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USE OF TABULATED THERMOCHEMICAL DATA

FOR PURE COMPOUNDS

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Abstract

Thermodynamic data for inorganic compounds is found in a variety of tabulations and computer databases. An extensive listing of sources of inorganic thermodynamic data is provided. The three major tabulations are the JANAF tables (1), Thermodynamic Properties of Individual Substances (2), and the tabulation by Barin (3). The notation and choice of standard states is different in each of these tabulations, so combining data from the different tabulations is often a problem. By understanding the choice of standard states, it is possible to develop simple equations for conversion of the data from one form to another.

Key Words: Computational Chemistry, Physical Chemistry, Tabulations, Thermodynamics,

I. Introduction

Thermodynamic data for the elements and compounds are tabulated in a variety of handbooks and electronic databases. Appendix I lists the tabulations (1-19) currently in common use, along with the format (tabular, analytic functions, electronic), and the quantities tabulated. These tabulations represent many years of intensive work—both in the measurements and the gathering and assessment of the data in these tables. The focus here will be on the first three tabulations. Most of the data in the remaining tabulations have been incorporated into these. Some of the data have been critically assessed for reliability, other data have not. Generally the JANAF (1) and TPIS (2) compendia are considered to have the highest degree of reliability.

The goal with each of these databases is to reliably and accurately calculate free energy changes in a reacting system and determine the resultant product assemblage. This is done either by (i) determining the free energy change of a single balanced reaction with reactants and products explicitly specified or (ii) with a free energy minimization computer code (20) where only the reactants are specified and the products and product amounts are determined by the code. To this end, each database presents the same basic thermodynamic information. However the form and choice of reference states differs for each database. Even the notation may differ from table to table. Appendix II lists the notation used in the first three tabulations. This report follows the JANAF tables (1) and the notation recommended in an IUPAC report (21) as closely as possible.

Bale and Eriksson (22) have reviewed eight integrated thermodynamic databases (ITDs). These are commercially available databases and codes for metallurgical thermochemistry. They discuss both the databases and the features of the accompanying codes. In addition a wealth of information on computer thermochemical codes is available on the directory of web sites in

Inorganic Chemical Thermodynamics--http://www.crct.polymtl.ca/FACT/websites.htm, maintained by Ecole Polytechnique of Montreal, Canada.

The emphasis here is on stand-alone databases for pure substances and their enthalpy, entropy, and Gibbs free energy at constant pressure—the quantities most often used in high temperature inorganic thermochemistry. The goal of this report is to describe the form of the data in each database and show how to easily convert the data from one form to another. The current trend in electronic databases is to store thermodynamic information as the Gibbs Energy Function, referenced to the standard state at 298.15 K. This function and standard state are not generally treated in thermodynamics textbooks and therefore will be discussed in detail here.

II. Tabulated Enthalpies

Heat capacity, $C_p^o(T)$, is often expressed as the following polynomial function.

$$C_p^o(T) = a + b\,T + cT^{-2} \tag{1}$$

Here T is the temperature in degrees Kelvin. A fourth term $d\,T^2$ is sometimes included (23).

Enthalpy, $H^o(T)$, is defined as:

$$H^o(T) - H^o(298) = \int_{298}^{T} C_p^o(T)\,dT \tag{2}$$

Integrating equation (1), we obtain:

$$H^o(T) - H^o(298) = aT + \frac{b}{2}T^2 - \frac{c}{T} - a(298) - \frac{b}{2}(298)^2 - \frac{c}{298} \qquad (3)$$

The enthalpy is only meaningful as a difference. $H^o(T)$ alone is only meaningful if a value for $H^o(298)$ is specified. In the JANAF tables (1) enthalpies are always expressed as the difference in equation (2). Thus the JANAF tables (1) list $H^o(T) - H^o(T_r)$ for every element and compound, with T_r equal to 298.15 K. This means that $H^o(T) - H^o(T_r)$ is zero at 298.15 K, negative when $T_r < 298.15\,K$, and positive when $T_r > 298.15\,K$. Table I gives an example of the JANAF (1) listing of $H^o(T) - H^o(T_r)$ for Al(cr):

T(K)	$H^{o}(T) - H^{o}(T_r)$
0	-4.539
100	-4.056
200	-2.254
250	-1.140
298.15	0.
300	0.045
350	1.280
400	2.553
450	3.856
500	5.186
900	7.921

Table I. Selected data for $H^{o}(T) - H^{o}(T_r)$ for Al(cr) from the JANAF (1) tables.

