermochemical data have both merits and shortcomings. The principal merit is the direct availability of $\Delta_f H_{300}$, S_{300}, and $C_p(T_i)$ values without having to evaluate polynomials. The main shortcoming is that it requires the user of data to do his own extrapolation and polynomization without providing the information for doing it properly.

Thermochemical Database

Thermochemical properties are calculated using statistical mechanics equations and conventions. These methods are described in the JANAF (1986) introduction to the database, and also by Gurvich Veits and Alcock (1989). The best presentation was recently put on the Internet by Irikura 1998. The present database is an enlarged and critically updated version of the earlier database (Burcat 1984). Extrapolation, where necessary, was done in an expert way. Otherwise original high temperature values were used.

Data for many additional species have been included, specifically organic radicals, large organic molecules related to fuels and soot formation, halogenated compounds important for waste incineration, fire extinguishing and air-pollution studies. A few new sulphur compounds were included. All together more than 850 species are included, of which more than 600 are new and the rest have been revised.

Updates of the Database

Since the database is available on the Internet (see below), and is periodically updated, it happens that sometimes the database is changed 3-4 times a month. Some of these changes are cosmetic, i.e., changing errors found in the text preceding each polynomial. Other changes are done in order to add new

species, and the most problematic ones are those which are done in order to exchange an existing polynomial with a new one. The reasons are publication of different molecular properties, correction of erroneous values used before to calculate the polynomial, or upgrade of the quality of the data on which the thermodynamic polynomial was based.

This procedure will cause that in principle nobody can ever know which data were used in order to calculate a certain chemical kinetic model, unless the modeler takes great care to write down the date of each of the polynomials used.

Recently there are kineticists and modelers that claim that a kind of "canonization" of the thermodynamic data values is necessary, and this is probably the reason behind the fact that the famous CHEMKIN themochemical database, is never corrected, just enlarged.

Thermochemical Polynomials

The thermodynamic and thermochemical data are represented as two sets of polynomial coefficients for each species. The first set reproduces data above 1000 K, the second set below 1000 K. The same 1000 K value is reproduced by both sets. This set is widely known as "The Old NASA polynomials". The following standard molar thermodynamic functions can be obtained from the polynomial coefficients:

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

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

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

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

$$-\frac{a_3}{6} T^2 - \frac{a_4}{12} T^3 - \frac{a_5}{20} T^4 + \frac{a_6}{T} - a_7$$

It should be noted that the H_T° value calculated is not the $H_T^\circ - H_{T_{ref}}^\circ$ function often appearing in tables but rather a thermochemical value used in engineering and usually called "absolute enthalpy" whose value is

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

The advantage of including $\Delta_f H_{298}^\circ$ in the function is that the values of H_T°/RT calculated from the polynomials can be used directly to compute standard enthalpies of reaction.

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

$$K_c = (RT)^{-\Delta \nu} \exp\left(\Delta a_1(\ln T - 1) + \frac{\Delta a_2 T}{2} \right.$$

$$\left. + \frac{\Delta a_3 T^2}{6} + \frac{\Delta a_4 T^3}{12} + \frac{\Delta a_5 T^4}{20} - \frac{\Delta a_6}{T} + \Delta a_7 \right)$$

The mole number change is $\Delta \nu = \Sigma \nu_j$ and the coefficient changes are $\Delta a_i = \Sigma \nu_j a_{ij}$ where the summations are over all reactant and product species j with the stoichiometric coefficients ν_j taken to be positive for products and negative for reactants. The reference state is the ideal gas at one bar pressure.

The change from 1 atm. to 1 bar as the thermochemical reference state, affect only the standard molar thermochemical values for gases, and for them it affects only thermodynamic functions that contain the entropy. The standard molar entropy when pressures are measured in bars is higher than the entropy when pressures are measured in atmospheres by the following amounts: for S/R, 0.013163; for S in Joules, 0.10944; and for S in calories 0.02616.

Data for a few liquid phase species, denoted by an (L) on the first data line, and

solids having an (S) on the first data line, have also been included. It is cautioned that computing equilibrium or dynamic properties must be done with these species using different methods than pertain to systems containing only ideal gases.

The information given prior to the coefficient lines indicate the nature of the procedures used to generate the input data for the fitting program (McBride and Gordon 1992).

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 one chosen was the most reliable, at the date of calculation of the polynomial coefficients. If no thermodynamic data were available in known tabulations or in the archival literature, the literature was searched for experimental or quantum mechanical calculated vibrational frequencies and moments of inertia, and independent calculations were performed. 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 & 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).

