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A Report on Some Thermodynamic Data for Desulfurization Processes

U.S. DEPARTMENT OF COMMERCE
National Bureau of Standards
Center for Chemical Physics
Chemical Thermodynamics Division
Washington, DC 20234

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Final

Prepared for
Department of Energy
Morgantown Energy Technology Center
Morgantown, West Virginia

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U.S. DEPARTMENT OF COMMERCE, Malcolm Baldrige, ***Secretary***
NATIONAL BUREAU OF STANDARDS, Ernest Ambler, ***Director***

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A REPORT ON SOME THERMODYNAMIC DATA FOR DESULFURIZATION PROCESSES

by

V. B. Parker, B.R. Staples, T.L. Jobe, and D. Neumann

Abstract

Tables are presented here of values of thermochemical properties and processes at 298.15 K for some substances of interest to DOE for flue gas desulfurization.

The substances covered are (1) the aqueous ions: OH^-, SO_3^{-2}, HSO_3^-, SO_4^{-2}, HSO_4^-, CO_3^{-2}, HCO_3^-, H^+, Mn^{+2}, Fe^{+2}, Mg^{+2}, Ca^{+2}, Na^+, and K^+, and (2) solid, liquid, aqueous, and gaseous compounds or species formed from these ions.

The tables contain the following:

1. The thermochemical property values, enthalpy of formation, $\Delta_f H°$, Gibbs energy of formation, $\Delta_f G°$, entropy, $S°$, and heat capacity, $C_p°$ all at 298.15 K, as well as the enthalpy difference between 298.15 K and 0 K, $H°-H_o°$, for the basic species cited above.

2. The predicted values for $\Delta H°$, $\Delta G°$, $\Delta S°$, and $\Delta C_p°$ as well as log K (equilibrium constant) for the processes, or reactions, of importance to DOE, calculated from (1).

3. The property values, ϕ_L, the relative apparent molar enthalpy, $\gamma_\pm$, the mean ionic activity coefficient, and ϕ, the osmotic coefficient, for the binary aqueous systems at 298.15 K, all as a function of concentration.

Some documentation for (2) and (3) is provided. All of the values given are consistent with the NBS TN 270 Series.

I GENERAL DESCRIPTION

1. Introduction

In this report tables of values of thermochemical properties and processes at 298.15 K for substances of interest to DOE for flue gas desulfurization processes are presented. This work is part of an ongoing evaluation of the various systems of interest. An analysis of the more recent data is underway and these data will be incorporated into these tables in a way which will preserve the total unity and consistency of the tables.

The substances covered are: (1) the aqueous ions: OH^-, SO_3^{-2}, HSO_3^-, SO_4^{-2}, HSO_4^-, CO_3^{-2}, HCO_3^-, H^+, Mn^{+2}, Fe^{+2}, Mg^{+2}, Ca^{+2}, Na^+, and K^+, and (2) solid, liquid, aqueous, and gaseous compounds or species formed from these ions.

The tables are arranged in three sections.

Section II contains the thermochemical property values, $\Delta_f H°$, $\Delta_f G°$, and $(H - H_0^\circ)$ in kcal/mol, and S° and C_p° in cal/(mol·K), all at 298.15 K, for the basic substances of interest. They are either obtained from the NBS Technical Note 270 Series, "Selected Values of Chemical Thermodynamic Properties of the Elements and Their Compounds," [81NBS][1], or have been selected to be compatible with those tables.

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[1] References are given in a chronologically ordered bibliography at the end of the report (section VII). They are cited in the text in coded form indicating year of publication and the first two authors. The pre 1900 references are listed before and separately from the post 1900 ones.

Section III contains the values, $\Delta H°$, $\Delta G°$ in kcal/mol, $\Delta S°$ and ΔC_p° in cal/(mol·K), and log K for some of the important processes in flue gas desulfurization. Emphasis has been given to the values for solution processes, i.e., $\Delta H°$ (soln), $\Delta G°$ (soln), $\Delta S°$ (soln), log K_s° and ΔC_p° for the salts and their hydrates at 298.15 K, as well as to the K's and ΔH's for ion pairing or complex ion formation. The process values are derived from the property values listed in section II as, for example:

$$\Delta H° = \Sigma\ \Delta_f H° \text{ (products) } - \Sigma\ \Delta_f H° \text{ (reactants).}$$

Section IV contains the following property values of various solutions as a function of concentration: $\Delta_f H$, and the derived ϕ_L, (the relative apparent molar enthalpy) and $\gamma_\pm$ (mean ionic activity coefficient) and ϕ (the osmotic coefficient).

Documentation for section III is provided in section V, as is documentation for section IV in section VI. Detailed analyses and complete documentation, however, are not given at this time since it is beyond the scope of this report. Many of the selections for the properties of the substances involve analysis of a complex network of thermodynamic data. In that process values for individual processes or substances may become modified in order to achieve a set of "best values." Some documentation, however, is provided on some processes where the experimental measurements on a particular process are the definitive ones for the predicted properties of that process or where newer data indicate the need for revision. Documentation is also provided for the activity coefficients given in the tables on solution properties.

Users of these tables are invited to comment on the selections, correct errors and bring new measurements to our attention. The support of the Department of Energy and Office of Standard Reference Data, NBS is gratefully acknowledged.

2. Explanation of the contents of the tables

The following material, adapted from [81NBS] provides definitions and conventions used in the tables.

2.1 Physical States

The physical state of the substance is appended to the chemical formula in parentheses: NaOH(c) = NaOH, crystalline. The abbreviations most commonly used to denote physical states are listed in Table I-1. Any other notations are explained in the tables.

2.2 Definition of Symbols for the Thermochemical Properties and Thermochemical Processes

The headings used in the tables in section II and their meanings are:

$\Delta_f H^\circ$	standard enthalpy of formation at 298.15 K;
$\Delta_f G^\circ$	standard Gibbs energy, G, of formation at 298.15 K;
$H^\circ - H^\circ_0$	enthalpy, H, of the compound in the indicated state at 298.15 K referred to its value at 0 K. If the indicated state at 298 K is gas, the corresponding state at 0 K is the hypothetical ideal gas; if the state at 298 K is solid or liquid, the corresponding state at 0 K is the thermodynamically stable crystalline solid, unless otherwise specifically indicated.
S°	standard entropy, S, at 298.15 K;
C°_p	heat capacity at constant pressure at 298.15 K.

The Gibbs energy is related to the other quantities by: $G = H-TS$, where T is the thermodynamic temperature. The enthalpy is related to the internal energy, E, by: $H = E + PV$, where P = pressure and V = volume.

All values refer to one mole of substance for the formula given.

For the processes listed in the tables in section III the headings and their meanings are:

$\Delta H°$	enthalpy change for the process under standard conditions, i.e., for the substances in their standard states, at 298.15 K
$\Delta G°$	Gibbs energy change for the process under standard conditions, etc.
$\Delta S°$	Entropy change for the process under standard conditions, etc.
$\Delta C_p°$	heat capacity change at constant pressure at 298.15 K
log K	The common logarithm of the equilibrium constant, equal to $-\Delta G°/2.3026RT$

The tables in section IV for the solution properties have the following headings and meanings.

ϕ_L	the relative apparent molar enthalpy
$\gamma_\pm$	the mean ionic activity coefficient
ϕ	the osmotic coefficient.

2.3 Conventions Regarding Pure Substances

The values of the thermodynamic properties of the pure substances given in the tables in section II are for the substances in their standard states. These standard states are defined as follows:

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

For a gas the standard state at any temperature 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 phase of a substance is indicated in parentheses at the end of the chemical formula. See section I-2.1.

The values of $\Delta_f H°$ and $\Delta_f G°$ given in the tables represent the change in the appropriate thermodynamic quantity when one mole 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 for the elements are indicated in the tables by the fact that the values of $\Delta_f H°$ and $\Delta_f G°$ are exactly zero.

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.

2.4 Convention Regarding Solutions

For all dissolved substances the composition of the solvent is indicated in parentheses following the chemical formula. Except in special cases, discussed below, the number of moles of the solvent associated with one mole of solute is stated explicitly. See section I- 2.1 and Table I-1 for the conventions used.

The standard state for a non-dissociated solute in aqueous solution is taken as the hypothetical ideal solution of unit molality, which has been designated as "std state, m = 1." For strong electrolytes in aqueous solution the conventional standard state is the ideal solution of unit activity (unit mean molality). 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 designation "a" is used for strong electrolytes in the standard state and "ao" for undissociated species in water solution. In non-aqueous media the standard state defined above is indicated by appending "X" to the formula of the solvent. The convention "std state, m = 1" is used only rarely for non-aqueous media. An "s" is appended to the formula of the solvent to designate this condition.

The value for $\Delta_f H$ for a solute in a solution of definite composition is the apparent enthalpy of the reaction of formation of the real solution from the elements comprising the solute, each in its standard reference state, and the appropriate total number of moles of solvent.

Elements + solvent → salt (dissolved in solvent). When using this representation for $\Delta_f H$ for the dissolved species the value of $\Delta_f H$ for the solvent is not required; the experimental value of an enthalpy of dilution can be obtained directly as the difference between the two values of $\Delta_f H$ at the corresponding concentrations.

It may be noted, to avoid confusion, that $\Delta_f H$ applies to the real solution, including any hydrolysis, ionization or other reaction that occurs upon solution of the solute.

The value for $\Delta_f H°$ for a solute in its standard state is equal to the apparent molar enthalpy of formation of the substance in an ideal solution containing the species of which the solute is assumed to be nominally composed. If this speciation is the same as that in the real solution at infinite dilution, then $\Delta_f H°$ is equal to $\Delta_f H^{\infty}$, the enthalpy of dilution of an ideal solution being zero. The assumed nominal composition of the solute is that at infinite dilution for non-dissociating substances, salts composed of ions that do not react further, such as NaI, and $KMnO_4$, and the common acids, such as HCl, H_2SO_4, H_3PO_4 and acetic acid. THe assumed nominal composition for salts containing ionizable or hydrolyzable species is not the same as the speciation in the real, infinitely dilute solution. For example, $NaHSO_4$ is composed of Na^+ and HSO_4^- ions in its standard state, while the infinitely dilute real solution contains Na^+, H^+ and SO_4^{2-} ions. THe difference between the $\Delta_f H$'s for these two solutions is the enthalpy of ionization of HSO_4^-.

The values of the thermodynamic properties tabulated for the individual ions in aqueous solution are based on the usual convention that the values of $\Delta_f H°$, $\Delta_f G°$, $S°$ and $C_p°$ for H^+ (aq, std. state, m = 1) are zero. For an ionic species e.g., HSO_4^- , the properties tabulated refer to that undissociated ion, i.e. they are not equal to the sum of those for its constituent ions. By adopting the above convention with respect to aqueous H^+, it follows that the thermodynamic relation $\Delta_f G° = \Delta_f H° - T[\Delta_f S° + [n/2]S°(H_2(gs))]$ where $\Delta_f S°$ has been calculated from tabulated entropies holds for individual ionic species, with n equal to the algebraic value of the charge. For neutral electrolyes, (and gaseous ions) the normal consistency relationship applies. See section I-4.

3. 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 4.184 joules exactly, 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 I-2.

The values in this table are consistent with the CODATA Fundamental Constants [73COD] and negligibly different from those listed in [81NBS].

The formula weights used in the tables are those listed in [81NBS]. Use of more recent atomic weights [80IUP] would produce only insignificant changes in the tabulated thermodynamic values.

4. Internal Consistency of the Tables

All of the values given in the tables of thermochemical properties 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 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 $\Delta_f H^\circ$, $\Delta_f G^\circ$, and S° at 298.15 K satisfy the relation:

$$\Delta_f G^\circ = \Delta_f H^\circ - T\ \Delta_f S^\circ.$$

to the precision given. The special case of solutions is discussed in section 2.4. 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 ΔH° or ΔG° for specific reactions may result from the introduction of such data. See section I-4.2.

There are, however, some substances [limited to the sodium and potassium salts of SO_4^{-2}(a), HCO_3^-(a) and CO_3^{-2}(a)] for which the G-H-S relationship has been relaxed, so that $\Delta_f G°(c)$ does not equal $\Delta_f H°(c) - T\ \Delta_f S°(c)$ within the stated uncertainty. These are designated in the tables (section II) by the statement:

G-H-S constraint has been relaxed.

The rationale is as follows:

Newer data on the entropies of solution and Third Law entropies of a number of salts have led to significantly different values of the entropies of these ions from those reported in TN 270-3 [81NBS] and used throughout the series. In order to retain the basic principle of those tables insofar as possible, namely that the values in the tables should yield "best" values for thermodynamic processes, values for $\Delta_f H°$, and $\Delta_f G°$ for the alkali metal salts have been selected such that the "best" values of ΔH° and ΔG° for the ideal solution process are maintained. The values of S° for the salts are selected from measurements independent of the solution process. In these cases the following thermodynamic relation:

$$\Delta S° \text{ (solution)} = [\Delta H° \text{ (solution)} - \Delta G° \text{ (solution)}]/T$$

will hold for the ideal solution process but the following relation may not be satisfied within the expected precision of the individual values of S°:

$$\Delta S°\text{(solution)} \neq \sum_{\text{ions}} S°\text{(a)} - S°\text{(c)}$$

Those processes affected in section II are designated.

See TN 270-8 [81NBS] for further details.

4.1 Uncertainties

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

In general, when uncertainties are not stated explicitly certain rules have been followed with respect to the number of significant figures recorded. Values are tabulated 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.

Each value, then, calculated for a process from the property values is given to one more decimal place than the property value with the least significant value.

4.2 Relationship to Other Tables of Thermodynamic Properties and Processes

The chemical thermodynamic properties and processes in the present tables may be combined with those published in TN 270 [81NBS] in order to calculate the change in another process. However we recommend against these values being combined with those in any other tabulation or with a property reported in an original research paper.

There are several reasons for avoiding the combination of thermochemical data from more than one source table. The most important is that different large-scale tables use different thermochemical properties of formation for substances that are ubiquitous in thermochemical measurements. Outstanding examples are the common inorganic acids and their ions. Another reason is that the groups preparing different tables may have relied on different measurements as the basis for selecting property values.

It is difficult to predict a priori how a change in one selected formation property or in a process would affect values assigned to other substances or processes because of the way these are linked by complex networks. In general, it may be expected that the advantage of internal consistency of a table will be lost if values from several sources are combined and that experimental measurements may be reproduced poorly.

No general, simple algorithm can be suggested for overcoming this problem. If it becomes necessary to extend a table of data to substances other than those tabulated, the user is advised to consult the group that prepared the table about the procedure that he plans to use.

Table I-1: Physical State Conventions

The following conventions are used to designate the physical state of a substance. This information appears in a parenthetical expression appended to the molecular formula.

