Cyanide and Antimony Thermodynamic Database for the Aqueous Species and Solids for the EPA-MINTEQ Geochemical Code

G. A. Sehmel

May 1989

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**Pacific Northwest Laboratory
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SUMMARY

Thermodynamic data for aqueous species and solids that contain cyanide and antimony were tabulated from several commonly accepted, published sources of thermodynamic data and recent journal articles. The review does not include gases or organic complexes of either antimony or cyanide, nor does the review include the sulfur compounds of cyanide. The basic thermodynamic data, ΔG_f^0 , ΔH_f^0 , and S_f^0 values, were chosen to represent each solid phase and aqueous species for which data were available in the appropriate standard state. From these data the equilibrium constants ($\log K_{r,298}^0$) and enthalpies of reaction ($\Delta H_{r,298}^0$) at 298 K (25°C) were calculated for reactions involving the formation of these aqueous species and solids from the basic components.

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LIST OF SYMBOLS, CONSTANTS, AND CONVERSION FACTORS

(a)	Descriptor for amorphous solid - Amorphous is defined as amorphous-like with minimal x-ray diffraction pattern
(aj)	Aqueous uncharged species
(am)	Descriptor for amorphous solid that gives no x-ray diffraction pattern - Most references do not differentiate between "a" and "am"
(cr)	Descriptor for a crystalline solid
cal	Thermochemical calorie, unit of energy, where 1 cal = 4.1840 joules absolute
e ⁻	Electron
F	Faraday constant, 23,061 cal/V•mol
(g)	Gaseous state
$\Delta G_{f,298}^{\circ}$	Gibbs free energy of formation at temperature 298.15K from the elements
$\Delta G_{r,298}^{\circ}$	Change in Gibbs free energy of formation for that specified reaction at temperature 298.15K
$\Delta H_{f,298}^{\circ}$	Heat or enthalpy of formation at temperature 298.15K from the elements
$\Delta H_{r,298}^{\circ}$	Change in heat of formation for that specified reaction at temperature 298.15K
γ_i	Activity coefficient of species i
I	Ionic strength
K	Temperature in degrees kelvin
$K_{r,T}^{\circ}$	Equilibrium "activity" constant for that specified reaction at temperature T
l	Liquid state
M	Molarity, moles of solute per liter of solution
R	Gas constant, 1.9872 cal/mol•K
(s)	Descriptor for compounds in the solid state

T	Temperature in degrees kelvin, unless otherwise noted as degrees Celsius
V	Volt
Z	Valence
298	Signifies 298.15K
⁰	Superscript indicating that the substance is in its standard state at 1 atmosphere pressure (1 atm = 1.013 bars = 1.013 x 10 ⁵ pascals)
{ }	Parentheses around an aqueous species indicate activities
[]	Brackets around an aqueous constituent indicate concentrations

INTRODUCTION

The U.S. Environmental Protection Agency's (EPA) development of proposed regulations for land disposal of solid wastes requires an understanding of the aqueous speciation, solubility constraints, and mobility of cyanide and antimony in ground-water environments. The EPA has selected the MINTEQ geochemical computer code as one of its important tools to assess the behavior of trace metals in natural waters. The MINTEQ geochemical computer code was developed for the EPA by Felmy, Girvin, and Jenne (1984) at the Pacific Northwest Laboratory.^(a) However, the MINTEQ thermodynamic database described by Felmy, Girvin, and Jenne (1984) and Felmy et al. (1984) does not contain thermodynamic data for cyanide and antimony, two elements of interest in land disposal of solid wastes.

To better predict the environmental behavior of antimony and cyanide, a review of the available thermodynamic data for these elements was completed. The scope of the literature review was limited to compilation and evaluation of thermodynamic data to the inorganic compounds of these two elements. This limitation in scope was necessary because the complexation of metals and metalloids with natural organic compounds is poorly understood and representative thermodynamic data are rarely available.

The objective of this review was to select chemical reactions and associated thermodynamic data that should be included in the MINTEQ equilibrium geochemical model database to represent the formation of antimony and cyanide aqueous species and solid phases. This report documents that data compilation and review.

