NBS TECHNICAL NOTE 270-5

Selected Values of Chemical Thermodynamic Properties

Tables for Elements 54 Through 61 in the Standard Order of Arrangement

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D. D. Wagman, W. H. Evans, V. B. Parker, I. Halow,
S. M. Bailey, R. H. Schumm, K. L. Churney

Physical Chemistry Division
Institute for Material Research
National Bureau of Standards
Washington, D.C. 20234

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ABSTRACT

Contains tables of values for the standard heats and Gibbs (free) energies of formation, entropies and enthalpies at 298.15 K and heats of formation at 0 K for compounds of vanadium, niobium, tantalum, titanium, zirconium, hafnium, scandium, and yttrium (elements 54-61 in the Standard Order of Arrangement). These tables are a continuation of the comprehensive revision of NBS Circular 500.

Key words: Enthalpy; entropy; Gibbs energy of formation; hafnium compounds; heat of formation; niobium compounds; scandium compounds; tantalum compounds; titanium compounds; vanadium compounds; yttrium compounds; zirconium compounds.

PREFACE

This is the fifth of a series of Technical Notes containing the tables of material prepared as a revision of National Bureau of Standards Circular 500, Selected Values of Chemical Thermodynamic Properties, by F. D. Rossini, D. D. Wagman, W. H. Evans, S. Levine and I. Jaffe. This Note contains data for compounds of eight elements, numbered 54 through 61 in the Standard Order of Arrangement. The Appendix contains a list of corrections for errors and misprints that have been detected in summary Note TN 270-3 and in TN 270-4.

The continued encouragement and support of the Office of Standard Reference Data of the National Bureau of Standards is gratefully acknowledged.

CONTENTS

INTRODUCTION

Substances and Properties Included in the Tables

The tables contain values where known of the enthalpy and Gibbs energy of formation, enthalpy, entropy and heat capacity at 298.15 K (25^0C), and the enthalpy of formation at 0 K, for all inorganic substances and organic molecules containing not more than two carbon atoms. In some instances such as metal-organic compounds, data are given for substances in which each organic radical contains one or two carbon atoms.

No values are given in these tables for metal alloys or other solid solutions, fused salts, or for substances of undefined chemical composition.

Physical States

The physical state of each substance is indicated in the column headed "State" as crystalline solid (c), liquid (liq), glassy or amorphous (amorp), or gaseous (g). Solutions in water are listed as aqueous (aq). For non-aqueous systems the physical state is that normal for the indicated solvent at 298.15 K.

Definition of Symbols

The symbols used in these tables are defined as follows: P = pressure; V = volume; T = absolute temperature; E = intrinsic or internal energy; S = entropy; H = E + PV = enthalpy (heat content); G = H - TS = Gibbs energy (formerly the free energy); $C_p = (dH/dT)_P$ = heat capacity at constant pressure.

Conventions Regarding Pure Substances

The values of the thermodynamic properties of the pure substances given in these tables are for the substances in their standard states (indicated by the superscript ° on the thermodynamic symbol). These standard states are defined as follows:

For a pure solid or liquid, the standard state is the substance in the condensed phase under a pressure of one atmosphere.

For a gas the standard state is the hypothetical ideal gas at unit fugacity, in which state the enthalpy is that of the real gas at the same temperature and at zero pressure.

The values of Δ Hf° and Δ Gf° given in the tables represent the change in the appropriate thermodynamic quantity when one gram-formula weight of the substance in its standard state is formed, isothermally at the indicated temperature, from the elements, each in its appropriate standard reference state. The standard reference state at 25 °C for each element except phosphorus has been chosen to be the standard state that is thermodynamically stable at 25 °C and at one atmosphere pressure. For phosphorus the standard reference state is the crystalline white form; the more stable forms have not been well characterized thermochemically. The same reference states have been maintained for the elements at 0 K except for the liquid elements bromine and mercury, for which the reference states have been chosen as the stable crystalline forms. The standard reference states are indicated in the tables by the fact that the values of Δ Hf° and Δ Gf° are exactly zero.

The values of $H^\circ_{298.} - H^\circ_0$ represent the enthalpy difference for the given substance between 298.15 K and 0 K. If the indicated standard state at 25 °C is the gas, the corresponding state at 0 K is the hypothetical ideal gas; if the state at 25 °C is solid or liquid, the corresponding state at 0 K is the thermodynamically stable crystalline solid, unless otherwise specifically indicated.

The values of S° represent the virtual or "thermal" entropy of the substance in the standard state at 298.15 K, omitting contributions from nuclear spins. Isotope mixing effects, etc., are also excluded except in the case of the hydrogen-deuterium (^{1}H-^{2}H) system. Where data have been available only for a particular isotope, they have been corrected when possible to the normal isotopic composition.

The values of the enthalpies of formation of gaseous ionic species are computed on the convention that the value of ΔHf° for the electron is zero. Conversions between 0 and 298.15 K are calculated using the value of $H^\circ_{298} - H^\circ_0$ = 1.481 kcal per mole of electrons, and assuming that the values of $H^\circ_{298} - H^\circ_0$ for the ionized and un-ionized molecules are the same.

Conventions Regarding Solutions

Solutions in water are designated as aqueous (aq); other solvents are designated by name or chemical formula. The concentration of the solution is expressed in terms of the number of moles of solvent associated with one mole of the solute. If no concentration is indicated, the solution is assumed to be "dilute".

The standard state for a solute in aqueous solution is taken as the hypothetical ideal solution of unit molality (indicated as "std. state, m = 1"). In this state the partial molal enthalpy and heat capacity of the solute are the same as in the infinitely dilute real solution. For non-aqueous solutions the standard state of the solute is the hypothetical ideal solution of unit mole fraction of solute ("std. state, $x_2 = 1$").

The value of Δ Hf° given in the tables for a solute in its standard state is the apparent molal enthalpy of formation of the substance in the infinitely dilute real solution. At this dilution the partial molal enthalpy is equal to the apparent molal quantity. At concentrations other than the standard state, the value of Δ Hf° represents the apparent enthalpy of the reaction of formation of the solution from the elements comprising the solute, each in its standard reference state, and the appropriate total number of moles of solvent. In this representation the value of Δ Hf° for the solvent is not required. The experimental value for a heat of dilution is obtained directly as the difference between the two values of Δ Hf° at the corresponding concentrations.

The values of the thermodynamic properties tabulated for the individual ions in aqueous solution are based on the usual convention that the values of ΔHf°, ΔGf°, S° and C_p° for H^+ (aq, std. state, m = 1) are zero. The properties of a neutral electrolyte in aqueous solution in the standard state are equal to the algebraic sum of these values for the appropriate kinds and number of individual ions assumed to constitute the molecule of the given electrolyte. When the undissociated species, rather than the sum of the ions, is meant, the notation "undissociated" or "un-ionized" is used. For an ionic species the properties tabulated refer to that undissociated ion. By adopting the above convention with respect to aqueous H^+, it follows that the thermodynamic relation Δ Gf° = Δ Hf° - T Δ Sf° will not hold for an individual ionic species. However no problem arises when neutral chemical systems are considered.