Basic Symbols	Explanation
(g)	Gaseous, e.g., $HCl(g)$
(gs)	Gaseous reference standard state for an element, e.g., $O_2(gs)$ for $O_2(g)$
(c)	Crystalline, e.g., $NH_4Cl(c)$
(cs)	Crystalline reference standard state for an element, e.g., Rb(cs) for Rb(c)
(l)	Liquid, e.g., $H_2O(l)$
(ls)	Liquid reference standard state for an element, e.g., $Br_2(ls)$ for $Br_2(l)$
(am)	Amorphous
(gl)	Glassy
(a)	Hypothetical standard state of the ideal aqueous solution at unit activity. For a neutral electrolyte the value of a property is equal to the algebraic sum of the values for the ions assumed to constitute the molecule of the electrolyte, e.g., $HCl(a)=H^+(a) + Cl^-(a)$. For an ionic species this notation is commonly used to refer to the undissociated ion as written. e.g., $HSO_4^-(a)$.

Basic Symbols	Explanation
(ao)	Hypothetical standard state of the ideal aqueous solution at unit activity of the undissociated (non-ionized) species, e.g., HF(ao), HF_2^-(ao). May also be used whenever the designation (a) could be ambiguous. Note that the descriptions HSO_4^-(a) and HSO_4^-(ao) are equivalent, but that HF(a) and HF(ao) are not.

TABLE I-2

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	8.35935×10^{-2}	1.036435×10^{-5}
1 cal/mol =	4.184	1	41.2928	1.162222×10^{-6}	1.798796	3.49755×10^{-1}	4.33644×10^{-5}
1 cm^3 atm/mol =	0.1013251	2.42173×10^{-2}	1	2.81458×10^{-8}	4.35619×10^{-2}	8.47011×10^{-3}	1.050166×10^{-6}
1 kWh/mol =	3,600,000	860,421	3.55292×10^{7}	1	1,547,721	300,937	37.3117
1 Btu/lb-mol =	2.32600	5.55927×10^{-1}	22.9558	6.46111×10^{-7}	1	1.944384×10^{-1}	2.41075×10^{-5}
1 cm^{-1}/molecule =	11.96266	2.85914	118.0622	3.32296×10^{-6}	5.14302	1	1.239852×10^{-4}
1 eV/molecule =	96484.56	23060.4	952,230	2.68013×10^{-2}	41480.9	8065.479	1

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

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

II Tables for the Thermochemical Property Values of Substances

The values tabulated are $\Delta_f H°$, $\Delta_f G°$ and $H° - H°_0$ in kcal/mol, $S°$ and $C°_p$ in cal/(mol·K), all at 298.15 K.

The tables are arranged in the following order:

Table II-1	The O, H, S, or C containing substances
II-2	The Fe - O, H, S, or C containing substances
II-3	The Mn - O, H, S, or C containing substances
II-4	The Mg - O, H, S, or C containing substances
II-5	The Ca - O, H, S, or C containing substances
II-6	The Na - O, H, S, or C containing substances
II-7	The K - O, H, S, or C containing substances

Table II-1

Enthalpy, Gibbs Energy of Formation, Entropy, and Heat Capacity

	Substance	$\Delta_f H^0$	$\Delta_f G^0$	$H^0 - H^0_0$	S^0	C_p^0
	Formula and Description	298.15 K (25°C)				
		kcal/mol			cal/(mol·K)	
1	O_2(gs)	0	0	2.0746	49.003	7.016
2	H^+(a)	0	0	-	0	0
3	H_2(gs)	0	0	2.0238	31.208	6.889
4	OH^-(a)	-54.970	-37.594	-	-2.57	-35.5
5	H_2O(l)	-68.315	-56.687	-	16.71	17.995
6	H_2O(g)	-57.796	-54.634	2.3667	45.104	8.025
7	S(cs,rh)	0	0	1.054	7.60	5.41
8	SO_2(g)	-70.944	-71.748	2.521	59.30	9.53
9	SO_2(ao)	-77.194	-71.871	-	38.7	-
10	SO_3(g)	-94.58	-88.69	2.796	61.34	12.11
11	SO_3^{-2}(a)	-151.9	-116.3	-	-7.	-
12	SO_4^{-2}(a)	-217.32	-177.97	-	4.8	-70.
13	$S_2O_5^{-2}$(a)	-	-	-	-	-

Table II-1 (cont'd)

Enthalpy, Gibbs Energy of Formation, Entropy, and Heat Capacity

	Substance	$\Delta_f H^0$	$\Delta_f G^0$	$H^0 - H^0_0$	S^0	$C_p{}^0$
	Formula and Description	298.15 K (25°C)				
		kcal/mol			cal/(mol·K)	
14	$HSO_3{}^-$(ao)	-149.67	-126.15	-	33.4	-
15	$HSO_4{}^-$(ao)	-212.08	-180.69	-	31.5	-20.
16	H_2SO_3(ao)	-145.51	-128.56	-	55.5	-
17	H_2SO_4(l)	-194.548	-164.938	6.748	37.501	33.20
18	H_2SO_4(a)	-217.32	-177.97	-	4.8	-70.
19	$H_2SO_4 \cdot H_2O$(l)	-269.508	-227.182	-	50.56	51.35
20	$H_2SO_4 \cdot 2H_2O$(l)	-341.085	-286.770	-	66.06	62.34
21	$H_2SO_4 \cdot 3H_2O$(l)	-411.186	-345.178	-	82.55	76.23
22	$H_2SO_4 \cdot 4H_2O$(l)	-480.688	-403.001	-	99.09	91.35
23	$H_2SO_4 \cdot 6.5H_2O$(l)	-653.264	-546.403	-	140.51	136.30
24	C(cs,graphite)	0	0	0.251	1.372	2.038
25	CO_2(g)	-94.051	-94.254	2.2378	51.06	8.87
26	CO_2(ao)	-98.90	-92.26	-	28.1	-
27	$CO_3{}^{-2}$(a)	-161.84	-126.17	-	-13.6	-
28	$HCO_3{}^-$(ao)	-165.39	-140.26	-	21.8	-
29	H_2CO_3(ao)	-167.22	-148.94	-	44.8	-

Table II-2

Enthalpy, Gibbs Energy of Formation, Entropy, and Heat Capacity

	Substance	$\Delta_f H^0$	$\Delta_f G^0$	$H^0 - H^0_0$	S^0	C_p^0
	Formula and Description	298.15 K (25°C)				
		kcal/mol			cal/(mol·K)	
30	Fe(cs)	0	0	1.073	6.52	6.00
31	Fe^{+2}(a)	-21.3	-18.85	-	-32.9	-
32	Fe^{+3}(a)	-11.6	-1.1	-	-75.5	-
33	$Fe_{0.947}O$(c)	-63.64	-58.59	2.26	13.74	11.50
34	FeO(c)	-65.0	-	-	-	-
35	Fe_2O_3(c)	-197.0	-177.4	3.719	20.89	24.82
36	Fe_3O_4(c)	-267.3	-242.7	5.87	35.0	34.28
37	$FeOH^+$(ao)	-77.6	-66.3	-	-7.	-
38	$FeOH^{+2}$(ao)	-69.5	-54.83	-	-34.	-
39	FeO(OH)(c)	-133.6	-	-	-	-
40	$Fe(OH)_2$(c)	-136.0	-116.3	-	21.	-
41	$Fe(OH)_2^+$(ao)	-	-104.7	-	-	-
42	$Fe(OH)_3$(c)	-196.7	-166.5	-	25.5	-
43	$Fe(OH)_3$(ao)	-	-157.6	-	-	-
44	$Fe(OH)_3^-$(ao)	-	-147.0	-	-	-
45	$Fe(OH)_4^{-2}$(ao)	-	-184.0	-	-	-

Table II-2 (cont'd)

Enthalpy, Gibbs Energy of Formation, Entropy, and Heat Capacity

	Substance Formula and Description	$\Delta_f H^o$	$\Delta_f G^o$	$H^o - H^o_0$	S^o	C_p^o
		298.15 K (25°C)				
		kcal/mol			cal/(mol·K)	
46	$Fe_2(OH)_2^{+4}$(ao)	-146.3	-111.68	-	-85.	-
47	$FeSO_3$(c)	-	-	-	-	-
48	$FeSO_3$(ao)	-	-	-	-	-
49	$FeSO_4$(c)	-221.9	-196.2	-	25.7	24.04
50	$FeSO_4$(a)	-238.6	-196.82	-	-28.1	-
51	$FeSO_4$(ao)	-	-	-	-	-
52	$FeSO_4^+$(ao)	-222.7	-184.7	-	-31.	-
53	$FeSO_4 \cdot H_2O$(c)	-297.25	-	-	-	-
54	$FeSO_4 \cdot 4H_2O$(c)	-508.9	-	-	-	-
55	$FeSO_4 \cdot 7H_2O$(c)	-720.50	-599.97	-	97.8	94.28
56	$Fe(SO_4)^-_2$(ao)	-	-364.4	-	-	-
57	$Fe_2(SO_4)_3$(c)	-617.0	-	-	-	-
58	$Fe_2(SO_4)_3$(a)	-675.2	-536.1	-	-136.6	-
59	$FeHSO_3^+$(ao)	-	-	-	-	-
60	$FeHSO_4^+$(ao)	-	-	-	-	-
61	$Fe(HSO_3)_2$(c)	-	-	-	-	-
62	$Fe(HSO_4)_3$(c)	-	-	-	-	-
63	$Fe(HSO_4)_3$(a)	-647.84	-543.17	-	-19.0	-
64	$FeCO_3$(c)	-177.00	-159.35	-	22.2	19.63
65	$FeCO_3$(a)	-183.14	-145.02	-	-46.5	-

Table II-3

Enthalpy, Gibbs Energy of Formation, Entropy, and Heat Capacity

	Substance Formula and Description	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$H^\circ - H^\circ_0$	S°	C_p°
		298.15 K (25°C)				
		kcal/mol			cal/(mol·K)	
66	Mn(cs,α)	0	0	1.194	7.65	6.29
67	Mn^{+2}(a)	-52.76	-54.5	-	-17.6	12.
68	MnO(c)	-92.07	-86.74	-	14.27	10.86
69	MnO_2(c)	-124.29	-111.18	-	12.68	12.94
70	$MnOH^+$(ao)	-107.7	-96.8	-	-4.	-
71	$Mn(OH)_2$(am)	-166.2	-147.0	-	23.7	-
72	$Mn(OH)_3^-$(ao)	-	-177.9	-	-	-
73	$MnSO_4$(c)	-254.60	-228.83	-	26.8	24.02
74	$MnSO_4$(a)	-270.1	-232.5	-	-12.8	-58.
75	$MnSO_4$(ao)	-266.7	-235.6	-	8.7	-
76	$MnSO_4 \cdot H_2O$(c,α)	-329.0	-	-	-	-
77	$MnSO_4 \cdot H_2O$(c,β)	-322.2	-	-	-	-
78	$MnSO_4 \cdot 4H_2O$(c)	-539.7	-	-	-	-
79	$MnSO_4 \cdot 5H_2O$(c)	-610.2	-	-	-	78.
80	$MnSO_4 \cdot 7H_2O$(c)	-750.3	-	-	-	-
81	$MnCO_3$(c,natural)	-213.7	-195.2	-	20.5	19.48
82	$MnCO_3$(c,precipitated)	-211.1	-	-	-	-
83	$MnCO_3$(a)	-214.60	-180.67	-	-31.2	-
84	$MnHCO_3^+$(ao)	-	-196.0	-	-	-

Table II-4

Enthalpy, Gibbs Energy of Formation, Entropy, and Heat Capacity

	Substance	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$H^\circ - H^\circ_0$	S°	C_p°
	Formula and Description	298.15 K (25°C)				
		kcal/mol			cal/(mol·K)	
85	Mg(cs)	0	0	1.195	7.81	5.95
86	Mg^{+2}(a)	-111.58	-108.7	-	-33.0	-
87	MgO(c,macro)	-143.81	-136.10	1.235	6.44	8.88
88	MgO(c,micro)	-142.92	-135.27	1.266	6.67	9.00
89	$Mg(OH)^{+}$(ao)	-	-149.8	-	-	-
90	$Mg(OH)_2$(c)	-220.97	-199.23	2.725	15.10	18.41
91	$Mg(OH)_2$(am)	-220.0	-	-	-	-
92	$Mg(OH)_2$(a)	-221.52	-183.9	-	-38.1	-
93	$MgSO_3$(c)	-241.0	-220.8*	-	21.0*	-
94	$MgSO_3$(a)	-263.48	-225.0	-	-40.0	-
95	$MgSO_3 \cdot 3H_2O$(c)	-461.7	-400.3*	-	50.0*	-
96	$MgSO_3 \cdot 6H_2O$(c)	-673.4	-570.2*	-	77.0*	-

* Not contained in NBS TN270-6 [81NBS] but consistent with it.

Table II-4 (cont'd)

Enthalpy, Gibbs Energy of Formation, Entropy, and Heat Capacity

	Substance Formula and Description	$\Delta_f H^o$	$\Delta_f G^o$	$H^o - H^o_0$	S^o	C_p^o
		298.15 K (25°C)				
		kcal/mol			cal/(mol·K)	
97	$MgSO_4$(c)	-307.1	-279.8	-	21.9	23.06
98	$MgSO_4$(a)	-328.90	-286.7	-	-28.2	-
99	$MgSO_4$(ao)	-324.1	-289.74	-	-1.7	-
100	$MgSO_4 \cdot H_2O$(c)	-382.9	-341.5	-	30.2	-
101	$MgSO_4 \cdot H_2O$(am)	-376.4	-335.8	-	33.0	-
102	$MgSO_4 \cdot 2H_2O$(c)	-453.2	-	-	-	-
103	$MgSO_4 \cdot 4H_2O$(c)	-596.7	-	-	-	-
104	$MgSO_4 \cdot 6H_2O$(c)	-737.8	-629.1	-	83.2	83.20
105	$MgSO_4 \cdot 7H_2O$(c)	-809.92	-686.4	-	89.	-
106	$MgSO_4 \cdot 3Mg(OH)_2 \cdot 8H_2O$(c)	-1543.3	-	-	-	-
107	$MgCO_3$(c)	-261.9	-241.9	-	15.7	18.05
108	$MgCO_3$(a)	-273.42	-234.87	-	-46.6	-
109	$MgCO_3 \cdot 3H_2O$(c)	-	-412.60	-	-	-
110	$MgCO_3 \cdot 5H_2O$(c)	-	-525.7	-	-	-
111	$MgHCO_3^+$(ao)	-	-250.3	-	-	-
112	$3MgCO_3 \cdot Mg(OH)_2 \cdot 3H_2O$(c)	-	-1100.3	-	-	-