In developing this database, we used the database reported in Deutsch and Krupka^(b) in their review of aqueous species, gases, and solids containing chromium, mercury, selenium, and thallium for EPA. We also exploited the

-
- (a) Operated for the U.S. Department of Energy by Battelle Memorial Institute under Contract DE-AC06-76RLO 1830.
 - (b) Deutsch, W. J., and K. M. Krupka. 1985. MINTEQ Geochemical Code: Compilation of Thermodynamic Database for the Aqueous Species, Gasses, and Solids Containing Chromium, Mercury, Selenium, and Thallium. Draft report submitted to the Environmental Protection Agency, Athens, Georgia. Unpublished. Cited in tables as code 85DK.

database for antimony compiled by Peterson et al. (1987) from Wagman et al. (1982).

In the next section, the methods used in data compilation, calculation and selection are described. The results of the reviews for cyanide and antimony are presented in separate chapters. In the final section, the conclusions of this study are briefly presented.

METHODS OF DATA COMPILATION, CALCULATION, AND SELECTION

The approach taken was to first compile all the available literature describing the thermodynamic data for cyanide and antimony compounds. This effort included tabulating any values presented in thermodynamic data compilations and collecting, if possible, the original articles describing the experimental methods. When necessary, the thermodynamic data were converted to $I = 0$ and temperature of 25°C (see below for a discussion of the recalculation methods) to be consistent with the existing MINTEQ thermodynamic database. Reactions and their associated thermodynamic constants were reformulated in terms of the basis species used by MINTEQ so that they could be evaluated for inclusion in the MINTEQ database. Based on this review, choices are made of the seemingly "best" values based on the sources of the thermodynamic values and the range in reported values. Finally, the chosen data are evaluated for a minimum acceptable level of internal consistency.

DATA COMPILATION

This review is based on a compilation of the available thermodynamic data from the published literature. To locate this literature a computerized search of Chemical Abstracts was completed for the years 1977 to 1987 for sources of thermodynamic data for antimony and cyanide. This time frame was selected to include the year 1982, during which the last National Bureau of Standards compilations of chemical thermodynamic properties were published (Wagman et al. 1982). A computer search was also completed for the March-October 1987 Citation Index.

All the data summarized during this study are listed in Appendices B and C for cyanide and antimony, respectively. It is anticipated that these complete summaries may be useful in the future for upgrading the database as additional thermodynamic data become available.

The sources of the selected thermodynamic data are identified in each table of this report by a reference code identical to that utilized by Smith and Martell (1976, p. xiii). The reference code lists 1) the last two digits of the year when the reference was published, 2) the first letter of the surnames of each of the first two authors listed for the reference, and 3) a

lower-case letter if duplication could exist between two or more reference codes. The reference codes and complete reference citations are listed together in the reference section at the end of this report.

Prime sources of thermodynamic data included in this review were published compilations of thermodynamic data, such as the U.S. National Bureau of Standards (NBS) publication (Wagman et al. 1982), Robie, Hemingway, and Fisher (1978), Smith and Martell (1976), and Naumov, Ryzhenko, and Khodakovsky (1974). In addition, data from recent journal articles are also included.

METHODS OF CALCULATION

To facilitate the comparison of thermodynamic data all the available data must be expressed in the same basic thermodynamic units. For this review, the comparison was made between the basic thermodynamic data values, $\Delta G_{f,298}^{\circ}$, $\Delta H_{f,298}^{\circ}$ and S_{298}° in kilocalories. Any thermodynamic data that was reported in other ways had to be recalculated to these terms and units. The final data must also be expressed in terms of the same standard state as defined by the ionic strength of the media and the reference state of temperature and atmospheric pressure used for the MINTEQ database. The calculation methods are explained below.