The JANAF tables (1) also list the heat of formation $\Delta_f H''(T)$ for each substance. For the elements in their conventional standard states, this is zero. However for the compounds, it is defined as follows. Following the notation of Barin (2), consider the formation of a compound B from the elements E_i:

$$v_1 E_1 + v_2 E_2 + \ldots = B \tag{4}$$

First consider the determination of $\Delta_f H''(298)$:

$$\Delta_f H''(298, B) = H''(298, B) - \sum_i v_i H''(298, E_i) \tag{5}$$

Next consider the determination of $\Delta_f H''(T)$:

$$\Delta_f H''(T, B) = H''(T, B) - \sum_i v_i H''(T, E_i) \tag{6}$$

Since the JANAF tables only present enthalpy data as the difference $H''(T) - H''(298)$, equation (5) can be subtracted from equation (6) to give:

$$\Delta_f H''(T, B) = \Delta_f H''(298, B) + \left[H''(T, B) - H''(298, B)\right] - \sum_i v_i \left[H''(T, E_i) - H''(298, E_i)\right] \tag{7}$$

Equation (7) is thus used to determine the enthalpy of formation of B at a temperature T. The TPIS compendium lists $\Delta_f H''(0)$ and $\Delta_f H''(298)$ as well as $H''(T) - H''(0)$. The enthalpy

of formation at any temperature $\Delta_f H^o(T)$ can be calculated in manner analogous to that described above.

$$\Delta_f H^o(T,B) = \Delta_f H^o(0,B) + \left[H^o(T,B) - H^o(0,B)\right] - \sum_i v_i \left[H^o(T,E_i) - H^o(0,E_i)\right]$$

(8)

Barin (3) also lists $H^o(T) - H^o(298)$, which is the same as the JANAF (1) $H^o(T) - H^o(T_r)$. In addition, Barin (3) lists the quantity $H^o(T)$. In order to do this he uses the standard element reference state (SER), taking $H^o(298)$ as zero for the elements in their most stable aggregation state at 298.15 K. The use of the standard element reference state avoid anomalies encountered when the reference state is taken at the temperature of interest (5). As will be discussed, the major computerized databases use data with this reference state. First consider equation (5). The summation term is zero for the elements at 298.15 K, so:

$$\Delta_f H^o(298,B) = H^o(298,B) \tag{8}$$

Adding $H^o(T,B) - H^o(298,B)$ to both sides leads to (24):

$$H^o(T,B) = \Delta_f H^o(298,B) + (H^o(T,B) - H^o(298,B)) \tag{9}$$

Equation (9) thus indicates how to convert from the JANAF data to the Barin $H^o(T)$.

III. Tabulated Entropies

Tabulations of entropies are more clear than those for enthalpies since there is an absolute value for entropy. At zero degrees Kelvin, the entropy equals to zero. Entropy can be determined from:

$$dS = \frac{C_p^o dT}{T} \tag{10}$$

Now this can be integrated to:

$$S''(T) = S''(298) + a \ln T + bT - \frac{c}{3}T^{-3} \tag{11}$$

$S''(298)$ can be determined from low temperature measurements:

$$S''(298) - S''(0) = S''(298) = \int_0^{298} \frac{C_p^o(T)\,dT}{T} \tag{12}$$

The major compendia—JANAF, TPIS, and Barin—list entropy exactly the same way.