Calculations

All calculations were performed with the McBride and Gordon PAC program. Over the years this program has been changed and extended. A new documentation was published (McBride and Gordon 1992). At least 4 versions of this program were used to produce the polynomials listed on the Internet. Those prepared before 1984 were produced with the PAC3 version in which internal rotations were not calculated so that these contributions had to be added separately. PAC4 written 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 it was arbitrarily set to 1000 K. In PAC4 the polynomials are pinned to the tabular value of 1000 K and therefore reproduce it exactly. The values at 298 K, however are not the original table values, but slightly different (depending on the local error of the polynomial coefficients). In the latest versions, PAC90 and PAC97 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 must not necessarily be the tabular one. These version also includes Wilhoit type extrapolations, as discussed by Burcat (1984), and optional use of estimated additivity group properties as described by Stein (1985). The values for some species were estimated using the Ritter and Bozzelli (1990) method, and Stein's (1985) method as used in the NIST database program (Stein *et al.*, 1991; Stein 1994). The difference

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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.

Accuracy of 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 the 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 & Bozzelli, were found to give generally excellent 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 & Bozzelli gives a maximum error for unknown species which is in the $\pm 8\%$ range for $\Delta_f H_{300}$. These are maximum values, and for most cases the errors are by far lower (see Reid, Prausnitz and Poling 1988, p. 196).

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, on 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 roundoffs, 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 form:

CPR=((((A5 * T + A4)* T + A3)* T + A2)* T + A1

Standard Enthalpies of Formation

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

a) those that were measured directly;

b) those for which the difference between their value and that of another compound is known;

c) those estimated on the basis of measured values of other compounds;

d) those estimated on the basis of other estimated compounds or structural groups.

Standard enthalpies of formation are quoted and requoted by different authors, making it difficult to find out to which of the four categories mentioned, a $\Delta_f H^\circ_{298}$ value belongs. When the measured values of individual compounds change with time due to better experimental systems or to errors found in previous measurements, it causes a need to change all the $\Delta_f H^\circ_{298}$ values of compounds belonging to categories (b-d) whose estimation was based on those values. But there are no means to do these changes other than minutious and continuous examination of each individual $\Delta_f H^\circ_{298}$ value. That is in part responsible for disputes between groups of researchers claiming a different heat of formation for an important specie. In this compilation, many decisions as to which value to adopt, had to be done arbitrarily for lack of established criteria.

Very few species of interest in combustion can be assigned standard enthalpies of formation with error limits so narrow that for combustion modeling purposes they may be taken to be exact. (Cox *et al.*, 1989; Cox and Pilcher 1979; Cohen 1996) The most accurately known of all (aside from 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, being known to the accuracy with which Planck's constant is known; a few diatomic and triatomic species whose electronic spectra have been successfully analyzed to 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 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 for what can be achieved in measuring or computing standard enthalpies of reaction,is in the vicinity of 0.1 to 0.2 kJ/mol.

Table 1. Standard enthalpies of formation in kJ/mol at 298.15 K for small gas-phase species of interest in combustion. [From Cox et al. 1989 and (NO and NO_2) Chase et al. 1985.]

Species	$\Delta_f H^\circ_{298}$	Species	$\Delta_f H^\circ_{298}$
C(g)	716.68 ± 0.45	NO(g)	90.29 ± 0.17
H(g)	217.998 ± 0.006	CO(g)	-110.53 ± 0.17
O(g)	249.18 ± 0.10	H_2O(g)	-241.826 ± 0.040
N(g)	472.68 ± 0.40	CO_2(g)	-393.51 ± 0.13
S(g)	276.98 ± 0.25	SO_2(g)	-296.81 ± 0.20
Cl(g)	121.190 ± 0.008	NO_2(g)	33.10 ± 0.8

The number of species important in combustion for which "directly measured" experimental values of standard enthalpies of formation can be assigned is small. All are based one way or another on chemical reactions to which enthalpy changes of reaction can be assigned 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 reaction can usually be arranged to occur with accurately measured stoichiometry. (Cox and Pilcher 1970)

Even for 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-kilojoule uncertainty in the enthalpy change of a reaction at 1000 K implies an uncertainty of 11% in its equilibrium constant.) 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, the asserted uncertainty ranges are about twice as large as for the values listed in Table 1.