Table II-5

Enthalpy, Gibbs Energy of Formation, Entropy, and Heat Capacity

	Substance Formula and Description	$\Delta_f H^0$	$\Delta_f G^0$	$H^0 - H^0_0$	S^0	C_p^0
		298.15 K (25°C)				
		kcal/mol			cal/(mol·K)	
113	Ca(cs)	0	0	1.364	9.90	6.05
114	Ca^{+2}(a)	-129.74	-132.30	-	-12.7	-
115	CaO(c)	-151.79	-144.37	-	9.50	10.23
116	CaO_2(c)	-156.0	-	-	-	-
117	$Ca(OH)^+$(ao)	-	-171.7	-	-	-
118	$Ca(OH)_2$(c)	-235.68	-214.76	-	19.93	20.91
119	$Ca(OH)_2$(a)	-239.68	-207.49	-	-17.8	-
120	$CaSO_3$(c)	-	-	-	24.23	21.92
121	$CaSO_3$(a)	-281.64	-248.6	-	-19.7	-
122	$CaSO_3 \cdot 0.5H_2O$(c)*	-313.5	-286.64	-	29.0	-
123	$CaSO_4$(c,α,soluble)	-340.64	-313.93	-	25.9	23.95
124	$CaSO_4$(c,β,soluble)	-339.58	-312.87	-	25.9	23.67
125	$CaSO_4$(c,insoluble,anhydrite)	-342.76	-315.93	-	25.5	0
126	$CaSO_4$(a)	-347.06	-310.27	-	-7.9	-
127	$CaSO_4 \cdot 0.5H_2O$(c,α)	-376.85	-343.41	-	31.2	28.54
128	$CaSO_4 \cdot 0.5H_2$(c,β)	-376.35	-343.18	-	32.1	29.69
129	$CaSO_4 \cdot 2H_2O$(c)	-483.42	-429.60	-	46.4	44.46
130	$CaCO_3$(c,calcite)	-288.46	-269.8	-	22.2	19.57
131	$CaCO_3$(c,aragonite)	-288.51	-269.55	-	21.2	19.42
132	$CaCO_3$(a)	-291.58	-258.47	-	-26.3	-

* Correction to NBS TN270-6 [81NBS]

Table II-6

Enthalpy, Gibbs Energy of Formation, Entropy, and Heat Capacity

	Substance	$\Delta_f H^o$	$\Delta_f G^o$	$H^o - H^o_0$	S^o	C_p^o
	Formula and Description	298.15 K (25°C)				
		kcal/mol			cal/(mol·K)	
133	Na(cs)	0	0	1.54	12.24	6.75
134	Na^+(a)	-57.39	-62.593	-	14.1	11.1
135	Na_2O(c)	-99.00	-89.74	2.964	17.94	16.52
136	NaOH(c)	-101.723	-90.709	2.507	15.405	14.23
137	NaOH(a)	-112.360	-100.187	-	11.5	-24.4
138	$NaOH \cdot H_2O$(c)	-175.560	-150.435	3.725	23.780	21.55
139	$NaOH \cdot 2H_2O$(l)	-243.565	-208.705	9.221	46.840	57.22
140	$NaOH \cdot 3.5H_2O$(l)	-348.900	-295.545	13.44	68.377	84.71
141	$NaOH \cdot 4H_2O$(l)	-383.64	-324.3	-	76.17	-
142	$NaOH \cdot 5H_2O$(l)	-452.75	-381.60	-	92.27	-
143	$NaOH \cdot 7H_2O$(l)	-590.11	-495.74	-	125.79	-
144	$NaSO_4^-$(ao)	-273.59	-241.56	-	26.0	-
145	Na_2SO_3(c)	-263.1	-242.0	5.36	34.88	28.74
146	Na_2SO_3(a)	-266.70	-241.50	-	21.0	-
147	$Na_2SO_3 \cdot 7H_2O$(c)	-755.8	-639.7	-	106.0	-

Table II-6 (cont'd)

Enthalpy, Gibbs Energy of Formation, Entropy, and Heat Capacity

	Substance	$\Delta_f H^o$	$\Delta_f G^o$	$H^o - H^o_0$	S^o	C_p^o
	Formula and Description	298.15 K (25°C)				
		kcal/mol			cal/(mol·K)	
148	Na_2SO_4(c,V,orthorhombic)♦	-331.52	-303.59	5.551	35.75	30.64
149	Na_2SO_4(c,III,metastable)	-	-	5.624	37.03	30.90
150	Na_2SO_4(a)	-332.10	-303.16	-	33.0	-48.
151	$Na_2SO_4 \cdot 10H_2O$(c)♦	-1034.24	-871.75	-	141.5	-
152	$NaHSO_3$(a)	-207.06	-188.74	-	47.5	-
153	$NaHSO_4$(c)	-269.0	-237.3	-	27.0	-
154	$NaHSO_4$(a)	-269.47	-243.28	-	45.6	-9.
155	$NaHSO_4 \cdot H_2O$(c)	-339.8	-294.4	-	37.	-
156	Na_2CO_3(c)♦	-270.24	-249.64	4.959	32.26	26.84
157	Na_2CO_3(a)	-276.62	-251.36	-	14.6	-
158	$NaCO_3^-$(ao)	-223.69	-189.50	-	-11.9	-
159	$Na_2CO_3 \cdot H_2O$(c)♦	-342.08	-307.22	6.296	40.18	34.80
160	$Na_2CO_3 \cdot 7H_2O$(c)♦	-764.81	-648.8	-	100.9+	-
161	$Na_2CO_3 \cdot 10H_2O$(c)♦	-975.46	-819.36	21.21	134.5+	131.53
162	$NaHCO_3$(c)♦	-227.25	-203.4	3.81	24.3	20.94
163	$NaHCO_3$(a)	-222.78	-202.85	-	35.9	-
164	$NaHCO_3$(ao)	-225.6	-203.1	-	27.2	-
165	$3NaHCO_3 \cdot Na_2CO_3$(c)	-951.9	-	-	-	-
166	$NaHCO_3 \cdot Na_2CO_3 \cdot 2H_2O$(c)	-641.7	-569.69	-	72.0	-

♦ G-H-S constraint has been relaxed. See section I-4.

+ Correction to NBS TN 270-8 [81NBS].

Table II-7

Enthalpy, Gibbs Energy of Formation, Entropy, and Heat Capacity

	Substance	$\Delta_f H^o$	$\Delta_f G^o$	$H^o - H^o_0$	S^o	C_p^o
	Formula and Description	298.15 K (25°C)				
		kcal/mol			cal/(mol·K)	
167	K(cs)	0	0	1.695	15.34	7.07
168	$K^+(a)$	-60.32	-67.70	-	24.5	5.2
169	$K_2O(c)$	-86.4	-	-	-	-
170	KOH(c)	-101.521	-90.61	2.904	18.85	15.5
171	KOH(a)	-115.29	-105.29	-	21.9	-30.3
172	$KOH \cdot H_2O(c)$	-179.0	-154.2	-	28.	-
173	$KOH \cdot 2H_2O(c)$	-251.2	-212.1	-	36.	-
174	$KSO_4^-(ao)$	-276.63	-246.69	-	36.1	-
175	$K_2SO_3(c)$	-269.0	-	-	-	-
176	$K_2SO_3(a)$	-272.5	-251.7	-	42.	-
177	$K_2SO_4(c)^{\#}$	-343.64	-315.83	6.079	41.96	31.42
178	$K_2SO_4(a)$	-337.96	-313.37	-	53.8	-60.
179	$KHSO_3(a)$	-209.99	-193.85	-	57.9	-
180	$KHSO_4(c)$	-277.4	-246.5	-	33.0	-
181	$KHSO_4(a)$	-272.40	-248.39	-	56.0	-15.
182	$K_2CO_3(c)^{\#}$	-275.1	-254.2	5.417	37.17	27.35
183	$K_2CO_3(a)$	-282.48	-261.57	-	35.4	-
184	$K_2CO_3 \cdot 1.5H_2O(c)^{\#}$	-384.60	-342.4	-	48.6	-
185	$KHCO_3(c)^{\#}$	-230.2	-206.4	-	27.6	-
186	$KHCO_3(a)$	-225.71	-207.96	-	46.3	-
187	$7K_2CO_3 \cdot 2CO_2 \cdot 9.5H_2O(c)$	-2843.7	-	-	-	-

G-H-S constraint has been relaxed. See Section I-4.

III Tables for the Thermochemical Values for Processes

The values tabulated are ΔH° and ΔG° in kcal/mol, ΔS° and ΔC_p° in cal/(mol·K), and log K for the processes listed.

The tables are arranged in the following order:

Table III-1	Processes involving O,H,S, or C containing substances
III-2	Processes involving Fe - O,H,S, or C containing substances
III-3	Processes involving Mn - O,H,S, or C containing substances
III-4	Processes involving Mg - O,H,S, or C containing substances
III-5	Processes involving Ca - O,H,S, or C containing substances
III-6	Processes involving Na - O,H,S, or C containing substances
III-7	Processes involving K - O,H,S, or C containing substances

Table III-1

Enthalpy and Gibbs Energy of Reaction, Entropy and Heat Capacity Changes of Reaction, and Equilibrium Constant

	Reaction	ΔH^0	ΔG^0	ΔS^0	ΔC_{p^0}	log K
		298.15 K (25°C)				
		kcal/mol		cal/(mol·K)		
1	$H_2(gs) + 0.5\ O_2(gs) \rightarrow H_2O(l)$	-68.315	-56.687	-39.000	7.598	41.5521
2	$H_2O(l) \rightarrow H^+(a) + OH^-(a)$	13.345	19.093	-19.28	-53.50	-13.995
3	$H_2O(l) \rightarrow H_2O(g)$	10.519	2.053	28.394	-9.970	-1.5049
4	$O_2(gs) + S(cs,rh) \rightarrow SO_2(g)$	-70.944	-71.748	2.697	-2.896	52.5919
5	$1.5\ O_2(gs) + S(cs,rh) \rightarrow SO_3(g)$	-94.58	-88.69	-19.764	-3.824	65.010
6	$SO_2(g) + 0.5\ O_2(gs) \rightarrow SO_3(g)$	-23.636	-16.942	-22.462	-0.928	12.419
7	$SO_2(g) + H_2O(l) \rightarrow H_2SO_3(ao)$	-6.251	-0.125	-20.55	-	0.0916
8	$H_2SO_3(ao) \rightarrow H^+(a) + HSO_3^-(ao)$	-4.16	2.41	-22.1	-	-1.766
9	$HSO_3^-(ao) \rightarrow H^+(a) + SO_3^{-2}(a)$	-2.23	9.85	-40.4	-	-7.220
10	$2\ HSO_3^-(ao) \rightarrow S_2O_5^{-2}(a) + H_2O(l)$	-	-	-	-	-

Table III-1 (cont'd)

Enthalpy and Gibbs Energy of Reaction, Entropy and Heat Capacity Changes of Reaction, and Equilibrium Constant

	Reaction	ΔH^0	ΔG^0	ΔS^0	ΔC_{p^0}	log K
		298.15 K (25°C)				
		kcal/mol		cal/(mol·K)		
11	$H_2SO_4(a) \rightarrow 2\ H^+(a) + SO_4^{-2}(a)$	0	0	0	0	0
12	$SO_4^{-2}(a) + H^+(a) \rightarrow HSO_4^-(ao)$	5.24	-2.72	26.7	50.	1.994
13	$SO_3(g) + H_2O(l) \rightarrow H_2SO_4(l)$	-31.653	-19.561	-40.549	3.095	14.338
14	$H_2SO_4(l) \rightarrow H_2SO_4(a)$	-22.772	-13.032	-32.70	-103.2	9.5526
15	$H_2SO_4(l) + H_2O(l) \rightarrow H_2SO_4 \cdot H_2O(l)$	-6.645	-5.557	-3.651	0.155	4.0733
16	$H_2SO_4(l) + 2\ H_2O(l) \rightarrow H_2SO_4 \cdot 2H_2O(l)$	-9.907	-8.458	-4.861	-6.850	6.1998
17	$H_2SO_4(l) + 3\ H_2O(l) \rightarrow H_2SO_4 \cdot 3H_2O(l)$	-11.693	-10.179	-5.081	-10.955	7.4613
18	$H_2SO_4(l) + 4\ H_2O(l) \rightarrow H_2SO_4 \cdot 4H_2O(l)$	-12.880	-11.315	-5.251	-13.830	8.2940
19	$H_2SO_4(l) + 6.5\ H_2O(l) \rightarrow H_2SO_4 \cdot 6.5H_2O(l)$	-14.668	-13.000	-5.60	-13.87	9.528
20	$CO_2(g) \rightarrow CO_2(ao)$	-4.849	1.994	-22.96	-	-1.462
21	$CO_2(ao) + H_2O(l) \rightarrow H^+(a) + HCO_3^-(ao)$	1.825	8.687	-23.01	-	-6.3676
22	$HCO_3^-(ao) \rightarrow H^+(a) + CO_3^{-2}(a)$	3.55	14.09	-35.4	-	-10.328

Table III-2

Enthalpy and Gibbs Energy of Reaction, Entropy and Heat Capacity Changes of Reaction, and Equilibrium Constant

	Reaction	ΔH^0	ΔG^0	ΔS^0	ΔC_{p}^0	log K
		298.15 K (25°C)				
		kcal/mol		cal/(mol·K)		
23	$Fe(cs) \rightarrow Fe^{+2}(a) + 2\ e-$	-21.3	-18.85	-8.21	-	13.817
24	$Fe(cs) \rightarrow Fe^{+3}(a) + 3\ e-$	-11.6	-1.1	-35.21	-	0.806
25	$Fe^{+2}(a) \rightarrow Fe^{+3}(a) + e-$	9.7	17.75	-27.00	-	-13.011
26	$0.947\ Fe(cs) + 0.5\ O_2(gs) \rightarrow Fe_{0.947}O(c)$	-63.64	-58.59	-16.936	2.310	42.947
27	$0.5\ Fe_2O_3(c) + 0.5\ H_2O(l) \rightarrow FeO(OH)(c)$	-0.94	-	-	-	-
28	$Fe(OH)_2(c) \rightarrow FeOH^{+}(ao) + OH^{-}(a)$	3.43	12.40	-30.6	-	-9.094
29	$Fe(OH)_2(c) \rightarrow Fe^{+2}(a) + 2\ OH^{-}(a)$	4.76	22.26	-59.0	-	-16.318
30	$FeOH^{+2}(ao) \rightarrow Fe^{+3}(a) + OH^{-}(a)$	2.93	16.14	-44.1	-	-11.828
31	$FeOH^{+2}(ao) + H_2O(l) \rightarrow Fe(OH)_2^{+}(ao)$	-	6.82	-	-	-4.997
32	$2\ FeOH^{+2}(ao) \rightarrow Fe_2(OH)_2^{+4}(ao)$	-7.3	-2.02	-17.	-	1.481
33	$Fe(OH)_3(c) \rightarrow Fe(OH)_3(ao)$	-	8.9	-	-	-6.524
34	$Fe(OH)_3(ao) \rightarrow Fe^{+3}(a) + 3\ OH^{-}(a)$	-	43.72	-	-	-32.046
35	$Fe(OH)_2(c) + OH^{-}(a) \rightarrow Fe(OH)_3^{-}(ao)$	-	6.89	-	-	-5.053
36	$Fe(OH)_2(c) + 2\ OH^{-}(a) \rightarrow Fe(OH)_4^{-2}(ao)$	-	7.49	-	-	-5.489

Table III-2 (cont'd)

Enthalpy and Gibbs Energy of Reaction, Entropy and Heat Capacity Changes of Reaction, and Equilibrium Constant