III. Tabulated Free Energies

III.A. JANAF $\Delta_f G''(T), FEF(298)$

The JANAF tables (1) present free energy functions referenced to 298.15 K and the Gibbs free energy of formation $\Delta_f G''(T)$. According to convention, the free energy of formation of the elements in their pure form, at the temperature of interest, is taken as zero. Thus $\Delta_f G^o(T)$ is zero for all pure elements. However it is not zero for compounds. The free energy function referenced to 298.15 K is extremely useful. It is defined as:

$$FEF(298) = \frac{\left[G''(T) - H''(298)\right]}{T} \tag{13}$$

Consider reaction (4). The Gibbs free energy of formation for compound B can be calculated from the free energy function as follows:

$$\frac{\Delta_f G(T,B)}{T} = FEF(298, B) - \sum_i v_i \left[FEF(298, E_i)\right] + \frac{\Delta_f H^o(298, B)}{T} \tag{14}$$

The ease of interpolation with the free energy function made it the favored choice for thermodynamic calculations until recently. However today, with near universal use of computers, polynomial expressions for free energies of formation are more widely used.

Table IIIa and IIIb illustrates the entries for these quantities from the JANAF tables (1).

T/K	$S^{o}(T)$	$-FEF(298)$	$H^{o}(T)-H^{o}(298)$	$\Delta_f H^{o}(T)$	$\Delta_f G^{o}(T)$
0	0		-3.218	0	0
100	3.833	33.351	-2.952	0	0
298.15	18.820	18.820	0	0	0
500	30.110	21.237	4.436	0	0
1000	47.329	30.387	16.942	0	0
1500	58.411	37.982	30.644	0	0

Table IIIa. Selected JANAF table (1) entries for Si(s)

T/K	$S^{o}(T)$	$\dfrac{-[G^{o}(T)-H^{o}(298)]}{T}$	$H^{o}(T)-H^{o}(298)$	$\Delta_f H^{o}(T)$	$\Delta_f G^{o}(T)$
0	0		-7.550	445.668	445.668
100	140.886	188.980	-4.809	448.142	434.437
298.15	167.980	167.980	0	450.000	405.528
500	179.204	170.456	4.374	449.938	375.391
1000	193.816	178.911	14.905	447.962	301.476
1500	202.360	185.396	25.447	444.803	228.879

Table IIIb. Selected JANAF table (1) entries for Si(g)

III.B. TPIS $FEF(0)$

The TPIS compendium (2) lists only the free energy function referenced to 0 K. This is defined as:

$$FEF(0) = \frac{[G''(T) - H''(0)]}{T} \tag{15}$$

This free energy function for gaseous molecules is readily calculated from spectroscopic data (25). In analogy with equation (14) above, the free energy of formation of compound B in reaction (4) can be calculated as:

$$\frac{\Delta_f G''(T,B)}{T} = FEF(0,B) - \sum_i \nu_i [FEF(0,E_i)] + \frac{\Delta_f H''(0,B)}{T} \tag{16}$$

The problem is that for this free energy of formation—and any free energy change calculation-- $\Delta_f H''(0)$ is needed and this not always available.

The free energy function referenced to 0 K can be converted to the free energy function referenced to 298.15 K, as follows:

$$FEF(0) = \frac{-[G'' - H''(298)]}{T} - \frac{[H''(298) - H''(0)]}{T} \tag{17}$$

The second term is calculated from the low temperature heat capacities. As pointed out by Lewis and Randall (25), reasonable estimates can be made for this which introduce little error. The free

energy function referenced to 298.15 K is given in the JANAF tables (1) and the compendium of Barin (3).

III.C. Barin $FEF(298), \Delta_f G^o(T), G^o(T)$

The tables of Barin (3) give the same $FEF(298)$ and $\Delta_f G^o(T)$, but they also include $G^o(T)$, which is the Gibbs energy (26). It should be noted that Barin (3) refers to the free energy function referenced to 298.15 K as the "Gibbs energy function" or the "free enthalpy function". This somewhat confusing nomenclature and the "free energy function" is more commonly used. Selected entries from Barin for Si(s) and Si(g) are given in Tables IVa and IVb.