Unit of Energy and Fundamental Constants

All of the energy values given in these tables are expressed in terms of the thermochemical calorie. This unit, defined as equal to 4.1840 joules, is generally accepted for the presentation of chemical thermodynamic data. Values reported in other units have been converted to calories by means of the conversion factors for molecular energy given in Table A.

The following values of the fundamental physical constants have been used in these calculations:

R = gas constant = 8.3143 ± 0.0012 J/deg mol = 1.98717 ± 0.00029 cal/deg mol

F = Faraday constant = 96487.0 ± 1.6 coulombs/mol = 23060.9 ± 0.4 cal/volt equivalent

Z = Nhc = 11.96258 ± 0.00107 J/cm^{-1} mol = 2.85912 ± 0.00026 cal/cm^{-1} mol

c_2 = second radiation constant = hc/k = 1.43879 ± 0.00015 cm deg

0°C = 273.15 K

These constants are consistent with those given in the Table of General Physical Constants, recommended by the National Academy of Sciences - National Research Council[1]. The formula weights in the tables have been calculated for the molecular formula given in the Formula and Description column using the 1961 Table of Relative Atomic Weights based on the atomic mass of ^{12}C = 12 exactly[2].

Internal Consistency of the Tables

All of the values given in these tables have been calculated from the original articles, using consistent values for all subsidiary and auxiliary quantities. The original data were corrected where possible for differences in energy units, molecular weights, temperature scales, etc. Thus we have sought to maintain a uniform scale of energies for all the substances in the tables. In addition the tabulated values of the properties of a substance satisfy all the known physical and thermodynamic relationships among these properties. The quantities Δ Hf°, Δ Gf°, and S° at 298.15 K satisfy the relation:

$$\Delta Gf° = \Delta Hf° - T \Delta Sf°.$$

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[1] NBS Technical News Bulletin, October 1963.

[2] A. E. Cameron and E. Wichers, J. Am. Chem. Soc. 84, 4192 (1962).

Furthermore the calculated value of any thermodynamic quantity for a reaction is independent of the path chosen for the evaluation.

In some cases newer data may have become available on certain substances after the values were selected for these tables. Because of the need to maintain the internal consistency of the tables, it is not always possible to incorporate these newer data into the tables without a detailed analysis of the effect of such a change. Unless great care is used, relatively significant errors in calculated values of $\Delta H°$ or $\Delta G°$ for specific reactions may result from the introduction of such data.

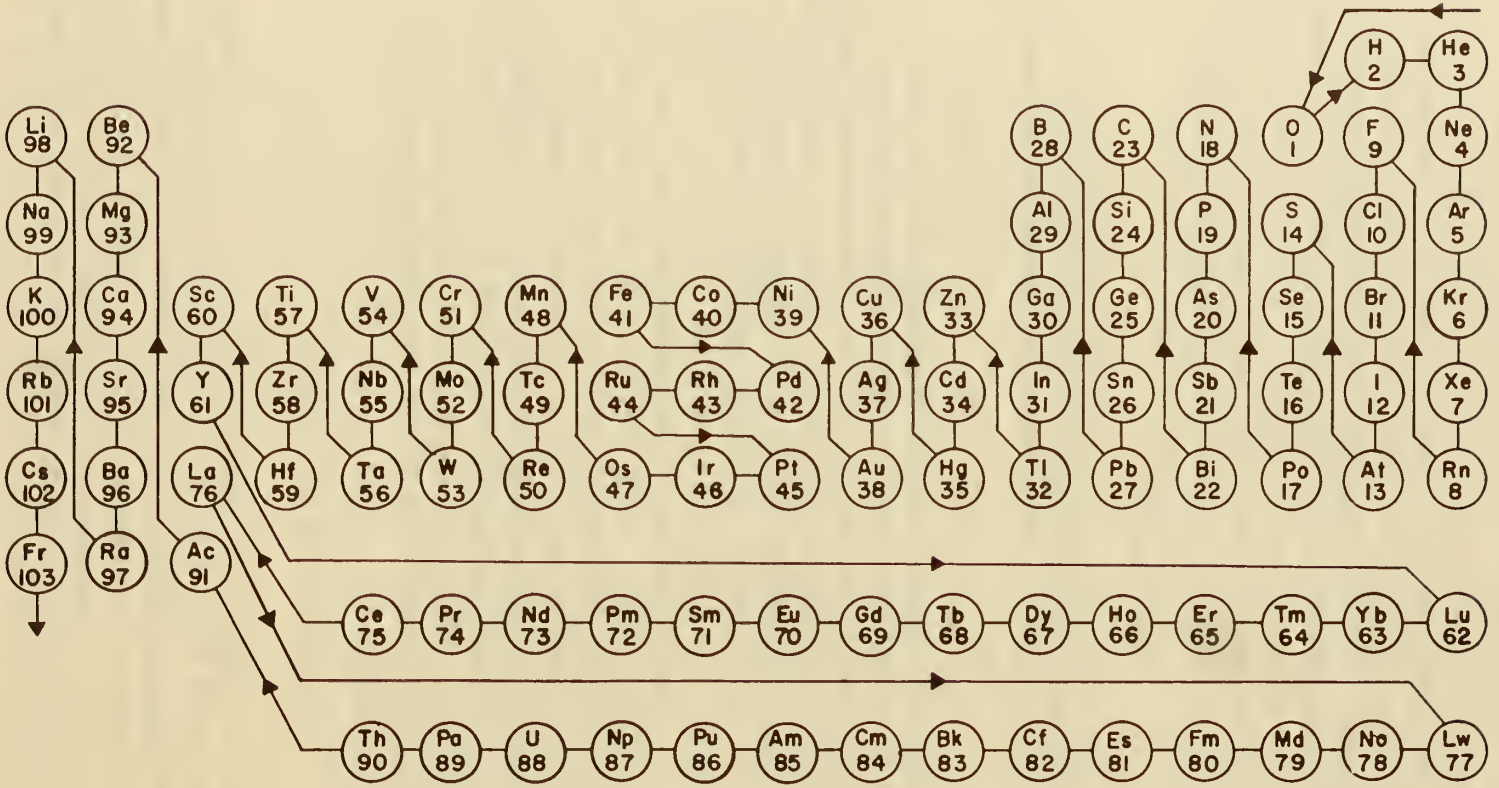
Uncertainties

The uncertainty in any value in the tables depends on the uncertainties of all the determinations in the total chain of reactions used to establish the value.

A discussion of the uncertainties will be included in the final publication of these tables in the National Standard Reference Data System. However we have followed certain rules with respect to significant figures to indicate these uncertainties. Values are tabulated in general such that the overall uncertainty lies between 2 and 20 units of the last figure. On the other hand, values are given so that the experimental data from which they are derived may be recovered with an accuracy equal to that of the original quantities. Thus the number of significant figures for any one value in the tables need not represent the absolute accuracy of that value. For solutions of varying composition values are frequently tabulated to more figures to make possible the recovery of enthalpies of solution and dilution. Similarly values of ΔHf°_{0} and $\Delta Hf^{\circ}_{298.15}$ may be given to different numbers of significant figures. In this instance the quantity with the lesser number of figures is used to represent the uncertainty estimate. The larger number of figures is used for the other quantity to retain the significance of the temperature correction term.