	Reaction	ΔH^0	ΔG^0	ΔS^0	ΔC_{p^0}	log K
		298.15 K (25°C)				
		kcal/mol		cal/(mol·K)		
37	$FeSO_3(c) \rightarrow Fe^{+2}(a) + SO_3{}^{-2}(a)$	-	-	-	-	-
38	$Fe(HSO_3)_2(c) \rightarrow Fe^{+2}(a) + 2\ HSO_3{}^{-}(ao)$	-	-	-	-	-
39	$Fe^{+2}(a) + SO_3{}^{-2}(a) \rightarrow FeSO_3(ao)$	-	-	-	-	-
40	$Fe^{+2}(a) + HSO_3{}^{-}(ao) \rightarrow FeHSO_3{}^{+}(ao)$	-	-	-	-	-
41	$Fe^{+3}(a) + SO_4{}^{-2}(a) \rightarrow FeSO_4{}^{+}(ao)$	6.22	-5.63	39.7	-	4.127
42	$FeSO_4(c) \rightarrow FeSO_4(a)$	-16.7	-0.62	-53.8	-	0.454
43	$FeSO_4 \cdot H_2O(c) \rightarrow FeSO_4(a) + H_2O(l)$	-9.66	-	-	-	-
44	$FeSO_4 \cdot 4H_2O(c) \rightarrow FeSO_4(a) + 4\ H_2O(l)$	-2.96	-	-	-	-
45	$FeSO_4 \cdot 7H_2O(c) \rightarrow FeSO_4(a) + 7\ H_2O(l)$	3.70	6.341	-8.9	-	-4.6480
46	$Fe_2(SO_4)_3(c) \rightarrow Fe_2(SO_4)_3(a)$	-58.2	-	-	-	-
47	$Fe^{+3}(a) + 2\ SO_4{}^{-2}(a) \rightarrow Fe(SO_4)^{-}{}_2(ao)$	-	-7.36	-	-	5.395
48	$Fe(HSO_4)_3(c) \rightarrow Fe(HSO_4)_3(a)$	-	-	-	-	-
49	$Fe^{+2}(a) + SO_4{}^{-2}(a) \rightarrow FeSO_4(ao)$	-	-	-	-	-
50	$Fe^{+2}(a) + HSO_4{}^{-}(ao) \rightarrow FeHSO_4{}^{+}(ao)$	-	-	-	-	-
51	$Fe^{+2}(a) + CO_3{}^{-2}(a) \rightarrow FeCO_3(a)$	0	0	0	-	0
52	$FeCO_3(c) \rightarrow FeCO_3(a)$	-6.14	14.33	-68.7	-	-10.504

Table III-3

Enthalpy and Gibbs Energy of Reaction, Entropy and Heat Capacity Changes of Reaction, and Equilibrium Constant

	Reaction	ΔH^0	ΔG^0	ΔS^0	ΔC_{p}^0	log K
		298.15 K (25°C)				
		kcal/mol		cal/(mol·K)		
53	$MnO(c) + H_2O(1) \rightarrow Mn(OH)_2(am)$	-5.82	-3.57	-7.28	-	2.619
54	$MnOH^+(ao) \rightarrow Mn^{+2}(a) + OH^-(a)$	-0.03	4.71	-16.2	-	-3.450
55	$Mn(OH)_3^-(ao) \rightarrow Mn^{+2}(a) + 3\ OH^-(a)$	-	10.62	-	-	-7.783
56	$MnSO_4(c) \rightarrow MnSO_4(a)$	-15.50	-3.67	-39.6	-82.0	2.690
57	$MnSO_4(ao) \rightarrow MnSO_4(a)$	-3.4	3.1	-21.5	-	-2.272
58	$MnSO_4.H_2O(c,\alpha) \rightarrow MnSO_4(a) + H_2O(1)$	-9.41	-	-	-	-
59	$MnSO_4 \cdot H_2O(c,\beta) \rightarrow MnSO_4(a) + H_2O(1)$	-16.21	-	-	-	-
60	$MnSO_4 \cdot 4H_2O(c) \rightarrow MnSO_4(a) + 4\ H_2O(1)$	-3.66	-	-	-	-
61	$MnSO_4 \cdot 5H_2O(c) \rightarrow MnSO_4(a) + 5\ H_2O(1)$	-1.48	-	-	-46.0	-
62	$MnSO_4 \cdot 7H_2O(c) \rightarrow MnSO_4(a) + 7\ H_2O(1)$	2.00	-	-	-	-
63	$MnSO_4.H_2O(c,\alpha) \rightarrow MnSO_4(c) + H_2O(g)$	16.60	-	-	-	-
64	$Mn^{+2}(a) + CO_3^{-2}(a) \rightarrow MnCO_3(a)$	0	0	0	-	0
65	$MnCO_3(c,natural) \rightarrow MnCO_3(a)$	-0.90	14.53	-51.7	-	-10.651
66	$MnCO_3(c,precipitated) \rightarrow MnCO_3(a)$	-3.50	-	-	-	-
67	$MnHCO_3^+(ao) \rightarrow Mn^{+2}(a) + HCO_3^-(ao)$	-	1.24	-	-	-0.909

Table III-4

Enthalpy and Gibbs Energy of Reaction, Entropy and Heat Capacity Changes of Reaction, and Equilibrium Constant

	Reaction	ΔH^0	ΔG^0	ΔS^0	$\Delta C_p{}^0$	log K
		298.15 K (25°C)				
		kcal/mol		cal/(mol·K)		
68	$MgO(c,macro) + H_2O(l) \rightarrow Mg(OH)_2(c)$	-8.845	-6.443	-8.05	-8.465	4.7228
69	$MgO(c,micro) + H_2O(l) \rightarrow Mg(OH)_2(c)$	-9.735	-7.273	-8.28	-8.585	5.3312
70	$Mg(OH)_2(c) \rightarrow Mg(OH)_2(a)$	-0.55	15.33	-53.20	-	-11.237
71	$Mg(OH)_2(am) \rightarrow Mg(OH)_2(a)$	-1.52	-	-	-	-
72	$Mg(OH)^+(ao) \rightarrow Mg^{+2}(a) + OH^-(a)$	-	3.50	-	-	-2.570
73	$MgSO_3(c) \rightarrow MgSO_3(a)$	-22.48	-4.2	-61.0	-	3.079
74	$MgSO_3 \cdot 3H_2O(c) \rightarrow MgSO_3(a) + 3\ H_2O(l)$	-6.72	5.24	-39.87	-	-3.840
75	$MgSO_3 \cdot 6H_2O(c) \rightarrow MgSO_3(a) + 6\ H_2O(l)$	0.03	5.08	-16.7	-	-3.722
76	$MgSO_3 \cdot 3H_2O(c) \rightarrow MgSO_3(c) + 3\ H_2O(g)$	47.31	15.60	106.31	-	-11.433
77	$MgSO_4(c) \rightarrow MgSO_4(a)$	-21.80	-6.9	-50.1	-	5.058
78	$MgSO_4(ao) \rightarrow MgSO_4(a)$	-4.80	3.04	-26.5	-	-2.228

Table III-4 (cont'd)

Enthalpy and Gibbs Energy of Reaction, Entropy and Heat Capacity Changes of Reaction, and Equilibrium Constant

	Reaction	ΔH^0	ΔG^0	ΔS^0	$\Delta C_p{}^0$	log K
		298.15 K (25°C)				
		kcal/mol		cal/(mol·K)		
79	$MgSO_4 \cdot H_2O(c) \rightarrow MgSO_4(a) + H_2O(l)$	-14.32	-1.89	-41.69	-	1.383
80	$MgSO_4 \cdot H_2O(am) \rightarrow MgSO_4(a) + H_2O(l)$	-20.82	-7.59	-44.49	-	5.561
81	$MgSO_4 \cdot H_2O(c) \rightarrow MgSO_4(c) + H_2O(g)$	18.00	7.07	36.80	-	-5.179
82	$MgSO_4 \cdot 2H_2O(c) \rightarrow MgSO_4(a) + 2\ H_2O(l)$	-12.33	-	-	-	-
83	$MgSO_4 \cdot 4H_2O(c) \rightarrow MgSO_4(a) + 4\ H_2O(l)$	-5.46	-	-	-	-
84	$MgSO_4 \cdot 6H_2O(c) \rightarrow MgSO_4(a) + 6\ H_2O(l)$	-0.99	2.28	-11.1	-	-1.670
85	$MgSO_4 \cdot 7H_2O(c) \rightarrow MgSO_4(a) + 7\ H_2O(l)$	2.82	2.89	-0.2	-	-2.119
86	$MgSO_4 \cdot 3Mg(OH)_2 \cdot 8H_2O(c) \rightarrow$ $3\ Mg(OH)_2(a) + MgSO_4(a) + 8\ H_2O(l)$	3.32	-	-	-	-
87	$MgCO_3(c) \rightarrow MgCO_3(a)$	-11.52	7.03	-62.3	-	-5.153
88	$MgCO_3 \cdot 3H_2O(c) \rightarrow MgCO_3(a) + 3\ H_2O(l)$	-	7.669	-	-	-5.6214
89	$MgCO_3 \cdot 5H_2O(c) \rightarrow MgCO_3(a) + 5\ H_2O(l)$	-	7.39	-	-	-5.420
90	$3MgCO_3 \cdot Mg(OH)_2 \cdot 3H_2O(c) \rightarrow$ $3\ MgCO_3(c) + Mg(OH)_2(c) + 3\ H_2O(l)$	-	5.31	-	-	-3.892
91	$MgHCO_3{}^+(ao) \rightarrow Mg^{+2}(a) + HCO_3{}^-(ao)$	-	1.34	-	-	-0.982

Table III-5

Enthalpy and Gibbs Energy of Reaction, Entropy and Heat Capacity Changes of Reaction, and Equilibrium Constant

	Reaction	ΔH^0	ΔG^0	ΔS^0	ΔC_{p^0}	log K
		298.15 K (25°C)				
		kcal/mol		cal/(mol·K)		
92	$CaO(c) + H_2O(l) \rightarrow Ca(OH)_2(c)$	-15.575	-13.703	-6.28	-7.315	10.044
93	$Ca(OH)_2(c) \rightarrow Ca(OH)_2(a)$	-4.00	7.27	-37.73	-	-5.329
94	$Ca(OH)^+(ao) \rightarrow Ca^{+2}(a) + OH^-(a)$	-	1.81	-	-	-1.324
95	$CaSO_3(c) \rightarrow CaSO_3(a)$	-	-	-43.93	-	-
96	$CaSO_3 \cdot 0.5H_2O(c) \rightarrow CaSO_3(a) + 0.5\ H_2O(l)$	-2.30	9.70	-40.34	-	-7.108
97	$CaSO_4(c,\alpha,soluble) \rightarrow CaSO_4(a)$	-6.42	3.66	-33.8	-	-2.683
98	$CaSO_4(c,\beta,soluble) \rightarrow CaSO_4(a)$	-7.48	2.60	-33.8	-	-1.906
99	$CaSO_4(c,insoluble,anhydrite) \rightarrow CaSO_4(a)$	-4.30	5.66	-33.4	-	-4.149
100	$CaSO_4 \cdot 0.5H_2O(c,\alpha) \rightarrow CaSO_4(a) + 0.5\ H_2O(l)$	-4.368	4.796	-30.74	-	-3.5158
101	$CaSO_4 \cdot 0.5H_2(c,\beta) \rightarrow CaSO_4(a) + 0.5\ H_2O(l)$	-4.868	4.566	-31.64	-	-3.3473
102	$CaSO_4 \cdot 2H_2O(c) \rightarrow CaSO_4(a) + 2\ H_2O(l)$	-0.270	5.956	-20.88	-	-4.3658
103	$CaCO_3(c,calcite) \rightarrow CaCO_3(a)$	-3.12	11.33	-48.5	-	-8.305
104	$CaCO_3(c,aragonite) \rightarrow CaCO_3(a)$	-3.07	11.08	-47.5	-	-8.122

Table III-6

Enthalpy and Gibbs Energy of Reaction, Entropy and Heat Capacity Changes of Reaction, and Equilibrium Constant

	Reaction	ΔH^0	ΔG^0	ΔS^0	ΔC_{p}^{0}	log K
		298.15 K (25°C)				
		kcal/mol		cal/(mol·K)		
105	$0.5\ Na_2O(c) + 0.5\ H_2O(l) \rightarrow NaOH(c)$	-18.066	-17.496	-1.920	-3.028	12.8244
106	$NaOH(c) \rightarrow NaOH(a)$	-10.637	-9.478	-3.90	-38.63	6.9474
107	$NaOH{\cdot}H_2O(c) \rightarrow NaOH(a) + H_2O(l)$	-5.115	-6.439	4.43	-27.96	4.7198
108	$NaOH{\cdot}2H_2O(l) \rightarrow NaOH(a) + 2\ H_2O(l)$	-5.425	-4.856	-1.92	-45.63	3.5595
109	$NaOH{\cdot}3.5H_2O(l) \rightarrow NaOH(a) + 3.5\ H_2O(l)$	-2.562	-3.046	1.61	-46.13	2.2331
110	$NaOH{\cdot}4H_2O(l) \rightarrow NaOH(a) + 4\ H_2O(l)$	-1.980	-2.63	2.17	-	1.931
111	$NaOH{\cdot}5H_2O(l) \rightarrow NaOH(a) + 5\ H_2O(l)$	-1.185	-2.022	2.78	-	1.4822
112	$NaOH{\cdot}7H_2O(l) \rightarrow NaOH(a) + 7\ H_2O(l)$	-0.455	-1.256	2.68	-	0.9206
113	$Na_2SO_3(c) \rightarrow Na_2SO_3(a)$	-3.60	0.50	-13.88	-	-0.366
114	$Na_2SO_3{\cdot}7H_2O(c) \rightarrow Na_2SO_3(a) + 7\ H_2O(l)$	10.90	1.39	32.0	-	-1.020
115	$Na^+(a) + SO_4^{-2}(a) \rightarrow NaSO_4^-(ao)$	1.12	-0.997	7.1	-	0.7308
116	$Na_2SO_4(c,V,orthorhombic) \rightarrow Na_2SO_4(a)$	-0.58	0.43	-3.39*	-78.6	-0.315
117	$Na_2SO_4{\cdot}10H_2O(c) \rightarrow Na_2SO_4(a) + 10.\ H_2O(l)$	18.99	1.72	57.92*	-	-1.261
118	$NaHSO_4(c) \rightarrow NaHSO_4(a)$	-0.47	-5.98	18.6	-	4.383
119	$NaHSO_4{\cdot}H_2O(c) \rightarrow NaHSO_4(a) + H_2O(l)$	2.02	-5.57	25.3	-	4.081

* Calculated from ΔH and ΔG for the processes given.