Much of the reported thermodynamic data is given as stability constants, $\log K_r^{\circ}$ values (the subscript r refers to reaction and the superscript o refers to standard state), and the enthalpy of reaction, $\Delta H_{r,298}^{\circ}$ values, as the thermodynamic data to characterize each chemical reaction. All aqueous- and solid-phase reactions are written as formation reactions in terms of designated basis species (Morel 1983), a minimum set of chemical species chosen to represent each chemical constituent in the water (Felmy, Girvin, and Jenne 1984). For example, the formation equilibrium for HCN° , in terms of designated basis species for the MINTEQ database, is written

The designated basis species representing a certain element or oxidation state of an element is generally, although not always, selected to be the

dominant species at approximately pH 7 and natural environmental conditions. However, the equilibrium constants, $\log K_r^0$, reported in the literature are often determined for different reactions and, therefore, must be reformulated in terms of the designated components to permit comparison and to permit inclusion in the MINTEQ thermodynamic database. The method for reformulating the equilibrium constants and recalculating the thermodynamic data consists of combining equilibria and adding or subtracting the appropriate equilibrium $\log K_r^0$ values and $\Delta H_{r,298}^0$ values. For example, for reformulating the equilibrium

with a $\log K_r^0$ of 12.8 in terms of Sb(OH)_3^0 , and H^+ , the equilibrium

with a $\log K_r^0$ value of -14.00 is used. Addition of the two equilibria and the appropriate stability constants results in the reformulated equilibrium

with a $\log K_r^0$ value of -1.2. Recalculation of $\Delta H_{r,298}^0$ values is accomplished in a similar manner. Further examples of the reformulation method and recalculation of stability constants, $\log K_r^0$ values, and the enthalpy of reaction can be found in Snoeyink and Jenkins (1980), Stumm and Morgan (1981), and Morel (1983).

In addition to recalculation of the equilibrium constants and enthalpy of reaction in terms of designated components, the thermodynamic data must be recalculated to be in terms of the designated standard and reference states. Equilibrium constants are typically expressed in terms of the concentration of the reactants and products at the stated ionic strength. Only in infinitely dilute solutions are the concentrations and activities equal. The designated standard state of the MINTEQ database is $I = 0$.

Knowing the value of the activity coefficient permits conversion from concentration to activities. Knowing the activity coefficient also permits recalculation of the equilibrium constants to $I = 0$ or recalculation in terms of the activities instead of the concentrations of the reactants and products. Although several methods have been proposed for calculating the activity coefficients (Lindsay 1979), one of the most widely used methods is the Davies equation

$$\log \gamma_i = -AZ_i^2 \left[\frac{\sqrt{I}}{1 + \sqrt{I}} - 0.3I \right] \quad (5)$$

where $A = 0.509$ for water at 25°C ; Z is the valence of the ion, i ; I is the ionic strength; and γ_i is the activity coefficient of the i th species. The conversion from the $\log K_r$ at a given ionic strength to $\log K_r^0$ at $I = 0$ is computed by

$$K_r^0(I = 0) = K_r(I = n) \cdot \pi\gamma(\text{products})/\pi\gamma(\text{reactants}) \quad (6)$$

where $\gamma(\text{products})$ is the multiplicative product of the γ values for each of the product components in the equilibria. The activity coefficients calculated using the Davies equation deviate progressively further from the actual activity coefficient as the ionic strength increases above $I = 0.1\text{M}$. At high ionic strengths (i.e., $I \geq 1\text{M}$), the deviation can result in considerable error in the equilibrium constant recalculated to $I = 0$. The amount of error depends on the form of the reaction, whether the species represents a major or minor portion of the element and the actual ionic strength. For further discussion see Linder and Murray (1982), and Sun, Harris, and Magnuson (1980). Although the extrapolation may become increasingly less accurate above ionic strengths of 0.1M , the Davies equation is used in this report to calculate the $\log K_r^0$ from values at the higher ionic strengths. Other methods that would be applicable at the higher ionic strengths require additional parameterization data which is not available for most chemical species.