T/K	$H^{o}(T)$	$H^{o}(T)-H^{o}(298)$	$\Delta_f H^{o}(T)$	$G^{o}(T)$	$\Delta_f G^{o}(T)$
298.15	0	0	0	-5.611	0
500	4.438	4.438	0	-10.619	0
1000	16.943	16.943	0	-30.390	0
1500	30.648	30.648	0	-56.979	0

Table IVa. Selected values from Barin (3) for Si(s). S and FEF(298) are the same as those in the

JANAF tables (1).

T/K	$H^{o}(T)$	$H^{o}(T)-H^{o}(298)$	$\Delta_f H^{o}(T)$	$G^{o}(T)$	$\Delta_f G^{o}(T)$
298.15	450.000	0	450.000	399.917	405.528
500	454.373	4.373	449.935	364.773	375.392
1000	464.903	14.903	447.960	271.090	301.480
1500	475.447	25.447	444.799	171.908	228.888

Table IVb. Selected values from Barin (3) for Si(g). S and FEF(298) are the same as those in the

JANAF tables (1).

Again, consider reaction (4). The free energy of formation of compound B can be calculated from the Gibbs energy functions as follows:

$$\Delta_f G''(T,B) = G''(T,B) - \sum_i v_i G''(T,E_i) \tag{18}$$

Thus if the free energy of formation of a compound is known from the JANAF tables (1) and the Gibbs energy functions for its constituent elements are known, the compound's Gibbs energy function is:

$$G''(T,B) = \Delta_f G''(T,B) + \sum_i v_i G''(T,E_i) \tag{19}$$

Using the JANAF table (1) data only, we can convert to Gibbs energy functions via the following:

$$G''(T) = H''(T) - T\,S''(T) = [\Delta_f H''(298) + (H''(T) - H''(298))] - T\,S''(T) \tag{20}$$

Also note that $G''(T)$ is the first term in the free energy function referenced to 298.15 K. Thus for pure elements, where $H''(298)$ is equal to zero:

$$G''(T) = -FEF(298)*T \tag{21}$$

For compounds where $H''(298)$ does not equal zero, we can use $FEF(298)$ to calculate $G''(T)$ as follows:

$$G''(T) = [\Delta_f H''(298) + (H''(T) - H''(298)] - T*[FEF(298)] \tag{22}$$

By definition the Gibbs energy is referenced to the elements in their most stable aggregation at 298.15 K. Dinsdale (5) has taken data from a range of sources and converted it to the Gibbs energy functions. These data is most commonly used in computer databases (eg SGTE database) for thermochemical calculations. It is often written as:

$$G - HSER \text{ or } G - H_{298} \tag{23}$$

Here HSER or H_{298} is the weighted average of the elements in the particular compound (27), which is zero. Thus the HSER in the above quantities is always zero and simply a mnemonic to specify the Gibbs energy referenced to 298.15 K. Typically $G - HSER$ is presented in the following functional form:

$$G - HSER = a + bT + cT\ln(T) + \sum_n d_n T^n \tag{24}$$

Generally the power terms are:

$$G - HSER = a + bT + cT\ln(T) + d_1 T^2 + d_2 T^3 + d_3 T^{-1} \tag{25}$$

This expression can be easily differentiated to obtain the entropy:

$$S = -\left(\frac{\partial(G - HSER)}{\partial T}\right)_p \tag{26}$$

the enthalpy:

$$H = \left(\frac{\partial [(G - HSER)/T]}{\partial (1/T)} \right)_p \tag{27}$$

and the heat capacity:

$$C_p = -T \left(\frac{\partial^2 (G - HSER)}{\partial T^2} \right)_p \tag{28}$$

Summary and Conclusions

There are numerous sources of thermochemical data for inorganic compounds at high temperatures. However the data in these compendia are often in very different forms. In this report we survey the main compendia and catalog the forms of the data presented. Equations are provided for easy conversion between the different data forms.

The most recent databases contain thermodynamic data in the form of the Gibbs energy function. This is referenced to 298.15 K. This function and its relation to Gibbs energies of formation and to free energy functions are discussed.