Table III-6 (cont'd)

Enthalpy and Gibbs Energy of Reaction, Entropy and Heat Capacity Changes of Reaction, and Equilibrium Constant

	Reaction	ΔH^0	ΔG^0	ΔS^0	ΔC_{p^0}	log K
		298.15 K (25°C)				
		kcal/mol		cal/(mol·K)		
120	$NaCO_3^-(ao) \rightarrow Na^+(a) + CO_3^{-2}(a)$	4.46	0.737	12.4	-	-0.5402
121	$Na_2CO_3(c) \rightarrow Na_2CO_3(a)$	-6.38	-1.72	-15.63*	-	1.261
122	$Na_2CO_3 \cdot H_2O(c) \rightarrow Na_2CO_3(a) + H_2O(l)$	-2.855	-0.827	-6.80*	-	0.6062
123	$Na_2CO_3 \cdot 7H_2O(c) \rightarrow Na_2CO_3(a) + 7\ H_2O(l)$	9.985	0.63	31.37*	-	-0.463
124	$Na_2CO_3 \cdot 10H_2O(c) \rightarrow Na_2CO_3(a) + 10.\ H_2O(l)$	15.69	1.13	48.83*	-	-0.828
125	$Na_2CO_3 \cdot 10H_2O(c) \rightarrow$ $Na_2CO_3 \cdot 7H_2O(c) + 3\ H_2O(l)$	5.705	0.50	18.49*	-	-0.366
126	$NaHCO_3(c) \rightarrow NaHCO_3(a)$	4.47	0.55	13.15*	-	-0.403
127	$NaHCO_3(ao) \rightarrow NaHCO_3(a)$	2.82	0.25	8.7	-	-0.183
128	$NaHCO_3 \cdot Na_2CO_3 \cdot 2H_2O(c) \rightarrow$ $NaHCO_3(a) + Na_2CO_3(a) + 2\ H_2O(l)$	5.67	2.106	11.92	-	-1.5437
129	$3NaHCO_3 \cdot Na_2CO_3(c) \rightarrow$ $3\ NaHCO_3(a) + Na_2CO_3(a)$	6.94	-	-	-	-

* Calculated from ΔH and ΔG for the processes given.

Table III-7

Enthalpy and Gibbs Energy of Reaction, Entropy and Heat Capacity Changes of Reaction, and Equilibrium Constant

	Reaction	ΔH^0	ΔG^0	ΔS^0	ΔC_{p^0}	log K
		298.15 K (25°C)				
		kcal/mol		cal/(mol·K)		
130	$0.5\ K_2O(c) + 0.5\ H_2O(l) \rightarrow KOH(c)$	-24.163	-	-	-	-
131	$KOH(c) \rightarrow KOH(a)$	-13.769	-14.68	3.05	-45.8	10.760
132	$KOH\cdot H_2O(c) \rightarrow KOH(a) + H_2O(l)$	-4.60	-7.78	10.6	-	5.700
133	$KOH\cdot 2H_2O(c) \rightarrow KOH(a) + 2\ H_2O(l)$	-0.72	-6.56	19.3	-	4.811
134	$K_2SO_3(c) \rightarrow K_2SO_3(a)$	-3.5	-	-	-	-
135	$K^+(a) + SO_4^{-2}(a) \rightarrow KSO_4^-(ao)$	1.01	-1.02	6.8	-	0.748
136	$K_2SO_4(c) \rightarrow K_2SO_4(a)$	5.68	2.46	10.80*	-91.4	-1.803
137	$KHSO_4(c) \rightarrow KHSO_4(a)$	5.00	-1.89	23.0	-	1.385
138	$K_2CO_3(c) \rightarrow K_2CO_3(a)$	-7.38	-7.37	-0.03*	-	5.402
139	$K_2CO_3\cdot 1.5H_2O(c) \rightarrow K_2CO_3(a) + 1.5\ H_2O(l)$	-0.352	-4.20	12.90*	-	3.079
140	$KHCO_3(c) \rightarrow KHCO_3(a)$	4.49	-1.56	20.29*	-	1.143
141	$7K_2CO_3\cdot 2CO_2\cdot 9.5H_2O(c) \rightarrow$ $7\ K_2CO_3(a) + 2\ CO_2(ao) + 9.5\ H_2O(l)$	19.55	-	-	-	-

* Calculated from ΔH and ΔG for the processes given.

IV Tables for the Property Values of Binary Aqueous Systems as a Function of Concentration.

The values tabulated are ϕ_L, the relative apparent molar enthalpy, $\gamma_\pm$, the mean ionic activity coefficient, and ϕ, the osmotic coefficient, as a function of the number of moles of H_2O, nH_2O, per mole of solute, and as a function of the number of moles of solute, mol/kg H_2O. Also included are the Δ_fH's as a function of the concentration obtained from NBS TN 270 [81NBS] and the parameters for the equations used to generate $\gamma_\pm$ and ϕ (for which see section VI). All values are reported at 298.15 K.

The following tabular summary indicates the substances covered, in the order presented, and the properties tabulated.

		ϕ_L	$\gamma_\pm$	ϕ			ϕ_L	$\gamma_\pm$	ϕ
IV-1	SO_2	✓			IV-10	CaS_2O_3	✓		
IV-2	H_2SO_3	✓			IV-11	Na_2SO_3	✓	✓	✓
IV-3	H_2SO_4	✓	✓	✓	IV-12	Na_2SO_4	✓	✓	✓
IV-4	$FeSO_4$	✓			IV-13	$NaHSO_4$	✓	✓	✓
IV-5	$Fe_2(SO_4)_3$	✓			IV-14	KOH	✓	✓	✓
IV-6	$Fe(HSO_4)_3$	✓			IV-15	K_2SO_3	✓		
IV-7	$MnSO_4$	✓	✓	✓	IV-16	K_2SO_4	✓	✓	✓
IV-8	$MgSO_4$	✓	✓	✓	IV-17	$KHSO_3$	✓		
IV-9	$CaSO_4$	✓	✓	✓	IV-18	$KHSO_4$	✓		

Table IV-1.
SO_2

n H_2O	$\Delta_f H$ kcal-mol^{-1}	ϕ_L cal-mol^{-1}	$\gamma\pm$	ϕ	m mol-kg^{-1}
100.00	-78.054	5531.			.55508
150.00	-78.226	5359.			.37005
200.00	-78.355	5230.			.27754
250.00	-78.458	5127.			.22203
300.00	-78.547	5038.			.18503
400.00	-78.691	4894.			.13877
500.00	-78.811	4774.			.11102
750.00	-79.036	4549.			.07401
1000.00	-79.201	4384.			.05551
1500.00	-79.461	4124.			.03701
2000.00	-79.642	3943.			.02775
2500.00	-79.776	3809.			.02220
3000.00	-79.891	3694.			.01850
3500.00	-79.989	3596.			.01586
4000.00	-80.068	3517.			.01388
5000.00	-80.209	3376.			.01110
7500.00	-80.443	3142.			.00740
10000.00	-80.584	3001.			.00555
∞	-83.585	0			0

$\Delta_f H^0$ = -83.585 kcal-mol^{-1} Number of molalities = 18

[completely ionized - See note on Table IV-2. H_2SO_3]

Enthalpy data taken from NBS TN 270-Series [81NBS]

Table IV-2.
H_2SO_3

n H_2O	Δ_fH kcal-mol^{-1}	ϕ_L cal-mol^{-1}	$\gamma_\pm$	ϕ	m mol-kg^{-1}
100.00	-146.369	5531.			.55508
150.00	-146.541	5359.			.37005
200.00	-146.670	5230.			.27754
250.00	-146.773	5127.			.22203
300.00	-146.862	5038.			.18503
400.00	-147.006	4894.			.13877
500.00	-147.126	4774.			.11102
750.00	-147.351	4549.			.07401
1000.00	-147.516	4384.			.05551
1500.00	-147.776	4124.			.03701
2000.00	-147.957	3943.			.02775
2500.00	-148.091	3809.			.02220
3000.00	-148.206	3694.			.01850
3500.00	-148.304	3596.			.01586
4000.00	-148.383	3517.			.01388
5000.00	-148.524	3376.			.01110
7500.00	-148.758	3142.			.00740
10000.00	-148.899	3001.			.00555
∞	-151.900	0			0

Δ_fH^0 = -151.900 kcal-mol^{-1} Number of molalities = 18

$[\ 2H^+ + SO_3^= \ ]$

Enthalpy data taken from NBS TN 270-Series [81NBS]

H_2SO_3 is thermodynamically equivalent to $SO_2 + H_2O$. They are not distinct species. Both the SO_2 and H_2SO_3 tables are for the formation of the real solution, including all effects of ionization.

Table IV-3.
H_2SO_4

n H_2O	Δ_fH kcal-mol^{-1}	ϕ_L cal-mol^{-1}	$\gamma\pm$	ϕ	m mol-kg^{-1}
1.00	-201.193	16127.	-	-	55.50807
1.50	-203.128	14192.	-	-	37.00538
2.00	-204.455	12865.	3.3732	2.4792	27.75403
2.50	-205.452	11868.	2.2343	2.3916	22.20323
3.00	-206.241	11079.	1.6038	2.3057	18.50269
3.50	-206.886	10434.	1.2214	2.2288	15.85945
4.00	-207.428	9892.	.9574	2.1440	13.87702
4.50	-207.889	9431.	.7708	2.0569	12.33513
5.00	-208.288	9032.	.6366	1.9726	11.10161
5.50	-208.637	8683.	.5381	1.8933	10.09238
6.00	-208.944	8376.	.4639	1.8196	9.25134
7.00	-209.458	7862.	.3620	1.6877	7.92972
8.00	-209.865	7455.	.2970	1.5740	6.93851
9.00	-210.190	7130.	.2530	1.4756	6.16756
10.00	-210.451	6869.	.2220	1.3903	5.55081
12.00	-210.835	6485.	.1823	1.2517	4.62567
15.00	-211.191	6129.	.1512	1.1034	3.70054
20.00	-211.500	5820.	.1293	.9542	2.77540
25.00	-211.660	5660.	.1213	.8706	2.22032
30.00	-211.755	5565.	.1187	.8202	1.85027
40.00	-211.869	5451.	.1193	.7651	1.38770
50.00	-211.944	5376.	.1225	.7362	1.11016
75.00	-212.068	5252.	.1326	.7004	.74011
100.00	-212.150	5170.	.1423	.6818	.55508
115.00	-212.192	5128.	.1477	.6741	.48268
150.00	-212.282	5038.	.1594	.6619	.37005
200.00	-212.387	4933.	.1743	.6527	.27754
300.00	-212.565	4755.	.2000	.6480	.18503
400.00	-212.709	4611.	.2219	.6510	.13877
500.00	-212.833	4487.	.2411	.6568	.11102
600.00	-212.950	4370.	.2582	.6636	.09251
700.00	-213.040	4280.	.2738	.6706	.07930
800.00	-213.128	4192.	.2879	.6775	.06939
900.00	-213.205	4115.	.3010	.6842	.06168
1000.00	-213.275	4045.	.3130	.6906	.05551
1500.00	-213.557	3763.	.3627	.7180	.03701
2000.00	-213.785	3535.	.4005	.7390	.02775
3000.00	-214.135	3185.	.4562	.7693	.01850
4000.00	-214.415	2905.	.4964	.7905	.01388

continued..

Table IV-3 continued.

H_2SO_4

$n\ H_2O$	$\Delta_f H$ kcal-mol^{-1}	ϕ_L cal-mol^{-1}	$\gamma\pm$	ϕ	m mol-kg^{-1}
5000.00	-214.620	2700.	.5276	.8064	.01110
7000.00	-214.945	2375.	.5738	.8293	.00793
10000.00	-215.285	2035.	.6211	.8516	.00555
15000.00	-215.665	1655.	.6717	.8744	.00370
20000.00	-215.900	1420.	.7050	.8889	.00278
30000.00	-216.232	1088.	.7482	.9069	.00185
50000.00	-216.545	775.	.7957	.9260	.00111
70000.00	-216.706	614.	.8229	.9366	.00079
100000.00	-216.855	465.	.8484	.9463	.00056
150000.00	-216.971	349.	.8735	.9557	.00037
200000.00	-217.042	278.	.8890	.9614	.00028
300000.00	-217.120	200.	.9080	.9682	.00019
500000.00	-217.187	133.	.9276	.9752	.00011
700000.00	-217.221	99.	.9383	.9789	.00008
1000000.00	-217.246	74.	.9479	.9823	.00006
2000000.00	-217.277	43.	.9628	.9874	.00003
∞	-217.320	0			0

$\Delta_f H^0$ = -217.320 kcal-mol^{-1} Number of molalities = 55

Enthalpy data taken from NBS TN 270-Series [81NBS]

Activity coefficient data from [81STA]

Constants for the activity coefficient equation below:

B1 = -7.26977066E+00 B4 = 9.96540329E+00 B7 = -1.92835211E-01
B2 = 1.27851225E+01 B5 = -4.32909954E+00 B8 = 1.76565010E-02
B3 = -1.42296622E+01 B6 = 1.17197320E+00 B9 = -6.89852000E-04

Equation for the activity coefficient of H_2SO_4:

$$\ln \gamma = \sum_{j=1}^{9} B_j\, m^{j/2}$$

Table IV-4.
$FeSO_4$

$n\ H_2O$	$\Delta_f H$ $kcal\text{-}mol^{-1}$	ϕ_L $cal\text{-}mol^{-1}$	$\gamma\pm$	ϕ	m $mol\text{-}kg^{-1}$
200.00	-237.100	1500.			.27754
40000.00	-237.800	800.			.00139
∞	-238.600	0			0

$\Delta_f H^0$ = -238.600 $kcal\text{-}mol^{-1}$ Number of molalities = 2

Enthalpy data taken from NBS TN 270-Series [81NBS]

Table IV-5.
$Fe_2(SO_4)_3$

$n\ H_2O$	$\Delta_f H$ $kcal\text{-}mol^{-1}$	ϕ_L $cal\text{-}mol^{-1}$	$\gamma\pm$	ϕ	m $mol\text{-}kg^{-1}$
400.00	-653.000	22200.			.13877
1000.00	-653.200	22000.			.05551
2000.00	-653.400	21800.			.02775
3000.00	-653.600	21600.			.01850
∞	-675.200	0			0

$\Delta_f H^o$ = -675.200 $kcal\text{-}mol^{-1}$ Number of molalities = 4

Enthalpy data taken from NBS TN 270-Series [81NBS]

Table IV-6.
$Fe(HSO_4)_3$

n H_2O	Δ_fH kcal-mol^{-1}	ϕ_L cal-mol^{-1}	$\gamma\pm$	ϕ	m mol-kg^{-1}
600.00	-646.500	1300.			.09251
∞	-663.560	-15760.			0

Δ_fH^0 = -647.800 kcal-mol^{-1} Number of molalities = 1

Enthalpy data taken from NBS TN 270-Series [81NBS]

Table IV-7.
$MnSO_4$

$n\ H_2O$	$\Delta_f H$ $kcal\text{-}mol^{-1}$	ϕ_L $cal\text{-}mol^{-1}$	$\gamma\pm$	ϕ	m $mol\text{-}kg^{-1}$
20.00	-267.580	2520.	.0439	.7307	2.77540
30.00	-268.020	2080.	.0428	.5562	1.85027
50.00	-268.180	1920.	.0510	.4823	1.11016
100.00	-268.330	1770.	.0734	.4846	.55508
200.00	-268.490	1610.	.1072	.5168	.27754
400.00	-268.640	1460.	.1540	.5572	.13877
1000.00	-268.850	1250.	.2399	.6248	.05551
2000.00	-269.070	1030.	.3236	.6842	.02775
3000.00	-269.140	960.	.3784	.7198	.01850
5000.00	-269.260	840.	.4509	.7631	.01110
10000.00	-269.400	700.	.5499	.8163	.00555
20000.00	-269.530	570.	.6427	.8610	.00278
50000.00	-269.680	420.	.7473	.9065	.00111
100000.00	-269.770	330.	.8103	.9317	.00056
∞	-270.100	0			0