Arrangement of the Tables

The compounds in the tables are entered according to the Standard Order of Arrangement, (see Figure 1), by the principle of latest position. In this scheme, a compound is listed under the element occurring latest in the list; water of hydration is neglected. Within a given element-table will be found all of the compounds of that element with elements occurring earlier in the order; the arrangement within a table follows the same ordering. An exception occurs in the carbon tables (Table 23), which is divided into subgroups consisting of all compounds with one carbon atom, then all with two carbon atoms, etc.



Standard Order of Arrangement of the Elements

Compounds are located in the Table for the element (in the compound) having the highest number in the above Figure.

Figure 1.

TABLE A

CONVERSION FACTORS FOR UNITS OF MOLECULAR ENERGY

	J/mol	cal/mol	cm^3 atm/mol	kWh/mol	Btu/lb-mol	cm^{-1}/molecule	eV/molecule
1 J/mol =	1	2.390057×10^{-1}	9.86923	2.77778×10^{-7}	0.429923	8.35940×10^{-2}	1.036409×10^{-5}
1 cal/mol =	4.18400	1	41.2929	1.162222×10^{-6}	1.798796	3.49757×10^{-1}	4.33634×10^{-5}
1 cm^3 atm/mol =	0.1013250	2.42173×10^{-2}	1	2.81458×10^{-8}	4.35619×10^{-2}	8.47016×10^{-3}	1.050141×10^{-6}
1 kWh/mol =	3,600,000	860,421	3.55292×10^{7}	1	1,547,721	300,938	37.3107
1 Btu/lb-mol =	2.32600	5.55927×10^{-1}	22.9558	6.46111×10^{-7}	1	1.944396×10^{-1}	2.41069×10^{-5}
1 cm^{-1}/molecule =	11.96258	2.85912	118.0614	3.32294×10^{-6}	5.14299	1	1.239812×10^{-4}
1 eV/molecule =	96487.0	23060.9	952,252	2.68019×10^{-2}	41482.0	8065.73	1

The underlined numbers represent the fundamental values used in deriving this table. The remaining factors were obtained by applying the relationships:

$$n_{ij} = n_{ik} \cdot n_{kj} \qquad n_{ii} = n_{ik} \cdot n_{ki} = 1$$

TABLES OF SELECTED VALUES OF PROPERTIES

SERIES I

Enthalpy of Formation at 0 K

Enthalpy of Formation at 298.15 K

Gibbs Energy of Formation at 298.15 K

Enthalpy at 298.15 K

Entropy at 298.15 K

Heat Capacity at 298.15 K

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Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 54(1) Vanadium

Substance	State	Formula Weight	ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°
Formula and Description			0 °K	298.15 °K (25 °C)				
			kcal/mol				cal/deg mol	
V	c	50.942	0	0	0	1.109	6.91	5.95
	g		122.12	122.90	108.32	1.8898	43.544	6.217
V^+	g		277.550	279.811				
V^{2+}	g		615.39	619.13				
V^{3+}	g		1292.69	1297.91				
V^{4+}	g		2369.8	2376.5				
V^{5+}	g		3874.1	3882.2				
V^{6+}	g		6828.6	6838.3				
V^{7+}	g		10291.7	10302.8				
V^{8+}	g		14297.2	14310.0				
V^{9+}	g		19043.3	19057.4				
V^{10+}	g		24359.	24374.				
VO	c	66.9414		-103.2	-96.6		9.3	10.86
	g		25.	25.	18.	2.10	55.8	7.3
VO^{2+} std. state	aq			-116.3	-106.7		-32.0	
VO_2	g	82.9408		-57.				
VO_2^+ std. state	aq			-155.3	-140.3		-10.1	
VO_3^- std. state	aq	98.9402		-212.3	-187.3		12.	
VO_4^{3-} std. state	aq	114.9396			-214.9			
V_2O_3	c	149.8822		-293.5	-272.3		23.5	24.67

SELECTED VALUES OF CHEMICAL THERMODYNAMIC PROPERTIES - SERIES I

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Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 54(2) — Vanadium

Substance				ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°
Formula and Description		State	Formula Weight	0°K	298.15°K (25°C)				
				kcal/mol				cal/deg mol	
V_2O_4	α	c	165.8816		-341.1	-315.1		24.5	27.96
V_2O_5		c	181.8810		-370.6	-339.3		31.3	30.51
$V_2O_7^{4-}$	std. state	aq	213.8798			-411.			
V_3O_5		c	232.8230		-465.	-434.		39.	
V_4O_7		c	315.7638		-635.	-591.		52.	
V_6O_{13}		c	513.6442		-1062.				
VO_2HO_2	std. state, undissoc.	aq	115.9476			-178.1			
HVO_4^{2-}	std. state	aq	115.9476		-277.0	-233.0		4.	
$[VO \cdot H_2O_2]^{3+}$	std. state	aq	100.9561			-125.1			
$[VO_2H_2O_2]^{+}$	std. state	aq	116.9555			-178.4			
$H_2VO_4^{-}$	std. state	aq	116.9555		-280.6	-244.0		29.	
$HV_2O_7^{3-}$	std. state	aq	214.8878			-428.4			
$H_3V_2O_7^{-}$	std. state	aq	216.9037			-445.5			
$V_2O_3(OH)_4$		g	166.9697		-489.7				
$HV_{10}O_{28}^{5-}$	std. state	aq	958.4112		-2078.	-1935.		369.	
$H_2V_{10}O_{28}^{4-}$	std. state	aq	959.4191			-1940.			
VF_3		c	107.9372					23.18	21.62
VF_4		c	126.9356		-335.4				
VF_5		liq	145.9340		-353.8	-328.2		42.0	

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Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 54(3) — Vanadium

Substance			ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°
Formula and Description	State	Formula Weight	0°K	298.15°K (25°C)				
			kcal/mol				cal/deg mol	
VF_5	g	145.9340	-340.96	-342.7	-327.4	4.634	76.67	23.56
VCl_2	c	121.848		-108.	-97.		23.2	17.26
	g			-61.3				
VCl_3	c	157.301		-138.8	-122.2		31.3	22.27
VCl_4	liq	192.754		-136.1	-120.4		61.	
	g		-125.32	-125.6	-117.6	5.21	86.6	23.0
VOCl	c	102.3944		-138.4				
VO_2Cl	c	118.3938		-185.6				
$VOCl_2$	c	137.8474		-165.0				
$VOCl_3$	liq	173.3004		-175.6	-159.8		58.4	
	g		-165.53	-166.25	-157.58	4.71	82.26	21.49
VBr_2	c	210.760		-87.3				
	g			-37.1				
VBr_3	c	290.669		-103.6				
	g			-56.8				
VBr_4	g	370.578		-80.5				
$VBrCl_3$	g	237.210		-120.				
VI_2	c	304.7508		-60.1				
	g			-1.				