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
$CH_4(g)$	-74.85 ± 0.29	-74.48 ± 0.42
$C_2H_6(g)$	-84.68 ± 0.50	-83.85 ± 0.29
$C_3H_8(g)$	-103.89 ± 0.59	-104.68 ± 0.50
$n\text{-}C_4H_{10}(g)$	-127.03 ± 0.67	-125.65 ± 0.67
$i\text{-}C_4H_{10}(g)$	-135.60 ± 0.54	-134.18 ± 0.63

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 calorimetries, values for radicals come from all sorts of measurements ranging

from photoionization mass spectroscopy to reaction rates. It is no surprise that the results are more contentious and less accurate. An overview of the present status for some of the common free radicals is given in Table 3, where the uncertainty ranges can be seen to be typically an order of magnitude greater than for stable hydrocarbon values.

Table 3. Standard enthalpies of formation in kJ/mol at 298.15 K for common radicals. Values for hydrocarbons accepted by the IUPAC Commitee for Revision of Radical Thermochemical Data, 2000.

Species	$\Delta_f H^\circ_{298}$	Species	$\Delta_f H^\circ_{298}$
$OH(g)$	39.3 ± 0.2	$CH(g)$	596.4 ± 1.2
$CN(g)$	$441. \pm 5$	$NH(g)$	$376.56 \pm 16.$
$SH(g)$	$143. \pm 3.0$	$CH_2OH(g)$	-17.8 ± 1.3
$HO_2(g)$	$14.6 \pm$	$CH_3O(g)$	17 ± 4
$CHO(g)$	42 ± 4	$C_3H_3(g)$	339 ± 4
$CH_2(g)$	390.4 ± 4.0	$C_2O(g)$	286.6 ± 63
$CH_3(g)$	147 ± 1	$C_3H_5(g)$	171 ± 3
$C_2H(g)$	565 ± 3.0	$n\text{-}C_3H_7(g)$	100 ± 2
$C_2H_3(g)$	299 ± 5	$i\text{-}C_3H_7(g)$	88 ± 2
$C_2H_5(g)$	119 ± 2	$C_6H_5(g)$	330 ± 3

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 data base 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).

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 data base used for setting group additivity parameters. For such molecules and radicals we recommend cautious use of the group additivity methods anyway, or, if that appears infeasible, even more cautious use of semi-empirical or semi-theoretical molecular electronic structure calculations. An extensive survey of the results of such calculations has been given by Dewar *et al.*, (1993).

Since the Enthalpies of Formation seems to be the most problematic of all the thermochemical values, Table 5 is dedicated entirely to this value, where we stress the errors if available. In Table 4 we mention for some species, in curled parenthesis {} additional values if different from the chosen.

Critical Evaluation

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 sum-

mation' method, for diatomic molecules and RRHO 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.

Species not included in this database

About 850 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 cyclo 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 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 & 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 3500 species. Many of these species are transition states. Unfortunately the thermochemical tables are not available to the public, and only limited thermochemical information ($\Delta_f H$ and $\Delta_f G$) was published with his molecular structure data. His published thermochemical values are of low reliability.

C) If you are looking for a solid or liquid specie (not ideal gas) like $CaSO_4$ or $MgCl_2$, 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.*). Other organometalic species of Ga and As can be found in an article by Tirtowidjojo & Pollard.

E) Ion of simple bi and tri-atomic species can be found in JANAF. The other compilation that mentions $\Delta_f H$ at 298 for ion species for some of the molecules and radicals included, is the above mentioned NIST S& P computerized database. This information 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 calorie = 4.184 joules
$\Re$ = 8.31451 kj/kg-mol-K
$\Re$ = 1.987216 cal/g-mol-K
cal/mol = 2.8591434 cm^{-1}
1 Bohr = 0.52917706 Å

$A.M.U.-Bohr^2 = 21.505458 \text{ g cm}^2 \times 10^{-39}$
$A.M.U.-Å^2 = 6.023 \text{ g cm}^2 \times 10^{-39}$
$A.M.U.-Å^2 = 5.05531 \text{ MHz}$
$1 \text{ Hz} = 1/2.99792458 \times 10^{10} \text{ cm}^{-1}$
$B = 16.85763/I_B(A.M.U.-Å^2)$
$B = 2.7988898*10^{-39}/I_B(\text{g cm}^2)$

Electronic Files

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

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

Transfer the file to your computer using download or browse through it with your Internet explorer.

Attention! The file is approximately 0.6 MB long and the transfer to remote computers may be long at busy hours. A table generator program written by B. McBride is included, to enable generation of thermodynamic properties from the given polynomials. The tables generated provide values of C_p, S, $H_T - H_{298}$, and $-(G_T - H_{298})/T$ as a function of T. Values of $\Delta_f H$ and $\log K_p$ can be added at any temperature interval within the polynomial's given limit.

A special file called THERM.DAT is a mirror database ready to be used with the CHEMKIN program.

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