$\Delta_f H^0$ = -270.100 $kcal\text{-}mol^{-1}$ Number of molalities = 14

Enthalpy data taken from NBS TN 270-Series [81NBS]

Activity coefficient data from [74PIT/MAY]

Constants for the activity coefficient equation (eqns. VI-1 thru 7) :

b = 1.20000000E+00 α_1 = 1.40000000E+00 α_2 = 1.20000000E+01

β^0 = 2.01000000E-01 β^1 = 2.98000000E+00 β^2 = 0.00000000E+00

C^ϕ = 1.82000000E-02

Table IV-8.
$MgSO_4$

n H_2O	$\Delta_f H$ kcal-mol^{-1}	ϕ_L cal-mol^{-1}	$\gamma\pm$	ϕ	m mol-kg^{-1}
20.00	-327.100	1800.	.0513	.8481	2.77540
25.00	-327.200	1700.	.0469	.7072	2.22032
50.00	-327.410	1490.	.0522	.5340	1.11016
75.00	-327.520	1380.	.0624	.5194	.74011
100.00	-327.590	1310.	.0718	.5228	.55508
200.00	-327.740	1160.	.1016	.5459	.27754
300.00	-327.820	1080.	.1238	.5633	.18503
400.00	-327.880	1020.	.1421	.5772	.13877
500.00	-327.930	970.	.1578	.5888	.11102
600.00	-327.970	930.	.1716	.5989	.09251
800.00	-328.040	860.	.1954	.6156	.06939
1000.00	-328.080	820.	.2154	.6291	.05551
2000.00	-328.202	698.	.2866	.6722	.02775
5000.00	-328.358	542.	.4003	.7334	.01110
10000.00	-328.467	433.	.4976	.7835	.00555
20000.00	-328.581	319.	.5969	.8328	.00278
50000.00	-328.707	193.	.7163	.8883	.00111
100000.00	-328.774	126.	.7898	.9202	.00056
∞	-328.900	0			0

$\Delta_f H^0$ = -328.900 kcal-mol^{-1} Number of molalities = 18

Enthalpy data taken from NBS TN 270-Series [81NBS]

Activity coefficient data from [74PIT/MAY]

Constants for the activity coefficient equation (eqns. VI-1 thru 7) :

b = 1.20000000E+00 α_1 = 1.40000000E+00 α_2 = 1.20000000E+01

β^0 = 2.21000000E-01 β^1 = 3.34300000E+00 β^2 = -3.72300000E+01

C^ϕ = 2.50000000E-02

Table IV-9.
$CaSO_4$

$n\ H_2O$	$\Delta_f H$ kcal-mol^{-1}	ϕ_L cal-mol^{-1}	$\gamma\pm$	ϕ	m mol-kg^{-1}
5000.00	-346.414	646.	.3714	.7111	.01110
7500.00	-346.518	542.	.4276	.7410	.00740
10000.00	-346.566	494.	.4695	.7631	.00555
20000.00	-346.685	375.	.5729	.8166	.00278
50000.00	-346.827	233.	.7000	.8784	.00111
100000.00	-346.915	145.	.7791	.9140	.00056
500000.00	-347.009	51.	.8986	.9633	.00011
1000000.00	-347.026	34.	.9284	.9746	.00006
∞	-347.060	0			0

$\Delta_f H^0$ = -347.060 kcal-mol^{-1} Number of molalities = 8

Enthalpy data taken from NBS TN 270-Series [81NBS]

Activity coefficient data from [74PIT/MAY]

Constants for the activity coefficient equation (eqns. VI-1 thru 7) :

b = 1.20000000E+00 α_1 = 1.40000000E+00 α_2 = 1.20000000E+01

β^0 = 2.00000000E-01 β^1 = 2.65000000E+00 β^2 = -5.57000000E+01

C^ϕ = 0.00000000E+00

Table IV-10.
CaS_2O_3

$n\ H_2O$	$\Delta_f H$ $kcal\text{-}mol^{-1}$	ϕ_L $cal\text{-}mol^{-1}$	$\gamma\pm$	ϕ	m $mol\text{-}kg^{-1}$
35.00	-284.560	1040.			1.58594
100.00	-284.800	800.			.55508
200.00	-284.950	650.			.27754
400.00	-285.020	580.			.13877
1000.00	-285.100	500.			.05551
∞	-285.600	0			0

$\Delta_f H^0$ = -285.600 $kcal\text{-}mol^{-1}$ Number of molalities = 5

Enthalpy data taken from NBS TN 270-Series [81NBS]

Table IV-11.
Na_2SO_3

$n\ H_2O$	$\Delta_f H$ kcal-mol^{-1}	ϕ_L cal-mol^{-1}	$\gamma\pm$	ϕ	m mol-kg^{-1}
30.00			.1989	.7124	1.85027
50.00			.2292	.7026	1.11016
100.00			.2866	.7281	.55508
200.00	-266.510	190.	.3529	.7580	.27754
800.00	-266.410	290.	.5029	.8177	.06939
2000.00			.6074	.8581	.02775
10000.00			.7705	.9195	.00555
50000.00			.8812	.9593	.00111
∞	-266.700	0			0

$\Delta_f H^0$ = -266.700 kcal-mol^{-1} Number of molalities = 8

Enthalpy data taken from NBS TN 270-Series [81NBS]

Activity coefficient data from [81GOL]

Constants for the activity coefficient equation (eqns. VI-8,9) :

B = 1.32416014E+00
C = -2.69200069E-01
D = 6.67319796E-02
E = 0.00000000E+00
F = 0.00000000E+00
G = 0.00000000E+00
H = 0.00000000E+00
I = 0.00000000E+00
J = 0.00000000E+00

Table IV-12.
Na_2SO_4

n H_2O	$\Delta_f H$ kcal-mol^{-1}	ϕ_L cal-mol^{-1}	$\gamma_\pm$	ϕ	m mol-kg^{-1}
18.00	-333.852	-1752.	.1389	.6735	3.08378
20.00	-333.800	-1700.	.1411	.6539	2.77540
25.00	-333.593	-1493.	.1494	.6303	2.22032
28.37	-333.491	-1391.	.1558	.6252	1.95658
30.00	-333.432	-1332.	.1590	.6244	1.85027
40.00	-333.165	-1065.	.1780	.6302	1.38770
50.00	-332.988	-888.	.1953	.6417	1.11016
60.00	-332.840	-740.	.2107	.6532	.92513
80.00	-332.605	-505.	.2367	.6726	.69385
100.00	-332.420	-320.	.2581	.6876	.55508
120.00	-332.275	-175.	.2762	.6996	.46257
140.00	-332.184	-84.	.2919	.7093	.39649
160.00	-332.122	-22.	.3058	.7175	.34693
180.00	-332.076	24.	.3183	.7246	.30838
200.00	-332.040	60.	.3296	.7308	.27754
250.00	-331.980	120.	.3540	.7435	.22203
300.00	-331.943	157.	.3743	.7537	.18503
350.00	-331.918	182.	.3919	.7622	.15859
400.00	-331.901	199.	.4072	.7694	.13877
500.00	-331.879	221.	.4333	.7813	.11102
600.00	-331.867	233.	.4549	.7910	.09251
800.00	-331.857	243.	.4894	.8060	.06939
1000.00	-331.855	245.	.5163	.8176	.05551
2000.00	-331.872	228.	.5991	.8520	.02775
3000.00	-331.892	208.	.6457	.8707	.01850
4000.00	-331.907	193.	.6774	.8832	.01388
5000.00	-331.920	180.	.7010	.8924	.01110
10000.00	-331.958	142.	.7677	.9178	.00555
20000.00	-331.992	108.	.8235	.9385	.00278
50000.00	-332.027	73.	.8805	.9589	.00111
∞	-332.100	0			0

$\Delta_f H^0$ = -332.100 kcal-mol^{-1} Number of molalities = 30

Enthalpy data taken from NBS TN 270-Series [81NBS]

Activity coefficient data from [81GOL]

Constants for the activity coefficient equation (eqns. VI-8,9) :

B = 1.21597315E+00 E = -4.86954126E-03 H = 0.00000000E+00
C = -3.55728552E-01 F = 0.00000000E+00 I = 0.00000000E+00
D = 8.29465562E-02 G = 0.00000000E+00 J = 0.00000000E+00

Table IV-13.
$NaHSO_4$

$n\ H_2O$	$\Delta_f H$ kcal-mol^{-1}	ϕ_L cal-mol^{-1}	$\gamma\pm$	ϕ	m mol-kg^{-1}
10.00	-269.590	-120.			5.55081
20.00	-270.020	-550.			2.77540
25.00	-270.040	-570.			2.22032
50.00	-270.120	-650.			1.11016
100.00	-270.145	-675.			.55508
200.00	-270.294	-824.			.27754
300.00	-270.470	-1000.			.18503
400.00	-270.604	-1134.			.13877
500.00	-270.710	-1240.			.11102
800.00	-270.970	-1500.			.06939
1000.00	-271.110	-1640.			.05551
2000.00	-271.580	-2110.			.02775
5000.00	-272.260	-2790.			.01110
∞	-274.710	-5240			0

$\Delta_f H^0$ = -269.470 kcal-mol^{-1} Number of molalities = 13

Enthalpy data taken from NBS TN 270-Series [81NBS]

Table IV-14.
KOH

$n\ H_2O$	Δ_fH $kcal\text{-}mol^{-1}$	ϕ_L $cal\text{-}mol^{-1}$	$\gamma\pm$	ϕ	m $mol\text{-}kg^{-1}$
3.00	-112.204	3086.	1673.	5.8770	18.50269
3.50	-112.644	2646.	257.9	4.6598	15.85945
4.00	-113.039	2251.	77.1172	3.8874	13.87702
4.50	-113.409	1881.	33.5041	3.3616	12.33513
5.00	-113.698	1592.	18.2855	2.9843	11.10161
6.00	-114.028	1262.	8.1041	2.4843	9.25134
8.00	-114.430	860.	3.3898	1.9579	6.93851
10.00	-114.657	633.	2.1575	1.6880	5.55081
12.00	-114.796	494.	1.6421	1.5250	4.62567
15.00	-114.920	370.	1.2786	1.3742	3.70054
20.00	-115.007	283.	1.0202	1.2349	2.77540
25.00	-115.034	256.	.9034	1.1566	2.22032
30.00	-115.050	240.	.8392	1.1066	1.85027
40.00	-115.072	218.	.7738	1.0471	1.38770
50.00	-115.086	204.	.7431	1.0132	1.11016
75.00	-115.104	186.	.7155	.9715	.74011
100.00	-115.114	176.	.7102	.9530	.55508
150.00	-115.129	161.	.7154	.9378	.37005
200.00	-115.139	151.	.7251	.9325	.27754
300.00	-115.156	134.	.7440	.9303	.18503
400.00	-115.166	124.	.7598	.9313	.13877
500.00	-115.175	115.	.7728	.9332	.11102
700.00	-115.188	102.	.7930	.9371	.07930
800.00	-115.193	97.	.8011	.9389	.06939
1000.00	-115.201	89.	.8144	.9422	.05551
1500.00	-115.215	75.	.8380	.9485	.03701
2000.00	-115.223	67.	.8538	.9531	.02775
3000.00	-115.234	56.	.8745	.9593	.01850
5000.00	-115.246	44.	.8976	.9665	.01110
7000.00	-115.252	38.	.9110	.9708	.00793
10000.00	-115.258	32.	.9236	.9748	.00555
20000.00	-115.267	23.	.9438	.9814	.00278
50000.00	-115.274	16.	.9632	.9878	.00111
100000.00	-115.279	11.	.9735	.9912	.00056
∞	-115.290	0			0

Δ_fH^0 = -115.290 $kcal\text{-}mol^{-1}$ Number of molalities = 34

Enthalpy data taken from NBS TN 270-Series [81NBS]

Activity coefficient data from [72HAM/WU]

Constants for the activity coefficient equation (eqns. VI-8,9) :

B = 1.15000000E+00 E = 2.99336000E-04 H = 0.00000000E+00
C = 2.30258509E-01 F = 3.91439000E-07 I = 0.00000000E+00
D = 6.04889000E-03 G = 0.00000000E+00 J = 0.00000000E+00

Table IV-15.
K_2SO_3

n H_2O	Δ_fH kcal-mol^{-1}	ϕ_L cal-mol^{-1}	$\gamma\pm$	ϕ	m mol-kg^{-1}
50.00	-272.200	300.			1.11016
100.00	-271.500	1000.			.55508
200.00	-271.200	1300.			.27754
350.00	-271.200	1300.			.15859
400.00	-271.300	1200.			.13877
500.00	-271.400	1100.			.11102
600.00	-271.500	1000.			.09251
1000.00	-271.900	600.			.05551
∞	-272.500	0			0

Δ_fH^0 = -272.500 kcal-mol^{-1} Number of molalities = 8

Enthalpy data taken from NBS TN 270-Series [81NBS]

Table IV-16.
K_2SO_4

$n\ H_2O$	$\Delta_f H$ kcal-mol^{-1}	ϕ_L cal-mol^{-1}	$\gamma\pm$	ϕ	m mol-kg^{-1}
50.00	-338.460	-500.	-	-	1.11016
60.00	-338.360	-400.	-	-	.92513
80.20	-338.180	-220.	.2236	.6743	.69212
100.00	-338.050	-90.	.2422	.6832	.55508
200.00	-337.820	140.	.3079	.7139	.27754
300.00	-337.770	190.	.3515	.7345	.18503
400.00	-337.730	230.	.3846	.7501	.13877
500.00	-337.720	240.	.4112	.7627	.11102
600.00	-337.708	252.	.4335	.7731	.09251
700.00	-337.706	254.	.4526	.7821	.07930
800.00	-337.707	253.	.4694	.7898	.06939
1000.00	-337.711	249.	.4976	.8028	.05551
1500.00	-337.720	240.	.5490	.8260	.03701
2000.00	-337.732	228.	.5851	.8418	.02775
3000.00	-337.751	209.	.6344	.8629	.01850
5000.00	-337.780	180.	.6927	.8870	.01110
8000.00	-337.806	154.	.7413	.9064	.00694
10000.00	-337.819	141.	.7625	.9147	.00555
20000.00	-337.854	106.	.8205	.9367	.00278
50000.00	-337.889	71.	.8791	.9582	.00111
100000.00	-337.909	51.	.9117	.9697	.00056
500000.00	-337.938	22.	.9587	.9860	.00011
∞	-337.960	0			0

$\Delta_f H^0$ = -337.960 kcal-mol^{-1} Number of molalities = 22

Enthalpy data taken from NBS TN 270-Series [81NBS]

Activity coefficient data from [81GOL]

Constants for the activity coefficient equation (eqns. VI-8,9) :

B = 9.43830073E-01 E = 0.00000000E+00 H = 0.00000000E+00
C = -8.85985775E-02 F = 0.00000000E+00 I = 0.00000000E+00
D = 0.00000000E+00 G = 0.00000000E+00 J = 0.00000000E+00

Table IV-17.
$KHSO_3$

n H_2O	$\Delta_f H$ kcal-mol^{-1}	ϕ_L cal-mol^{-1}	$\gamma\pm$	ϕ	m mol-kg^{-1}
400.00	-209.900	90.			.13877
∞	-212.220	-2230.			0

$\Delta_f H^0$ = -209.990 kcal-mol^{-1} Number of molalities = 1

Enthalpy data taken from NBS TN 270-Series [81NBS]

Table IV-18.
$KHSO_4$

n H_2O	Δ_fH kcal-mol^{-1}	ϕ_L cal-mol^{-1}	$\gamma\pm$	ϕ	m mol-kg^{-1}
20.00	-273.500	-1100.			2.77540
25.00	-273.500	-1100.			2.22032
50.00	-273.500	-1100.			1.11016
100.00	-273.600	-1200.			.55508
200.00	-273.800	-1400.			.27754
220.00	-273.840	-1440.			.25231
400.00	-273.840	-1440.			.13877
800.00	-274.180	-1780.			.06939
1000.00	-274.560	-2160.			.05551
2000.00	-274.680	-2280.			.02775
5000.00	-275.050	-2650.			.01110
9000.00	-275.700	-3300.			.00617
∞	-277.640	-5240.			0

Δ_fH^0 = -272.400 kcal-mol^{-1} Number of molalities = 12

Enthalpy data taken from NBS TN 270-Series [81NBS]

V Documentation for the Thermochemical Values for Some Processes

The arrangement is as follows:

V-1 Processes involving Fe
V-2 Processes involving Mg
V-3 Processes involving Ca
V-4 Processes involving Na

V-1. Processes involving Fe

The Dissociation of $FeOH^+$ (ao) (reaction 28)

[63BOL/ARV] determined the hydrolysis K of Fe^{+2}(a) to $FeOH^+$(ao) as a function of T.