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 54(4) Vanadium

Substance			ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°
Formula and Description	State	Formula Weight	0°K	298.15°K (25°C)				
			kcal/mol				cal/deg mol	
VI_3	c	431.6552		-64.7				
VI_4	g	558.5596		-29.3				
V_2S_3	c	198.076		-227.				
$VOSO_4$	c	163.003		-312.9	-279.6		26.0	
std. state, undissoc.	aq				-282.6			
VN	c	64.9487		-51.9	-45.7		8.91	9.08
NH_4VO_3	c	116.9788		-251.7	-212.3		33.6	30.91
$NOVF_6$	c	194.9385		-396.2	-348.6		40.	
$(VO)_3(PO_4)_2$ std. state	aq	390.7670			-775.6			
$VC_{0.88}$	c	61.5118		-24.3	-23.7		6.2	7.66
V_2C	c	113.8952					12.2	13.3
$[VO(C_2O_4)_2]^{2-}$ std. state	aq	242.9812			-415.6			
$V(CO)_6$	g	219.0053		-236.				
$VOSCN^+$ std. state	aq	125.0232		-98.	-86.		8.	
VSi_2	c	107.114		-73.				
V_2Si	c	129.970		-37.				
V_3Si	c	180.912		-26.				

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Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 54(5) — Vanadium

Substance			ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°
Formula and Description	State	Formula Weight	0°K	298.15°K (25°C)				
			kcal/mol				cal/deg mol	
V_5Si_3	c	338.968		-94.				
$Pb_2V_2O_7$	c	628.260		-509.7				
$Pb_3(VO_4)_2$	c	851.449		-567.4				
VAl_3	c	131.8865		-26.				
V_5Al_8	c	470.5620		-70.				
$TlVO_3$	c	303.3102			-206.3			
$Tl_4V_2O_7$	c	1031.3598			-467.3			
$AgVO_3$	c	206.8102			-214.3			
Ag_2HVO_4	c	331.6876			-288.6			
$Ag_2HVO_4 \cdot AgOH$	c	456.5650			-358.6			
$Fe(VO_3)_2$	c	253.7274		-453.8				
$Mn(VO_3)_2$	c	248.8184		-477.9				

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Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 55(1) Niobium

Substance		State	Formula Weight	ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°
Formula and Description				0°K	298.15°K (25°C)				
				kcal/mol				cal/deg mol	
Nb		c	92.906	0	0	0	1.255	8.70	5.88
		g		172.758	173.5	162.8	1.997	44.490	7.208
Nb^+		g		330.32	332.54				
Nb^{2+}		g		660.55	664.25				
Nb^{3+}		g		1238.0	1243.1				
Nb^{4+}		g		2121.3	2127.9				
Nb^{5+}		g		3287.0	3295.1				
Nb^{6+}		g		5653.0	5662.6				
Nb^{7+}		g		8536.	8547.				
NbO		c	108.9054		-97.0	-90.5		11.5	9.86
		g		51.2	51.	44.	2.099	57.09	7.36
NbO_2		c	124.9048	-189.19	-190.3	-177.0	2.222	13.03	13.74
		g			-51.3	-52.3		61.0	
NbO_3^-	ionic strength = 1	aq				-222.8			
Nb_2O_5	(high temp. form)	c	265.809	-451.63	-454.0	-422.1	5.325	32.80	31.57
		aq			-458.8				

National Bureau of Standards — Washington, D. C.

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 55(2) — Niobium

Substance: Formula and Description	State	Formula Weight	ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°
			0°K	298.15°K (25°C)				
			kcal/mol				cal/deg mol	
$Nb(OH)_4^+$ ionic strength = 1	aq				-288.9			
$Nb(OH)_5$ undissoc.; ionic strength = 1	aq				-346.2			
NbF_5	c	187.898	-432.68	-433.5	-406.1	5.707	38.3	32.2
	g		-413.76	-415.8	-401.1	4.49	76.9	23.2
$NbCl_{2.33}$	c	175.630		-113.4				
$NbCl_{2.67}$	c	187.448		-128.6				
$NbCl_3$	g	199.265		-86.				
$NbCl_{3.13}$	c	203.874		-144.7				
$NbCl_4$	c	234.718		-166.0				
	g			-134.				
$NbCl_5$	c	270.171		-190.6	-163.3		50.3	35.4
	g		-167.83	-168.2	-154.4	6.370	95.71	28.88
$NbOCl_2$	c	179.8114		-185.1				
$NbOCl_3$	c	215.2644		-210.2	-187.		34.	
	g		-179.16	-179.8	-171.6	4.931	85.6	22.0

SELECTED VALUES OF CHEMICAL THERMODYNAMIC PROPERTIES - SERIES I

National Bureau of Standards — Washington, D. C.

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 55(3) — Niobium

Substance			ΔHf_0°	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°
Formula and Description	State	Formula Weight	0°K	298.15°K (25°C)				
			kcal/mol				cal/deg mol	
$NbBr_5$	c	492.451		-132.9				
	g			-104.8				
$NbBrO_3$	c	220.8132		-179.3				
NbI_5	c	727.428		-64.2				
$Nb_{1.136}S_2$	c	169.669		-92.8				20.
NbN	c	106.9127	-55.35	-56.2	-49.2	1.439	8.25	9.32
Nb_2N	c	199.8187		-59.9				
NbC	c	104.9172	-33.2	-33.2	-32.7	1.495	8.46	8.81
Nb_2C	c	197.8232		-45.4	-44.4		15.3	14.48
$NbGe_{0.15}$	c	103.795		-4.0				
$NbGe_{0.54}$	c	132.105		-14.6				
$NbGe_{0.67}$	c	141.541		-15.4				
$NbGe_2$	c	238.086		-20.8				
$NbB_{1.875}$	c	113.177		-58.8				
$NbB_{1.963}$	c	114.128				1.620	8.91	11.42

National Bureau of Standards — Washington, D. C.

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 55(4) Niobium

Substance			ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C°_p
Formula and Description	State	Formula Weight	0°K	298.15°K (25°C)				
			kcal/mol				cal/deg mol	
$NbCo_2$	c	210.7724		-13.7	-13.2		22.	
$NbCo_3$	c	269.7056		-14.1	-13.7		29.	
$NbFe_2$	c	204.600		-11.1	-11.8		24.	13.0
$NbCr_2$	c	196.898		-5.0	-5.0	3.231	19.97	17.45

National Bureau of Standards — Washington, D. C.

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 56(1) Tantalum

Substance		State	Formula Weight	ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°
Formula and Description				0°K	298.15°K (25°C)				
				kcal/mol				cal/deg mol	
Ta		c	180.948	0	0	0	1.347	9.92	6.06
		g		186.765	186.9	176.7	1.482	44.241	4.985
Ta^+		g		368.72	370.33				
TaO		g	196.9474	60.3	60.	53.	2.10	57.6	7.31
TaO_2		g	212.9468	-40.7	-41.	-43.	3.1	64.	12.5
Ta_2O_5	β	c	441.8930		-489.0	-456.8		34.2	32.30
		aq			-496.7				
Ta_2H		c	181.9560	-6.93	-7.8	-16.5	2.84	18.9	21.7
TaF_5		c	275.9400		-454.97				
	std. state, undissoc.	aq				-137.6			
TaF_6^-	std. state	aq	294.9384			-209.2			
TaF_7^{2-}	std. state	aq	313.9368			-280.2			
$TaCl_{2.5}$		c	269.5801		-114.5				
$TaCl_3$		c	287.307		-132.2				
$TaCl_4$		c	322.760		-167.7				
		g			-134.0				

National Bureau of Standards — Washington, D. C.