Appendix I. Tabulations of Thermochemical Data

Author, Title, Date	Format	Quantities	Ref
Chase, et. al., <u>JANAF Thermochemical Tables</u> (1998)	Tabular, Electronic	$C_p^o(T), S^o(T), FEF(298), H^o(T) - H^o(T_r),$ $\Delta_f H^o(T), \Delta_f G^o(T), \log K_f, \Delta_{tr} H$	1
Gurvich, et. al., <u>Thermochemical Properties of Indivual Substances</u> (1989)	Tabular, Electronic	$C_p^o(T), FEF(0), H^o(T) - H^o(0), S^o(T),$ $\log K_f, \Delta_f H^o(0), \Delta_f H^o(298), \Delta_{tr} H^o$	2
Barin, <u>Thermochemical Data of the Indivual Substances</u> (1989)	Tabular	$C_p^o(T), S^o(T), FEF(298), H^o(T),$ $H^o(T) - H^o(298), G^o(T), \Delta_f H^o(T),$ $\Delta_f G^o(T), \log K_f, \Delta_{tr} H$	3
Pankratz, <u>Thermodynamic Properties of Elements and Oxides</u> (1982) Pankratz, <u>Thermodynamic Properties of Halides</u> (1984) Pankratz, Mah, and Watson, <u>Thermodynamic Properties of Sulfides</u> (1987) Pankratz, <u>Thermodynamic Properties of Carbides, Nitrides, and other Selected Substances</u> (1994) Pankratz, Stuve, and Gokcen,	Tabular, Functional Tabular	$C_p^o, S^o(T), FEF(298), H^o(T) - H^o(298),$ $\Delta_f H^o, \Delta_f G^o(T), \log K_f, \Delta_{tr} H$ $C_p^T, S^o(T), H^o(T) - H^o(298),$ $\Delta_f H^o(T), \Delta_f G^o(T)$	4

Thermodynamic Data for Mineral Technology (1984)			
Dinsdale, SGTE Data for Pure Elements (1991)	Functional	$G - HSER$	5
SGTE Database	Electronic	$G - HSER$ for most compounds $C_p^o, \Delta_f H^o(298)$ for some compounds	6
Database for HSC	Electronic Functional	$\Delta_f H^o(298), S^o(298), C_p^o(T)$	7
Cox, et al., CODATA Key Values for Thermodynamics (1989)	Tabular	$C_p^o(T), FEF(0), H^o(T) - H^o(0)$	8
Hultgren, et. al., Selected Values of the Thermodynamic Properties of the Elements (1973)	Tabular	$C_p^o, H^o(T) - H^o(298), S^o(T) - S(298),$ $FEF(298), \Delta_{vap}G^o, \Delta_{vap}H^o, \Delta_{tr}H, \log P(vapor)$	9
Robie and Hemingway, Thermodyanamic Properties of Minerals and Related Substances at 298.15 K and 1 Bar Pressure and Higher Temperatures	Tabular	$S^o(298), \Delta_f H^o(298), \Delta_f G^o(298)$ for many minerals $C_p^o(T), S_T^o(T), H^o(T) - H^o(298), FEF(298),$ $\Delta_f H^o(T), \Delta_f G^o(T), \log K_f, \Delta_{tr}H(T)$ for selected minerals	10
Kubachewski, The Thermodynamic Properties of Double Oxides	Functional	$\Delta_f G$	11
Kubachewski, Alcock, and Spencer, Materials Thermochemistry	Tabular, Functional	$C_p^o(T), S^o(298), \Delta_f H^o(298), \Delta_{tr}H$	12