The Solution Process for $Fe(OH)_2$(c) (reactions 29,35,36)

[83THO] measured the ΔH for the precipitation of $Fe(OH)_2$ from $FeSO_4$(aq) with KOH(aq). [53LEU/KOL] and [63DAU/DAU] measured the K's for the formation of $FeOH^+$(ao). [56GAY/WOO] obtained the K's for the formation of $Fe(OH)_3^{-1}$(ao) and $Fe(OH)_4^{-2}$(ao) from $Fe(OH)_2$(c).

The Solution Process for $FeSO_4 \cdot nH_2O$(c) (n=7,4,1,0) (reactions 42-45)

[63ADA/KEL] measured the ΔH soln in HCl (aq) of $FeSO_4 \cdot H_2O$(c) and $FeSO_4 \cdot 7H_2O$(c). [14FOR] measured the ΔH (soln) of all the hydrates, as well as the anhydrous salt, in H_2O. H_2O vapor pressure measurements of the hydrates have been made by [64KOH/ZAS] and [14BIL].

The Solution Process for $FeCO_3$(c) (reaction 52)

[35KEL/AND] cite the K to be 3.14×10^{-11}. [(18)75BER] measured the ΔH for the precipitation from $FeSO_4$(aq) and K_2CO_3(aq).

V-2. Processes involving Mg

The Formation Properties of MgO(c,macro) and MgO(c,micro) (reactions 68,69)

$\Delta_f H°$'s of MgO(Macro-crystal) and MgO(micro-crystal) are obtained primarily from the measurements of [43SHO/HUF] on the ΔH's of solution of Mg(c) and MgO in aqueous HCl, the direct combustion measurements on Mg(cs) by [51HOL/HUB], and the measurements of [49GIA] on ΔH(trans) MgO(macro) $\rightarrow$ MgO(micro).

The Relationship between MgO(macro and micro) and $Mg(OH)_2(c)$ (reactions 68, 69)

The ΔH measurements of [37WEL/TAY] and [38TAY/WEL] on the solution of MgO(c,macro) and $Mg(OH)_2(c)$ in 2N HCl, as well as the measurements of [37GIA/ARC], (micro), [48TOR/SAH],and [43SHO/HUF] on the solution of MgO(c, micro) and $Mg(OH)_2(c)$ in 1N HCl, are used to determine the relationship. The decomposition measurements of $Mg(OH)_2(c)$ by [37GIA/ARC] are in agreement.

The Dissociation of $MgOH^+(aq)$ (reaction 72)

The log K = -2.58 is obtained from the tabulation of [64SIL/MAR] and [63HOS2].

The Precipitation of $Mg(OH)_2$(amorp) (reaction 71)

[83THO] and [87BER] measured the ΔH (pptn) of $Mg(OH)_2$ from $MgSO_4$ solutions with KOH(aq) and NaOH(aq), respectively. In addition, [87BER] measured the ΔH from $MgCl_2(aq)$ with NaOH(aq).

The Solution Process for $MgSO_3 \cdot nH_2O(c)$ (n-6,3,0) (reactions 73-77)

The ΔH measurement of [87HAR] on the solution of $MgSO_3 \cdot 6H_2O(c)$, $MgSO_3 \cdot 3H_2O(c)$, and $MgSO_3(c)$ in HCl(aq) and on the solution of a mixture of $MgSO_3 \cdot 6H_2O(c)$ and $MgCl_2 \cdot 6H_2O(c)$ in $H_2SO_3(aq)$ result in values for the $\Delta_f H°$'s for $MgSO_3(c)$ and the two hydrates. The ΔH soln is thus calculated from $\Sigma\ \Delta_f H°$ (aq products) $-\Delta_f H°$ Mg $SO_3 \cdot nH_2O(c)$.

The tabulated ΔG°(soln) for $MgSO_3 \cdot 6H_2O$ = 5.036 kcal/mol is obtained from the solubility, 0.062 moles $MgSO_3$/kg H_2O given by [65SEI/LIN] and an estimated $\gamma_{\pm}$ (at I = 0.25) = 0.23 obtained from the Davies equation (see [68HAM]). The calculated ΔS°(soln) results in S° $MgSO_3 \cdot 6H_2O(c)$ = 77 cal/(mol·K), a reasonable value. S° $MgSO_3 \cdot 3H_2O(c)$ and S° $MgSO_3(c)$ are estimated and are used to obtain the other tabulated ΔG°'s for the solution processes.

<u>The Solution Process for $MgSO_4 \cdot nH_2O(c)$ (n=7,6,4,2,1,0)</u> (reactions 77,79-85)

The ΔH° (soln) of $MgSO_4(c)$ in H_2O is obtained from the ΔH (soln) measurements of [83THO], [83BER/ILO], and [85PIC] and the tabulated ϕ_L values for $MgSO_4(nH_2O)$ at the appropriate concentrations.

The measurements of [25MAR], [59DEW/RIC], and [55KNO/STA] on the decomposition of $MgSO_4(c)$ to $MgO(c)$ and $SO_2(g)$ or $SO_3(g)$ lead to independent values for $\Delta_f H°$ $MgSO_4(c)$ and ΔH° (soln) which are in poor agreement.

The determination of ΔH° (soln) $MgSO_4 \cdot H_2O(c)$ is based on the measurements of [56JAM/FRO], [83THO], and[85PIC]. The ΔH° (soln) for $MgSO_4 \cdot H_2O$ (amorph) was also determined by [56JAM/FRO]. The ΔH° (soln) of $MgSO_4 \cdot 2H_2O(c)$, $MgSO_4 \cdot 4H_2O(c)$ and $MgSO_4 \cdot 6H_2O(c)$ were obtained primarily from the measurements of [83THO]. The ΔH(soln) of $MgSO_4 \cdot 7H_2O$ as a function of concentration was measured by [51KAG/MIS] and [30PER]. These measurements as well as those of [52KAP/SAM], [83THO], and [85PIC] determined the ΔH°(soln) $MgSO_4 \cdot 7H_2O(c)$.

[65SEI/LIN] lists the saturated solution to be 3.167 mol/kg H_2O for $MgSO_4(aq)$ in equilibrium with $MgSO_4 \cdot 6H_2O(c)$ (metastable at 298 K) and 3.026 mol/kg H_2O in equilibrium with $MgSO_4 \cdot 7H_2O(c)$. The activity coefficient and osmotic coefficient obtained from [59ROB/STO] are 0.0517 and 0.974 respectively at 3.167 mol/kg H_2O, and 0.0496 and 0.930 respectively at 3.026 mol/kg H_2O so that ΔG° (soln) for the hexahydrate and heptahydrate are 2.539 and 2.735 kcal/mol respectively.

The ΔG° (soln) and the ΔH° (soln) for the heptahydrate results in a calculated S° $MgSO_4 \cdot 7H_2O(c)$ = 88.5 cal/(mol·K). In addition [40BEL] and [64KOH/ZAS] measured the $H_2O(g)$ decomposition pressure of the heptahydrate to the hexahydrate, resulting in values of 89.0 and 87.4 cal/(mol·K), respectively. The ΔH obtained by [40BEL] and [64KOH/ZAS] for this decomposition are consistent with the ΔH(soln) measurements. The [64KOH/ZAS] measurements on the hexahydrate/tetrahydrate decomposition are reasonably consistent with the solution measurements. For the lower hydrate decomposition their measurements are not.

[64NEW] measured the ΔH (soln) of $MgSO_4 \cdot 7H_2O(c)$ and $3Mg(OH)_2 \cdot MgSO_4 \cdot 8H_2O(c)$ in HCl(aq). Combining these measurements with those of [38TAY/WEL] on the ΔH(soln) of $Mg(OH)_2(c)$ in HCl(aq) results in $\Delta H° = + 2.1$ kcal for $3Mg(OH)_2 \cdot MgSO_4 \cdot 8H_2O(c) \rightarrow MgSO_4 \cdot H_2O(c) + 3Mg(OH)_2(c) + H_2O(l)$.

<u>The Dissociation Process for $MgSO_4(ao)$</u> (reaction 78)

The tabulated values are obtained from [58NAI/NAN]. Other values are listed by [64SIL/MAR].

<u>The Solution Process for $MgCO_3 \cdot nH_2O(c)$ (n = 5,3,0)</u> (reactions 87-89)

[65LAN] reviewed the data on the stability relationships in the $MgO\text{-}CO_2\text{-}H_2O$ system. His interpretation and calculations were accepted for the ΔG°(soln) processes for $MgCO_3 \cdot H_2O(c)$ and $MgCO_3 \cdot 3H_2O(c)$, and for the ΔG° for decomposition of $MgCO_3 \cdot 3H_2O(c)$. The value obtained from these and accepted for the ΔG°(soln) $MgCO_3(c)$ = 7.0 kcal/mol is not in agreement with the log $K_s = -7.46$ obtained by [62HAL]. The ΔH°(soln) $MgCO_3(c)$ from the accepted ΔG°(soln) and S° $MgCO_3(c)$ is = -11.50 kcal/mol which is supported by the measurements of [54KAP/STA] on the ΔH (soln) measurements of $MgCO_3$(c) and MgO(c) which result in ΔH = 23.5 kcal/mol for the decomposition of $MgCO_3$(c). The accepted ΔH for this decomposition is 24.0 kcal/mol in agreement with [41ROT], but in sharp contrast with the measurements of [13MAR/SIM], [62ELL/MOR], and [58FOL/KLI], which indicate a ΔH 2 to 4 kcal/mol greater than the accepted. This system needs reinvestigation.

The Dissociation Process for $Mg(HCO_3)^+$ (ao) (reaction 91)

[63HOS] reported the pK = 0.95 for the dissociation.

V-3. Processes Involving Ca

The Formation Properties of CaO(c)

The $\Delta_f H°$ is obtained from the combustion measurements of [56HUB/HOL].

The Relationship Between CaO(c) and $Ca(OH)_2(c)$ (reaction 92)

This relationship is obtained from the measurements of [38TAY/WEL], [37WEL/TAY], and [35SCH/PRA] on ΔH's of solution of CaO(c) and $Ca(OH)_2(c)$ in HCl solutions. The measurements are in good agreement.

Solution Process for $Ca(OH)_2(c)$ (reaction 93)

[65HOP/WUL] measured (and corrected for $CaOH^+$ (ao) formed) ΔH(soln) $Ca(OH)_2$. Their corrected value is 4.36 kcal/mol. They also corrected the solubility = .0203 mol/kg H_2O [56BAT/BOW] for the presence of $CaOH^+$(ao), obtaining m Ca^{+2}(aq) = 0.0145, m OH^-(aq) = 0.0345, γ Ca^{+2}(aq) = 0.507 and γ OH^-(aq) = 0.838 (obtained from the extended Debye-Hückel relation), resulting in ΔG° (soln) = 7.11 kcal/mol or log K_s° = -5.21. The tabulated values differ slightly from these because of the influence of other measurements on related compounds.

The Dissociation of $CaOH^+$(ao) (reaction 94)

The dissociation constant was determined by [59BAT/BOW], [54GIM/MON], [53BEL/GEO], and [51DAV/HOY]. The values range from K = 0.07 to 0.04. K = 0.05 was selected. [54GIM/MON] and [53BEL/GEO] also obtained ΔH° = -1.25 and -1.19 kcal/mol respectively for this. [65HOP/WUL] obtained ΔH° = -2.0 kcal/mol from a least squares analysis of measurements on $Ca(OH_2(c)$.

Solution Process for $CaSO_3 \cdot 5H_2O(c)$ (reaction 96)

[23BIC] measured the solubility and reported ΔG° (soln) = 9.74 kcal/mol or $K_s^\circ = 7.25 \times 10^{-8}$ assuming the dihydrate was the equilibrium solid phase.

This value is assigned to the hemihydrate equilibrium phase. [70RAD] reports K_s° to be 8.4 X 10^{-8} in fair agreement, with the solid phase the hemihydrate. The entropy of the hydrate is estimated as 29.0 cal/(mol·K), so that with ΔS° ≃ -41.4 cal/(mol·K) and ΔG° (soln) ≃ 9.70 kcal/mol, ΔH° (soln) = -2.3 kcal/mol. This is a correction to TN270-6 [81NBS].

The Solution Process for $CaSO_4 \cdot nH_2O$(c) (n=2,0.5 and 0) (reactions 97-102)

[46WAL], [25LAN/DUR], and [30LAN/MON] measured the ΔH (soln) of the dihydrate. They are in good agreement. The tabulated ΔG° (soln) is based on $K_s^\circ = 4.22 \times 10^{-5}$ from [64SIL/MAR]. More recent evidence, [69GAR/GLU], [76LIL/BRI], and [75YOK/YAM] indicates that a better ΔG° (soln) corrected for ion pairing, is 6.25 kcal/mol based on a solubility = 0.01518 mol/kg H_2O, $\gamma_\pm = 0.338$ and $a_w = 0.9995$. This would result in ΔS° (soln) = -21.9 cal/(mol·K).

[41KEL/SOU] reviewed the relationships between the various hydrates. These were accepted. More recent measurements by [64MCA], on the ΔH's of solution of the various hydrates, are in agreement with [41KEL/SOU]. A reanalysis of the ΔG°'s of solution will be made.