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 56(2) Tantalum

Substance			ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°
Formula and Description	State	Formula Weight	0 °K	298.15 °K (25 °C)				
			kcal/mol				cal/deg mol	
$TaCl_5$	c	358.213		-205.3				
	g			-181.3				
$TaOCl_3$	g	303.3064		-186.6				
$TaBr_5$	c	580.493		-143.0				
	g			-115.6				
TaS_2	c	245.076		-111.				
TaN	c	194.9547		-60.1				9.7
Ta_2N	c	375.9027		-65.				
NH_4TaCl_6	c	411.7046		-270.8				
TaC	c	192.9592	-34.96	-35.0	-34.6	1.56	10.11	8.79
Ta_2C	c	373.9072		-51.0	-50.8		20.7	
$TaSi_2$	c	237.120		-28.				
Ta_5Si_3	c	988.998		-76.				
TaB_2	c	202.570		-46.				

National Bureau of Standards — Washington, D.

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 57(1) Titanium

Substance		State	Formula Weight	ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C°_r
Formula and Description				0°K	298.15°K (25°C)				
				kcal/mol				cal/deg mol	
Ti		c	47.90	0	0	0	1.149	7.32	5.98
		g		111.65	112.3	101.6	1.802	43.066	5.839
Ti^+		g		268.9	271.1				
Ti^{2+}		g		582.1	585.7				
Ti^{3+}		g		1216.0	1221.1				
Ti^{4+}		g		2213.8	2220.4				
Ti^{5+}		g		4501.9	4509.9				
Ti^{6+}		g		7254.4	7264.0				
Ti^{7+}		g		10501.	10512.				
Ti^{8+}		g		14387.	14400.				
Ti_2		g	95.80		170.				
TiO	α	c	63.899	-123.49	-124.2	-118.3	1.48	8.31	9.55
		g		4.	4.	-3.	2.29	56.0	7.81
TiO^{2+}	in $HClO_4$ medium	aq			-164.9				
TiO_2	anatase	c	79.899	-223.44	-224.6	-211.4	2.062	11.93	13.26
	Brookite	c			-225.1				
	rutile	c		-224.6	-225.8	-212.6	2.065	12.03	13.15
		amorp			-210.				
	hydrated ppt				-219.8				
		g			-60.				

National Bureau of Standards — Washington, D. C.

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 57(2) Titanium

Substance	State	Formula Weight	ΔHf_0°	ΔHf°	ΔGf°	$H_{298}^\circ - H_0^\circ$	S°	C_p°
Formula and Description			0 °K	298.15 °K (25 °C)				
			kcal/mol				cal/deg mol	
Ti_2O_3	c	143.798	-361.52	-363.5	-342.8	3.431	18.83	23.27
Ti_3O_5	c	223.697	-584.69	-587.8	-553.9	5.52	30.9	37.00
TiH_2	c	49.916	-26.61	-28.6	-19.2	1.18	7.1	7.2
TiF_4	amorp	123.894	-393.68	-394.2	-372.7	4.841	32.02	27.31
	g			-371.0				
H_2TiF_6	aq	163.906		-573.7				
$TiCl_2$	c	118.806	-122.64	-122.8	-111.0	3.18	20.9	16.69
$TiCl_3$	c	154.259	-172.86	-172.3	-156.2	5.00	33.4	23.22
	g			-129.5				
$TiCl_4$	c	189.712	-195.75					
	liq			-192.2	-176.2		60.31	34.70
	g		-182.04	-182.4	-173.7	5.17	84.8	22.8
in 1600 H_2O	aq			-250.3				
in 2N $HClO_4$:	aq							
$m = 0.77 \times 10^{-2}$				-249.86				
$m = 1.4 \times 10^{-4}$				-250.16				
$m = 0$				-250.20				

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Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 57(3) Titanium

Substance	State	Formula Weight	ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C°_p
Formula and Description			0°K	298.15°K (25°C)				
			kcal/mol				cal/deg mol	
$TiCl_4$ in 3N $HClO_2$	aq							
$m = 1.3\times10^{-2}$				-247.00				
$m = 0$				-247.30				
in 4N $HClO_4$	aq							
$m = 1.2\times10^{-2}$				-244.3				
$m = 0$				-244.80				
in 5N $HClO_4$	aq							
$m = 1.2\times10^{-2}$				-240.5				
$m = 2.2\times10^{-4}$				-241.92				
$m = 0$				-241.95				
TiOCl	c	99.352		-180.				
$TiBr_2$	c	207.718		-96.				
$TiBr_3$	c	287.627	-126.65	-131.1	-125.2	5.49	42.2	24.31
$TiBr_4$	c	367.536	-141.36	-147.4	-140.9	6.825	58.2	31.43
	g		-124.14	-131.3	-135.8	5.71	95.2	24.1
$TiCl_3Br$	g	234.168				5.25	89.5	23.1
$TiClBr_3$	g	323.080				5.49	94.7	23.7

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Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 57(4) Titanium

Substance	State	Formula Weight	ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°
Formula and Description			0°K	298.15°K (25°C)				
			kcal/mol				cal/deg mol	
TiI_2	c	301.709		-63.				
	g			-13.				
TiI_4	c	555.518		-89.8	-88.8		59.6	30.03
	g			-66.4				
in benzene; std. state, $x_2 = 1$				-82.5	-85.8		74.	
TiS	c	79.964		-57.				
	g			73.				
TiS_2	c	112.028					18.73	16.23
$TiCl_4 \cdot 1H_2S$	c	223.792		-205.9				
$TiCl_4 \cdot 2H_2S$	c	257.872		-218.0				
$TiBr_4 \cdot 1H_2S$	c	401.616		-160.8				
$TiBr_4 \cdot 2H_2S$	c	435.696		-172.6				
TiN	c	61.907	-79.93	-80.8	-74.0	1.311	7.23	8.86
TiP	c	78.874		-67.6				

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Table 57(5) — Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity
Titanium

Substance			ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°
Formula and Description	State	Formula Weight	0°K	298.15°K (25°C)				
			kcal/mol				cal/deg mol	
$TiCl_4 \cdot POCl_3$	c	344.044		-349.				
$TiCl_4 \cdot 2POCl_3$	c	496.376		-484.0				
$TiCl_4 \cdot PH_3$	c	223.710		-209.5				
$TiCl_4 \cdot 2PH_3$	c	257.708		-219.0				
$TiBr_4 \cdot PH_3$	c	401.534		-162.1				
$TiBr_4 \cdot 2PH_3$	c	435.532		-172.6				
TiAs	c	122.822		-35.8				
TiSb	c	169.65		-67.2				
TiC	c	59.911	-43.80	-44.1	-43.2	1.101	5.79	8.04
$TiF_4 \cdot CH_3CN$	c	164.947		-381.1				
$TiCl_4 \cdot 2CH_3CN$	c	271.818		-178.8				
$TiBr_4 \cdot 2CH_3CN$	c	449.642		-121.1				

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Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 57(6) Titanium

Substance		State	Formula Weight	ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°
Formula and Description				0°K	298.15°K (25°C)				
				kcal/mol				cal/deg mol	
$TiSi$	γ	c	75.986		-31.				
$TiSi_2$	β	c	104.072		-32.				
Ti_5Si_3	ϵ	c	323.758		-138.				
TiB_2		c	69.522	-77.0	-77.4	-76.4	1.333	6.81	10.58
$TiAl$		c	74.882		-18.0				
$TiAl_3$		c	128.844		-35.0				
Ti_3Al		c	170.682		-23.5				
Al_2TiO_5		c	181.860					26.2	32.60
Tl_2TiCl_6		c	669.358		-318.				
$ZnTiO_3$		c	161.268		-311.3				
Zn_2TiO_4		c	242.638		-393.8	-366.7		34.2	32.82
Ni_3Ti	γ	c	224.03		-33.2				
$NiTi_2$	ϵ	c	154.51		-19.2				

SELECTED VALUES OF CHEMICAL THERMODYNAMIC PROPERTIES - SERIES I

National Bureau of Standards — Washington, D. C.