Elliot and Glieser, Thermochemistry for Steel Making	Tabular	$C_p^o(T), S^o(T), FEF(298), H^o(T) - H^o(T_r),$ $\Delta_f H^o(T), \Delta_f G^o(T), \log K_f, \Delta_{tr} H$	13
Mills, Thermodynamic Data for Inorganic Sulfides, Selenides, and Tellurides (1974)	Tabular	$C_p^o(T), S^o(T), FEF(298),$ $H^o(T) - H^o(298), \Delta_f H^o(T),$ $\Delta_f G^o(T), \log K_p$	14
Chang and Ahmad, Thermodynamic Data on Metal Carbonates and Related Oxides (1982)	Tabular	$C_p^o(T), S^o(T), FEF(298), H^o(T) - H^o(298),$ $\Delta_f G^o(T)$ for the carbonate from the metal oxide and CO_2	15
Schick, Thermodynamics of Certain Refractory Compounds (1966)	Tabular	$C_p^o(T), S^o(T), FEF(298), H^o(T) - H^o(298),$ $\Delta_f H^o(T), \Delta_f G^o(T), \log K_p$	16
Rossini, et. al., Selected Values of Chemical Thermodynamic Properties (1961)	Tabular	$C_p^o(298), S^o(298), \Delta_f H^o(0),$ $\Delta_f H^o(298), \Delta_f G^o(298)$	17
Stull and Sinke, Thermodynamic Properties of the Elements (1956)	Tabular	$C_p^o(T), H^o(T) - H^o(298), S^o(T)$ $FEF(298), \Delta_f H^o(T), \Delta_f G^o(T)$	18
Wagman, et. al., Selected Values of Chemical Thermodynamic Properties (1965)	Tabular	$C_p^o(T), S^o(298), \Delta_f H^o(0), \Delta_f H^o(298),$ $\Delta_f G^o(298), H^o(298) - H^o(0)$	19

Appendix II. Notation in the JANAF (1), TPIS(2), Barin (3), and this report.

JANAF (1)	TPIS (2)	Barin (3)	This Report	Meaning
T	T	T	T	Absolute temperature, degrees Kelvin
C_p^o	$C_p^o(T)$	C_p	$C_p^o(T)$	Heat Capacity at constant Pressure
S^o	$S^o(T)$	S	$S^o(T)$	Absolute entropy of a given substance, equal to zero at 0 K
$[G^o - H^o(T_r)]/T$		$(G - H298)$	$FEF(298)$	Free energy function referenced to 298.15 K
	$\Phi^o(T)$		$FEF(0)$	Free energy function Referenced to 0 K
	$H^o(T) - H^o(0)$			Enthalpy difference between enthalpy at temperature T and 0 K
		H	$H^o(T, B)$	Enthalpy for compound B—B not always included if it is clear from the context
$H^o - H^o(T_r)$		$H - H298$		Enthalpy difference between Enthalpy at temperature T and 298.15 K
$\Delta_f H^o$	$\Delta_f H^o(T)$	ΔH_f	$\Delta_f H^o(T)$	Enthalpy of formation of a given substance from the elements in their conventional standard states at a temperature T
		G	$G^o(T),$ $G - HSER$	Gibbs energy function
$\Delta_f G^o$		ΔG_f	$\Delta_f G^o(T)$	Gibbs energy of formation from the elements in their conventional standard states at a temperature T

K_f	$K''(T)$	K_f	K_f	Equilibrium constant for the formation of the compounds from their elements in conventional reference states
Superscript $^\circ$	Superscript $^\circ$		Superscript $^\circ$	Conventional standard state—1 bar, temperature of interest, most stable form of the element at that temperature of interest
			SER	Standard Element Reference State— 1 bar, 298.15 K, most stable form of the element at 298.15 K
$\Delta_{tr} H_T^\circ$		L	$\Delta_{tr} H$	Enthalpy of transformation

Annotated Bibliography for Main Text and Appendices:

1. The JANAF are perhaps the most widely used thermochemical tables. This data has been carefully assessed. A detailed description is given for the source of each data set. It is now in its fourth edition, although the second and third editions are still in common use:

1a. Stull, D. R. and Prophet, H. *JANAF Thermochemical Tables, 2nd ed.*; NSRDS—NBS 37, National Bureau of Standards: Washington, DC, 1971.