The Solution Process for $CaCO_3$(c, calcite) and (c, aragonite) (reactions 103,104)

The decomposition pressure measurements of [36SAN], [56HIL/WIN], [36SOU/ROY], [33MAT/BIT], [60JAN/LOR], and [62BAK] on calcite, and the difference in the ΔH's of solution of CaO(c) and $CaCO_3$(c) measured by [63MEA/RIC], [25BAC], [41ROT/BER], [37WEL/TAY], and [28ROT/CHA] result in ΔH° = 42.62 kcal/mol for the decomposition to CaO(c) and CO_2(g). The K_s° measurements of [60GAR/THO], [60BIA/GHI], [58TRO], [29FRE/JOH], and [68HAL/TAS], are in good agreement and lead to the tabulated ΔG°(soln) = 11.33 kcal/mol. However, more recent determinations, such as [74JAC/LAN] indicate that log K = -8.42

($\Delta G°$(soln) = 11.49 kcal/mol) if ion pairing is ignored and log K = -8.47 ($\Delta G°$ (soln) = 11.55 kcal/mol) if $CaCO_3$(ao) and $CaHCO_3^+$ (ao) are assumed. The $\Delta H°$(soln) with the latter approach is -2.6 kcal/mol with ΔC_p = -109 ± 2 cal/(mol·K) and $\Delta S°$ = -47.4 ± 1.0 cal/(mol·K). The values for the aragonite process are obtained from the transition properties calcite → aragonite, given by [35KEL/AND], [53JAM], and [56MAC].

The Solution Process for $NaOH(c)$, $NaOH \cdot H_2O(c)$ and $NaOH \cdot nH_2O(l)$ (reactions 106-112)

The ΔH°'s for the solution processes are taken from the measurements of [62MUR/GIA] who also measured the low temperature C_p's (corrected by [69SIE/GIA]). [69SIE/GIA] also measured the solubility of $NaOH \cdot H_2O(c)$ to be 27.312 mol/kg H_2O. From [72HAM/WU] $\gamma_{\pm} = 31.88$ and $\phi = 2.715$ resulting in $\Delta G°(\text{soln}) = -6.438$ kcal/mol. The vapor pressure measurements are in agreement. The solution processes for the liquid NaOH hydrates are taken from the measurements of [69SIE/GIA].

The Formation of $NaSO_4^-(ao)$ (reaction 115)

[75REA], [50JEN/MON], and [69IZA/EAT] measured the K. The values are in good agreement. [62AUS/NAI] reported the ΔH (corrected to $\mu = 0$).

The Solution Process for $Na_2SO_3(c)$ and $Na_2SO_3 \cdot 7H_2O(c)$ (reactions 113,114)

The solid phase in equilibrium with the saturated solution of Na_2SO_3 (solubility = 2.42 mol/kg H_2O) is $Na_2SO_3 \cdot 7H_2O(c)$. With $\gamma \pm = 0.190$ and $\phi = 0.738$, $\Delta G°$ (soln) = 0.96 kcal/mol. From the extrapolation of the data above 308 K the solubility for the anhydrous $Na_2SO_3(c)$ would be 2.32 mol/kg H_2O with $\gamma_{\pm} = 0.191$ and $\phi = 0.73$ so that ΔG° for this process is 0.62 kcal/mol. This solubility is now believed to be incorrect. The $\Delta G°(\text{soln})$ would most likely be close to zero. A reexamination is underway. ΔH° = -3.55 kcal/mol for solution of the anhydrous salt from the measurements of [84FOR] who also measured the ΔH for the solution of the heptahydrate (ΔH° = + 11.00 kcal/mol). The vapor pressure measurements of [28TAR] and [28ARI] on the heptahydrate lead to ΔG° = 15.87 and 15.36 kcal, respectively for the dehydration. All these values plus the measured S° $Na_2SO_3(c)$ (see [61KEL/KIN]) were used to obtain the selected tabulated values.

The Solution Process for Na_2SO_4(c) and $Na_2SO_4 \cdot 10H_2O$(c) (reactions 116,117)

The ΔG° soln = 1.677 kcal/mol for the decahydrate is obtained from the solubility = 1.96 mol/kg H_2O [49ROS], $\gamma_\pm$ = 0.156 and ϕ = 0.621 [59ROB/STO]. The ΔH°(soln) = 18.84 kcal/mol is obtained from the measurements of [38PIT/COU].

For the anhydrous Na_2SO_4(c,V, orthorhombic) the measurements of [69GAR/JEK] lead to ΔH° = -0.58 kcal/mol. ΔG° for the solution process = + 0.420 kcal/mol is obtained from m = 3.63 mol/kg H_2O [49ROS] and $\gamma_\pm$ = 0.137 from [59ROB/STO].

In addition to these measurements, the H_2O vapor pressure measurements of [37HIG] and [29MAT/OGU] on the decahydrate result in ΔG° = 21.79 kcal/mol $Na_2SO_4 \cdot 10H_2O$(c). The tabulated values result from this input data. The S° $Na_2SO_4 \cdot 10H_2O$(c) includes a 1.08 cal/(mol·K) correction for a zero point entropy.

VI Documentation and Discussion of the Aqueous Solution Property Values

The arrangement is as follows:

VI-1. A general description of the methods and equations used to obtain $\gamma_{\pm}$, the mean ionic activity coefficient, and ϕ. the osmotic coefficient is described. Included are the concentration ranges for which the equations used for $\gamma_{\pm}$ and ϕ are valid.

VI-2. Some specific sources of information for ϕ_L, the relative apparent molar enthalpy, is provided for $FeSO_4$, $MgSO_4$, $CaSO_4$, Na_2SO_3, and Na_2SO_4, as well as comments on $\gamma_{\pm}$ at saturation for these substances.

VI-1. Activity and Osmotic Coefficients

Activity and osmotic coefficients can be calculated using various semi-theoretical equations. There have been two major efforts towards the evaluation of activity and osmotic coefficients during the past 10 years. Pitzer and coworkers have formulated a set of equations of the virial coefficient type consistent with both the modern statistical mechanical description of electrolyte solutions and the basic principles of thermodynamics of solutions. The Electrolyte Data Center at NBS (see [78GOL/NUT]) has completed many detailed critical evaluations of electrolytes using an extensive data base of all available experimental data and has used extended forms of the Lietzke-Stoughton-Hamer-Wu equations [62LIE/STO,72HAM/WU], and more recently, extensions of the Pitzer equations [74PIT/MAY]. Both of these types of equations have been employed in the representation of activity data here.

For this report, the activity and osmotic coefficient of 2 : 2 charge type electrolytes ($MgSO_4$, $CaSO_4$, and $MnSO_4$) have been calculated from the Pitzer equations.

For the activity coefficient of these 2 : 2 salts, the equation is

$$\ln\gamma = 4f^{\gamma} + mB^{\gamma}_{MX} + m^2C^{\gamma}_{MX} \tag{VI-1}$$

where

$$f^{\gamma} = -A_{\phi}[I^{1/2}/(1 + bI^{1/2}) + (2/b)\ln(1 + bI^{1/2})] \tag{VI-2}$$

and

$$B^{\gamma}_{MX} = 2\beta^{(0)}_{MX} + (2\beta^{(1)}_{MX}/\alpha_1^2 I)\,[1 - (1 + \alpha_1 I^{1/2} - \tfrac{1}{2}\alpha_1^2 I)e^{-\alpha_1 I^{1/2}}] \tag{VI-3}$$

$$+ (2\beta^{(2)}_{MX}/\alpha_2^2 I)[1 - (1 + \alpha_2 I^{1/2} - \tfrac{1}{2}\alpha_2^2 I)e^{-\alpha_2 I^{1/2}}]$$

and

$$C^{\gamma}_{MX} = \tfrac{3}{2}C^{\phi}_{MX} \tag{VI-4}$$

The osmotic coefficient equation is

$$\phi - 1 = 4f^{\phi} + mB^{\phi}_{MX} + m^2C^{\phi}_{MX}$$

where

$$f^{\phi} = -A_{\phi}[I^{1/2}/(1 + bI^{1/2})] \qquad \text{(VI-6)}$$

and

$$B^{\phi}_{MX} = \beta^{(0)}_{MX} + \beta^{(1)}_{MX} e^{-\alpha_1 I^{1/2}} + \beta^{(2)}_{MX} e^{-\alpha_2 I^{1/2}} \qquad \text{(VI-7)}$$

Here, I is the ionic strength, $1/2\Sigma m z_i^2$ and MX is the general salt formed from the M ions. Definition of terms and a more detailed discussion of these equations are given in reference [74PIT/MAY]; parameters for these equations are given in the appropriate tables (section IV).

For the uni-univalent compounds, and the unsymmetrical charge-types, uni-bi and bi-univalent compounds, the activity and osmotic coefficients have been calculated from the Hamer-Wu, Lietzke-Stoughton equations used in previous evaluations [77STA/NUT].

The equation for the osmotic coefficient is:

$$\begin{aligned} \emptyset = 1 + \{ &|z_+ z_-| A_m[-(1+B\ I^{1/2}) + 2\ln(1+B\ I^{1/2}) \\ &+ 1/(1 + B\ I^{1/2}] + 1/2Cm + 2/3Dm^2 + 3/4Em^3 + \ldots \} \end{aligned} \qquad \text{(VI-8)}$$

and the activity coefficient:

$$\ln\gamma_{\pm} = \frac{-|z_+ z_-| A I^{1/2}}{1 + B\ I^{1/2}} + Cm + Dm^{3/2} + Em^2 + \ldots . \qquad \text{(VI-9)}$$

The parameters for these equations are tabulated in the appropriate tables in section IV. Activity coefficients for these charge-types may also be calculated from the Pitzer equations for the uni-univalent and uni-bi and bi-univalent salts. In these cases, the Pitzer equations are sometimes applicable to a more limited concentration range. Each table references the sources of data.

<u>Caution</u> should be exercised in the use of these equations because the equations are only valid over a specific concentration range. The valid ranges of concentrations are summarized in Table VI-1.

Table VI-1.

Limitations on the Use of Activity and Osmotic Coefficient Equations at 298 K.

Compound	Valid Concentration Range mol/kg H_2O
H_2SO_4	0.001-28.0
$MnSO_4$	0.1-4.0
$MgSO_4$	0.006-3.0
$CaSO_4$	0.004-0.0011
Na_2SO_3	0-2.0
Na_2SO_4	0-4.5
KOH	0-20.0
K_2SO_4	0-0.7

VI-2. The Relative Apparent Molar Enthalpy, ϕ_L

All values for $\Delta_f H$ as a function of concentration are obtained from the tabulations in [81NBS]. ϕ_L is retrieved from the relationship:

$$\phi_L = \Delta_f H(MX(n\ H_2O)) - \Delta_f H^\circ(MX(a))$$

where $\Delta_f H^\circ$ is the enthalpy of formation in the standard state. See section I-2.4 for conventions used in defining $\Delta_f H^\circ$ for electrolytes.

Normally, for simple salts and acids, ϕ_L is the negative of the enthalpy of dilution to infinite dilution. However, for salts such as $NaHSO_4$, having an ion that can itself ionize, ϕ_L differs from the enthalpy of dilution to infinite dilution by ΔH for the ionization of the acid anion.

Specific sources for ϕ_L for some systems follows.

$\underline{FeSO_4}$

The dilution values have been obtained from the various solution reactions involving Fe^{+2} aqueous solutions with SO_4^{-2} aqueous solutions measured by [83THO] and [1873BER].

$\underline{MgSO_4}$

As indicated under the section for the solution process for $MgSO_4 \cdot nH_2O(c)$ [51KAG/MIS] and [30PER] determined the ΔH (soln) of $MgSO_4 \cdot 7H_2O(c)$ as a function of concentration. These measurements were converted to ΔH's (diln) and merged with the measured ΔH's (diln) of [28LAN], [31LAN/STR], [32PLA], [27LAN/MES], [27LAN/MES], and [83THO] to obtain a smooth curve for ϕ_L. The extrapolation to infinite dilution was made to follow as closely as possible the limiting Debye-Huckel slope. The ΔH measurements of [83THO] on the ΔH (mix) of aqueous solutions of $MgCl_2$ or $Mg(NO_3)_2$ with coefficients have been calculated from [74PIT/MAY] and at $m = 3.167$ mol/kg H_2O, $\gamma_\pm$ is 0.0569 which differs slightly from the value cited in section V from [81NBS], (0.0517). Similarly, the activity of water differs, 0.964 compared with 0.974 in section V taken from TN 270-6 [81NBS]. These differences will be resolved.

The enthalpies of dilution were obtained from the measurements of [30LAN/MON] and [31LAN/STR]. The activity coefficients have been calculated from [74PIT/MAY]. The activities at saturation, 0.01518 mol/kg H_2O, agree well (0.331) when compared to 0.338 cited in section V-4 from [81NBS].

Na_2SO_3 and Na_2SO_4

The dilution heats for Na_2SO_3 are based on the neutralization measurements of [83THO] and [31RAM/HAN] with NaOH(aq).

The ϕ_L values for Na_2SO_4 are based on the measurements of [77SOL/VLA], [74THO/SMI], [41WAL/ROB], and [58BRO/GIA].

The activities calculated from [81GOL] agree well with those used in [81NBS] for saturated solutions of Na_2SO_3 and Na_2SO_4.

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11. ABSTRACT *(A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)*

Tables are presented here of values of thermochemical properties and processes at 298.15 K for substances of interest to DOE for flue gas desulfurization.

The substances covered are (1) the aqueous ions: OH^-; SO_3^{-2}, HSO_3^-, SO_4^{-4}, HSO_4^-, CO_3^{-2}, HCO_3^-, H^+, Mn^{+2}, Fe^{+2}, Mg^{+2}, Ca^{+2}, Na^+, and K^+, and (2) solid, liquid, aqueous, and gaseous compounds or species formed from these ions.

The tables contain the following:

1. The thermochemical property values, enthalpy of formation, $\Delta_f H°$, Gibbs energy of formation, $\Delta_f G°$, entropy, $S°$, and heat capacity, $C_p°$ all at 298.15 K, as well as the enthalpy difference between 298.15 K and 0 K, $H°-H_0°$, for the basic species cited above.
2. The predicted values for $\Delta H°$, $\Delta G°$, $\Delta S°$, and $\Delta C_p°$ as well as log K (equilibrium constant) for the processes, or reactions, of importance to DOE, calculated from (1).
3. The property values, ϕ_L, the relative apparent molar enthalpy, $\gamma_\pm$, from the mean ionic activity coefficient, and ϕ, the osmotic coefficient, for binary aqueous systems at 298.15 K, all as a function of concentration.

Some documentation for (2) and (3) is provided. All of the values given are consistent with the NBS TN 270 Series.

12. KEY WORDS *(Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)*

Activity coefficients; binary aqueous systems; enthalpy; enthalpies of dilution; entropy; flue gas desulfurization; Gibbs energy, osmotic coefficients; thermochemical tables; H^+; OH^-; S ions; CO_3^{-2} and HCO_3^-; Mn^{-2}; Fe^{+2}; Mg^{+2}; Ca^{+2}; Na^+; K^+

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