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 58(1) — Zirconium

Substance		State	Formula Weight	ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°
Formula and Description				0 °K	298.15 °K (25 °C)				
				kcal/mol				cal/deg mol	
Zr	α, hexagonal	c	91.22	0	0	0	1.322	9.32	6.06
		g		145.19	145.5	135.4	1.629	43.32	6.37
Zr^+		g		302.9	304.7				
Zr^{2+}		g		605.7	609.0				
Zr^{3+}		g		1135.9	1140.6				
Zr^{4+}		g		1927.8	1934.0				
Zr^{5+}		g		3807.	3815.				
ZrO		g	107.219		15.				
ZrO_2	α, monoclinic		123.219	-261.734	-263.04	-249.24	2.091	12.04	13.43
ZrO_2	hydrated ppt				-260.4				
		g			-75.				
ZrO_3	ppt		139.218		-241.				
ZrH_2	zirconium hydride	c	93.236	-38.34	-40.4	-30.8	1.284	8.37	7.40
$ZrOOH^+$		aq	124.227		-270.1				
ZrF_2		g	129.217		-135.				
ZrF_3		g	148.215		-265.				
ZrF_4	β, monoclinic	c	167.214	-455.44	-456.8	-432.6	4.183	25.00	24.79
		g		-398.99	-400.0	-391.1	4.53	76.3	20.9
$ZrF_4 \cdot H_2O$		c	185.229		-527.6				
$ZrF_4 \cdot 3H_2O$		c	221.260		-669.9				

National Bureau of Standards — Washington, D. C.

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 58(2) — Zirconium

Substance	State	Formula Weight	ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°
Formula and Description			0°K	298.15°K (25°C)				
			kcal/mol				cal/deg mol	
$ZrCl$	c	126.673		-63.				
	g			60.				
$ZrCl_2$	c	162.126		-120.				
	g			-40.				
$ZrCl_3$	c	197.579		-179.				
	g			-121.				
$ZrCl_4$	c	233.032	-234.60	-234.35	-212.7	5.957	43.4	28.63
	g		-207.69	-208.0	-199.7	5.401	88.0	23.49
	aq			-293.3				
in 55 $HCOOC_2H_5$				-260.8				
in 50 $CH_3COOC_2H_5$				-260.2				
in 35 $C_3H_7COOC_2H_5$				-259.4				
in 80 $C_6H_5NO_2$				-244.8				
$ZrOCl_2$	aq	178.125		-280.3				
$ZrOCl_2 \cdot 2H_2O$	c	214.156		-400.9				
$ZrOCl_2 \cdot 3.5H_2O$	c	241.179		-510.4				
$ZrOCl_2 \cdot 6H_2O$	c	286.217		-689.5				
$ZrOCl_2 \cdot 8H_2O$	c	322.248		-829.8				

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National Bureau of Standards — Washington, D. C.

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 58(3) — Zirconium

Substance	State	Formula Weight	ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°
Formula and Description			0°K	298.15°K (25°C)				
			kcal/mol				cal/deg mol	
$ZrBr_4$	c	410.856		-181.8				
	g			-153.8				
in 100 $HCOOC_2H_5$				-209.0				
in 85 $CH_3COOC_2H_5$				-207.5				
in 65 $C_3H_7COOC_2H_5$				-207.4				
$ZrOBr_2$	aq	267.037		-259.9				
$Zr\ Br_2 \cdot 3.5H_2O$	c	330.091		-490.0				
$ZrOBr_2 \cdot 8H_2O$	c	411.160		-808.4				
ZrI_4	c	598.838		-115.1				
	g			-84.1				
in 250 $CH_3COOC_2H_5$				-139.8				
ZrS_2	c	155.348		-135.3				
$Zr(SO_4)_2$	c	283.343		-529.9				41.
$Zr(SO_4)_2 \cdot H_2O$	c	301.359		-610.4				
$Zr(SO_4)_2 \cdot 4H_2O$	c	355.405		-825.6				
$ZrO(SO_4)_2^{2-}$	aq	299.343		-630.1				
ZrN	c	105.227	-86.42	-87.2	-80.4	1.575	9.29	9.66
	g			134.				

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Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 58(4) Zirconium

Substance			ΔHf_0°	ΔHf°	ΔGf°	$H_{298}^\circ - H_0^\circ$	S°	C_p°
Formula and Description	State	Formula Weight	0°K	298.15°K (25°C)				
			kcal/mol				cal/deg mol	
$ZrF_4 \cdot NH_4F$	c	204.251		-576.6				
$ZrF_4 \cdot NH_4F \cdot H_2O$	c	222.266		-647.3				
$ZrF_4 \cdot 2NH_4F$	c	241.288		-692.8				
$ZrF_4 \cdot 3NH_4F$	c	278.325		-804.6				
ZrC	c	103.231	-48.33	-48.5	-47.7	1.401	7.96	9.06
$ZrCl_4 \cdot 2CH_3CN$	c	315.138		-200.6				
$ZrBr_4 \cdot 2CH_3CN$	c	492.962		-151.0				
ZrSi	c	119.306		-37.				
$ZrSi_2$	c	147.392		-38.				
Zr_2Si	c	210.526		-50.				
Zr_3Si	c	301.746		-52.				
Zr_3Si_2	c	329.832		-92.				
Zr_5Si_3	c	540.358		-138.				
Zr_6Si_5	c	687.750		-205.				
$ZrSiO_4$	c	183.304	-483.32	-486.0	-458.7	3.562	20.1	23.58
ZrB_2	c	112.842	-77.69	-78.0	-77.0	1.590	8.59	11.53

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Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 59(1) Hafnium

Substance		State	Formula Weight	ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°
Formula and Description				0°K	298.15°K (25°C)				
				kcal/mol				cal/deg mol	
Hf	α, hexagonal	c	178.49	0	0	0	1.397	10.41	6.15
		g		147.92	148.0	137.8	1.481	44.642	4.972
Hf^+		g		309.	311.				
Hf^{2+}		g		653.	656.				
Hf^{3+}		g		1190.	1195.				
Hf^{4+}		g		1958.	1964.				
HfO		g	194.489		12.				
HfO_2		c	210.489		-273.6	-245.5		14.18	14.40
	hydrous ppt				-269.0				
$HfOOH^+$		aq	211.497		-279.5				
HfF_4	monoclinic	c	254.484		-461.4	-437.5		27.	
		g			-399.1				
$HfCl_4$		c	320.302		-236.70	-215.42		45.6	28.80
		g			-211.4				
		aq			-302.7				
	in 80 $C_6H_5NO_2$				-247.9				

National Bureau of Standards — Washington, D. C.