1b. Chase, M. W. Jr., Davies, C. A., Downey, J. R. Jr., Frurip, D. J., McDonald, R. A., and Syerud, A. N. *JANAF Thermochemical Tables, 3rd ed.; Journal of Physical and Chemical Reference Data,* Volume 14, 1985, American Chemical Society and American Physical Society for National Bureau of Standards: New York, NY, 1986.

1b. Chase, M. W. Jr. *NIST-JANAF Thermochemical Tables, 4th ed.; Journal of Physical and Chemical Reference Data,* Monograph No. 9, American Chemical Society and American Physical Society for National Bureau of Standards: New York, NY, 1998.

1c. Some of the JANAF tables and a good deal of useful information is available on the NIST Chemistry Web Page: http://webbook.nist.gov/chemistry/

2. The Russian tables "Thermodynamic Properties of Individual Substances" (TPIS) are also carefully assessed data. A detailed text describes the sources of the data and a level of accuracy is given to each substance. Listed below are three versions—the Russian version, the English translation of Volumes 1-3, Volume 4 is expected out soon, and the electronic version. The

electronic version has the option of selecting the format of the output: JANAF form, TPIS form, or functional form of C_p'', $FEF(0)$, $FEF(298)$, $H''(T) - H''(0)$, $H''(T) - H''(298)$, and $S''(T)$.

2.a. Glusko, V. P., Gurvich, L. V., Bergman, G. A., Veitz, I. V., Medvedev, V. A., Khachkuruzov, G. A., and Jungman, V. S. *Thermodynamic Properties of Pure Substances, 3rd ed., Volumes I-IV,* Nauka Publishers: Moscow, 1982 (in Russian).

2.b.i. Gurvich, L. V., Veyts, I. V., and Alcock, C. B. *Thermodynamic Properties of Indivual Substances, 4th ed., Volumes I and II,* Hemisphere Publishing Corporation: New York, 1989.

2.b.ii. Gurvich, L. V., Veyts, I. V., and Alcock, C. B. *Thermodynamic Properties of Indivual Substances, 4th ed., Volume III,* Begell House: New York, 1989.

2.b.iii. Gurvich, L. V., Veyts, I. V., and Alcock, C. B. *Thermodynamic Properties of Indivual Substances, 4th ed., Volume IV,* Begell House: New York, to be published 1999.

2.c. Gurvich, L. V., Iorish, V. S., Chekhovskoi, D. V., Yungman, V. S. *IVTANTHERMO—A Thermodynamic Database and Software System for the Personal Computer,* NIST Special Database 5, National Institutes of Standards and Technology: Gathersburg, MD, 1993.

3. The tables of Barin and Knacke do not appear to be as thoroughly assessed data. The tables are the only major tables to contain data in the form of the Gibbs energy function, as discussed in the text. The older version gives the heat capacity in both tabular and functional form, as opposed to the newer version, which only gives the heat capacity in tabular form.

3.a.i Barin, I. and Knacke, O. *Thermochemical Properties of Inorganic Substances,* Springer-Verlag: Berlin, 1973.

3.a.ii. Barin, I., Knacke, O., and Kubachewski, O. *Thermochemical Properties of Inorganic Substances*, Springer-Verlag: Berlin, 1977.

3b. Barin, I. *Thermochemical Data of Pure Substances, Volumes 1 and 2*, VCH: Wienheim, Germany, 1989.

4. This is a series of Bulletins from the former US Bureau of Mines.

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9.   Hultgren, R., Desai, P. D., Hawkins, D. T., Gleiser, M., Kelley, and Wagman, D. D. *Selected Values of the Thermodynamic Properties of the Elements*, American Society for Metals: Metals Park, OH, 1973.

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12. The textbook by Kubachewski, Alcock and Spencer is a classic, now in its sixth edition. It contains a wealth of information on experimental thermochemistry as well as extensive tables.

Kubachewski, O., Alcock, C. B., and Spencer, P. J. *Materials Thermochemistry, 6th ed.,* Pergamon Press: New York, 1993.

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13a. Elliot, J. F. and Gleiser, M. *Thermochemistry for Steelmaking, Volume 1,* Addison-Wesley Publishing Company: Reading, MA, 1960.

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