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 59(2) Hafnium

Substance			ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C°_p
Formula and Description	State	Formula Weight	0 °K	298.15 °K (25 °C)				
			kcal/mol				cal/deg mol	
HfN	c	192.497		-88.3				
HfC	c	190.501		-60.1				
HfB	c	189.301		-47.				
HfB_2	c	200.112	-80.09	-80.3	-79.4	1.77	10.2	11.89

SELECTED VALUES OF CHEMICAL THERMODYNAMIC PROPERTIES - SERIES I

National Bureau of Standards — Washington, D. C.

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 60(1) — Scandium

Substance	State	Formula Weight	ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°
Formula and Description			0°K	298.15°K (25°C)				
			kcal/mol				cal/deg mol	
Sc	c	44.956	0	0	0	1.247	8.28	6.10
	g		89.87	90.3	80.32	1.674	41.75	5.28
Sc^+	g		240.69					
Sc^{2+}	g		535.87					
Sc^{3+}	g		1106.86					
std. state, m = 1	aq			-146.8	-140.2		-61.	
Sc^{4+}	g		2801.1					
Sc^{5+}	g		4914.9					
Sc^{6+}	g		7477.					
Sc^{7+}	g		10659.					
Sc^{8+}	g		14319.					
Sc^{9+}	g		18470.					
Sc^{10+}	g		23666.					
Sc^{11+}	g		29428.					
Sc^{12+}	g		45245.					
Sc^{13+}	g		62667.					
Sc^{14+}	g		81803.					
Sc^{15+}	g		103157.					

National Bureau of Standards — Washington, D. C.

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 60(2) — Scandium

Substance		State	Formula Weight	ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°
Formula and Description				0 °K	298.15 °K (25 °C)				
				kcal/mol				cal/deg mol	
Sc_2		g	89.912	155.	154.9	141.6	2.4	61.	8.7
ScO		g	60.955	-13.5	-13.68	-19.90	2.100	53.65	7.38
Sc_2O		g	105.911	-6.	-6.9		2.7		11.2
Sc_2O_3		c	137.910	-453.95	-456.22	-434.85	3.34	18.4	22.52
$ScH_{1.97}$		c	46.942		-32.2				
$Sc(OH)^{2+}$	std. state, m = 1	aq	61.963		-205.9	-191.5		-32.	
$Sc(OH)_3$		c	95.978		-325.9	-294.8		24.	
ScF		g	63.9544	-33.	-33.2	-39.3	2.138	53.11	7.74
ScF_2		g	82.9528	-153.	-153.5	-156.6	2.84	67.0	11.5
ScF_3		c	101.9512		-389.4	-371.8		22.	
		g		-297.4	-298.	-295.	3.83	71.8	16.2
ScCl		g	80.409	27.	26.9	20.6	2.246	56.00	8.40
$ScCl^{2+}$	std. state, m = 1	aq			-189.6	-172.7		-54.	
$ScCl_2$		g	115.862				3.1	72.5	12.6
$ScCl_2^+$	std. state, m = 1	aq			-233.6	-206.		-46.	

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 60(3) Scandium

Substance		State	Formula Weight	ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°
Formula and Description				0°K	298.15°K (25°C)				
				kcal/mol				cal/deg mol	
$ScCl_3$		c	151.315		-221.1				
	in 5500 H_2O	aq			-268.8				
$ScCl_3 \cdot 6H_2O$		c	259.411		-671.6				
$Sc(OH)_2Cl$		c	114.424		-303.	-276.3		26.	
$Sc_2(OH)_5Cl$		c	210.402			-535.4			
$ScBr^{2+}$	std. state, m = 1	aq	124.865		-177.0	-166.2		-41.	
$ScBr_2$		g	204.774				3.3	77.6	13.0
$ScBr_2^+$	std. state, m = 1	aq			-207.5	-191.4		-25.	
$ScBr_3$		c	284.683		-177.6				
ScI_2		g	298.765				3.4	81.6	13.3
ScS		g	77.020	41.9	41.8	29.7	2.2	56.3	8.0
$Sc(SO_4)^+$	std. state, m = 1	aq	141.018			-321.7			
$Sc(SO_4)_2^-$	std. state, m = 1	aq	237.079			-501.5			
$Sc_2(SO_4)_3$		c	378.097						62.0

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Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 60(4) Scandium

Substance			ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°
Formula and Description	State	Formula Weight	0°K	298.15°K (25°C)				
			kcal/mol				cal/deg mol	
$Sc(SeO_4)^+$ std. state, m = 1	aq	187.91		-293.9	-248.2		-53.	
$Sc(SeO_4)_2^-$ std. state, m = 1	aq	330.87		-409.	-354.7		57.	
$Sc_2(SeO_3)_3 \cdot 10H_2O$	c	650.94		-1326.5				
$Sc(NO_3)^{2+}$ std. state, m = 1	aq	106.961			-168.4			
ScAs	c	119.8776		-64.				
ScC_2	g	68.978	143.	143.6				
$Sc(HCO_2)_3$	c	180.009						54.
$Sc_2(C_2O_4)_3$	c	353.971						124.
$Sc(CNS)^{2+}$ std. state, m = 1	aq	103.038			-119.6			

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Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 61(1) Yttrium

Substance			ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C°_p
Formula and Description	State	Formula Weight	0 °K	298.15 °K (25 °C)				
			kcal/mol				cal/deg mol	
Y	c	88.905	0	0	0	1.426	10.62	6.34
	g		100.49	100.7	91.1	1.639	42.87	6.18
Y^{+}	g		247.62					
Y^{2+}	g		529.88					
Y^{3+}	g		1003.1					
std. state, m = 1	aq			-172.9	-165.8		-60.	
Y^{4+}	g		2428.					
Y^{5+}	g		4204.					
Y^{6+}	g		6349.					
Y^{7+}	g		9024.					
Y^{8+}	g		11999.					
Y^{9+}	g		15370.					
Y^{10+}	g		19775.					
Y^{11+}	g		24525.					
Y^{12+}	g		33150.					
Y_2	g	177.810	164.	163.5	150.7	2.4	64.	8.7

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 61(2) Yttrium

Substance			ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°
Formula and Description	State	Formula Weight	0°K	298.15°K (25°C)				
			kcal/mol				cal/deg mol	
YO	g	104.9044	-9.	-9.3	-15.5	2.115	55.88	7.53
Y_2O	g	193.8094	2.	1.0		2.9		11.7
Y_2O_2	g	209.8088	-126.	-127.4		3.5		15.8
Y_2O_3	c	225.8082	-453.40	-455.38	-434.19	3.983	23.68	24.50
YH_2	c	90.9209	-35.45	-37.5	-27.8	1.403	9.17	8.24
Y^2H_2	c	92.9332				1.659	10.29	10.77
YH_3	c	91.9289	-44.45	-47.3	-33.2	1.613	10.02	10.36
Y^2H_3	c	94.9473				2.025	12.03	13.73
$Y(OH)^{2+}$ std. state, m = 1	aq	105.9124			-210.1			
$Y(OH)_3$	c	139.927			-308.6			
$Y_2(OH)_2^{4+}$ std. state, m = 1	aq	211.8247			-425.5			
YF	g	107.9034	-32.7	-33.	-39.	2.163	55.38	7.92
YF^+	g		145.	146.2				
YF_2	g	126.9018				2.9	69.3	11.7
YF_3	c	145.900		-410.8	-393.1		24.	
	g		-307.4	-308.0	-305.4	3.98	74.5	16.8

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 61(3) Yttrium

Substance		State	Formula Weight	ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C°_p
Formula and Description				0 °K	298.15 °K (25 °C)				
				kcal/mol				cal/deg mol	
YCl		g	124.358	48.	47.8	41.5	2.286	58.33	8.56
YCl^+		g		164.	165.2				
YCl^{2+}	std. state, m = 1	aq			-214.0	-198.7		-46.	
YCl_2		g	159.811				3.2	75.0	12.9
YCl_2^+		g		127.	128.1				
YCl_3		c	195.264		-239.0				
		g		-179.	-179.3		4.4		18.
	in 4000 H_2O	aq			-291.96				
YCl_3^+		g		116.	117.2				
$YCl_3 \cdot 6H_2O$		c	303.356		-691.3	-592.1		92.	
$Y_2Cl_5^+$		g	355.075		-95.				
$(YCl_3)_2$		g	390.528		-384.				
$Y(OH)_2Cl$		c	158.373			-297.9			
$Y_2(OH)_5Cl$		c	298.300			-609.3			
YBr^{2+}	std. state, m = 1	aq	168.814		-203.8	-191.6		-43.	
YBr_2		g	248.723				3.4	80.0	13.2

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 61(4) Yttrium

Substance			ΔHf_0°	ΔHf°	ΔGf°	$H_{298}^\circ - H_0^\circ$	S°	C_p°
Formula and Description	State	Formula Weight	0 °K	298.15 °K (25 °C)				
			kcal/mol				cal/deg mol	
YI_2	g	342.7138				3.5	84.0	13.5
YI_3	c	469.6182		-147.4				
$Y(IO_3)_3$	c	613.6128			-271.2			
YS	g	120.969	42.	41.7	29.7	2.2	58.	8.2
$Y(SO_4)^+$ std. state, m = 1	aq	184.967		-386.1	-347.1		-29.	
$Y(SO_4)_2^-$ std. state, m = 1	aq	281.028		-602.0	-526.2		-17.	
$Y_2(SO_4)_3$	c	465.995			-866.8			138.
$Y_2(SO_4)_3 \cdot 8H_2O$	c	610.118			-1332.1			
$Y_2(SeO_3)_3$	c	558.68		-721.8				
$Y(NO_3)^{2+}$ std. state, m = 1	aq	150.9099			-192.4			
YAs	c	163.8266		-77.4				
YC_2	c	112.9274		-26.	-26.		13.	
	g		142.	142.6	128.4	2.5	61.	10.7

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Table 61(5) — Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity
Yttrium

Substance		State	Formula Weight	ΔHf_0°	ΔHf°	ΔGf°	$H_{298}^\circ - H_0^\circ$	S°	C_p°
Formula and Description				0°K	298.15°K (25°C)				
				kcal/mol				cal/deg mol	
$Y(C_2O_4)^+$	std. state, m = 1	aq	176.9248			-335.8			
$Y(C_2O_4)_2^-$	std. state, m = 1	aq	264.9446			-501.8			
$Y(C_2O_4)_3^{3-}$	std. state, m = 1	aq	352.9644			-664.7			
$Y_2(CO_3)_3$		c	357.8379			-752.4			
$Y_2(C_2O_4)_3 \cdot 9H_2O$		c	604.007			-1363.8			
$Y(C_2H_3O_2)^{2+}$		aq	147.9499		-285.8				
$Y(C_2H_3O_2)_2^+$		aq	206.9948		-399.8				
$Y(C_2H_3O_2)_3$		aq	226.0397		-516.1				
$YCl_3 \cdot CH_3NH_2$		c	266.322		-264.9				
$YCl_3 \cdot 2CH_3NH_2$		c	257.379		-286.				
$YCl_3 \cdot 3CH_3NH_2$		c	288.437		-305.				
$YCl_3 \cdot 4CH_3NH_2$		c	319.495		-321.				
$Y(CNS)^{2+}$	std. state, m = 1	aq	146.9868			-144.7			
YZn		c	154.275		-20.1	-18.4		15.	
YZn_2	α	c	219.645		-34.2	-31.4		21.	
YZn_3		c	285.015		-39.3	-35.6		28.	
YZn_4		c	350.385		-44.5	-40.2		36.	

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Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table 61(6) — Yttrium

Substance			ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C°_p
Formula and Description	State	Formula Weight	0°K	298.15°K (25°C)				
			kcal/mol				cal/deg mol	
YZn_5	c	415.755		-52.1	-46.4		41.	
YZn_{11}	c	807.98		-74.9	-67.7		96.	
Y_2Zn_{17}	c	1289.10		-144.8	-131.3		145.	
$Y(ReO_4)_3$	c	839.5		-701.9	-629.4		88.	
$YNbO_4$	c	245.809						27.6

APPENDIX

Errata for Technical Note 270-3 and 270-4

(See also TN 270-4, page 139)

TN	Page				
3	48	H_2S_2(liq)	$\Delta Hf°_{298}$ =	-4.33	kcal/mol
		H_2S_2(g)	=	3.71	kcal/mol
		H_2S_3(liq)	=	-3.57	kcal/mol
		H_2S_3(g)	=	7.29	kcal/mol
		H_2S_4(liq)	=	-2.99	kcal/mol
		H_2S_4(g)	=	10.57	kcal/mol
		H_2S_5(liq)	=	-2.49	kcal/mol
		H_2S_5(g)	=	13.84	kcal/mol
		H_2S_6(liq)	=	-1.99	kcal/mol
3	87	H_3PO_4 in 0.75 H_2O	=	-304.35	kcal/mol
3	97	$AsCl_3$(liq)	$\Delta Gf°_{298}$ =	-62.0	kcal/mol
			S° =	51.7	cal/deg mol
		$AsCl_3$(g)	$\Delta Hf°_0$ =	-62.12	kcal/mol
			$\Delta Hf°_{298}$ =	-62.5	kcal/mol
			$\Delta Gf°_{298}$ =	-59.5	kcal/mol
3	208	Al_2O_3(c); the third, fourth and fifth lines should read:			
		(ρ)	$\Delta Hf°_{298}$ =	-391.	kcal/mol
		(κ)	=	-397.	kcal/mol
			(Delete value for $\Delta Gf°_{298}$)		
		(γ)	$\Delta Hf°_{298}$ =	-395.	kcal/mol
4	3	HgI(g)	$\Delta Hf°_0$ =	32.9	kcal/mol
			$\Delta Hf°_{298}$ =	31.64	kcal/mol
			$\Delta Gf°_{298}$ =	21.14	kcal/mol
4	108	$MnI_2 \cdot 4H_2O$(c)	$\Delta Hf°_{298}$ =	-343.9	kcal/mol
	113	MnC_2O_4(c)	=	-246.2	kcal/mol
		$MnC_2O_4 \cdot 2H_2O$(c)	$\Delta Hf°_{298}$ =	-389.2	kcal/mol
			S° =	48.	cal/deg mol
		$MnC_2O_4 \cdot 3H_2O$(c)	$\Delta Hf°_{298}$ =	-459.1	kcal/mol

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