In some cases, the equilibrium constant is reported for a temperature other than 25°C , the standard state used in the MINTEQ code. Because the

equilibrium constant is dependent on temperature, it should be converted from the reported temperature to the standard state temperature. This recalculation uses the van't Hoff equation, which is

$$\ln K_{T_2} = \ln K_{25} + \Delta H_{r,298}^{\circ} / R (1/298.15 - 1/T_2) \quad (7)$$

where K_{25} and K_{T_2} are the equilibrium constants at 25°C and the new temperature, T_2 , respectively, and R is the gas constant. This equation also includes the enthalpy of the reaction, $\Delta H_{r,298}^{\circ}$, which is assumed to be independent of temperature. If no $\Delta H_{r,298}^{\circ}$ value is reported in the available thermodynamic data, then the $\log K_r^{\circ}$ value is assumed to be independent of temperature.

Once the $\log K_r^{\circ}$ and $\Delta H_{r,298}^{\circ}$ values have been calculated for the formation of the desired aqueous species or solid phase in terms of the basis species and the standard state, these values can be used to calculate the basic thermodynamic data, $\Delta G_{f,298}^{\circ}$, $\Delta H_{f,298}^{\circ}$, and S_{298}° , for the aqueous complexes and solid phases of antimony and cyanide.

The standard state free energies of formation, $\Delta G_{f,298}^{\circ}$, for the aqueous complexes and solid phases can be calculated from the $\log K_r^{\circ}$ values, from electropotential data, or from the standard state enthalpy and entropy of formation. Equilibrium constant data are used to compute the $\Delta G_{r,298}^{\circ}$ value according to the equation:

$$\Delta G_{r,298}^{\circ} = -2.303RT \log K_r^{\circ} \quad (8)$$

where R is the gas constant (0.001987 kcal T/Mol) and T is 298.15K. Using the $\Delta G_{r,298}^{\circ}$ value, the free energy of formation of the desired species or solid phase can be calculated using the following relationship and the equilibrium reaction:

$$\Delta G_{r,298}^{\circ} = \sum \Delta G_{f,298}^{\circ} (\text{products}) - \sum \Delta G_{f,298}^{\circ} (\text{reactants}) \quad (9)$$

To compute the $\Delta G_{f,298}^{\circ}$ for a complex using this equation, the $\Delta G_{f,298}^{\circ}$ must be known for all products and reactants in the reaction except the one of

interest. If electropotential data are available, the $\Delta G_{r,298}^0$ value can also be calculated from the relationship

$$\Delta G_{r,298}^0 = -nFE^0 \quad (10)$$

where n is the number of electrons involved in the reaction, F is the Faraday constant (23.061 kcal volt/equivalent), and E^0 is the standard cell potential.

The standard enthalpy of reaction, $\Delta H_{r,298}^0$, and the standard entropy of reaction, $S_{r,298}^0$, can be computed from the free energy of reaction using the following relationship:

$$\Delta G_{r,298}^0 = \Delta H_{r,298}^0 - T\Delta S_{298}^0 \quad (11)$$

where T is 298.15K. The standard enthalpy, $\Delta H_{f,298}^0$, and the entropy, S_{298}^0 , of formation for the species of interest can be calculated from the $\Delta H_{r,298}^0$ and S_{298}^0 values using the following relationships:

$$\Delta H_{r,298}^0 = \sum \Delta H_{f,298}^0 \text{ (products)} - \sum \Delta H_{f,298}^0 \text{ (reactants)} \quad (12)$$

$$\Delta S_{298}^0 = \sum S_{298}^0 \text{ (products)} - \sum S_{298}^0 \text{ (reactants)}. \quad (13)$$

As can be seen, to compute the $\Delta G_{f,298}^0$, $\Delta H_{f,298}^0$, and ΔS_{298}^0 values for the cyanide and antimony species, $\Delta G_{f,298}^0$, $\Delta H_{f,298}^0$, and S_{298}^0 values must be accepted for the other reactants. The accepted values for these reactants and the basis or parent Sb and CN species are given in Table 1. These accepted values come primarily from Wagman et al. (1968) and CODATA (1972, 1975, 1976, 1977, 1978).

DATA SELECTION

After all the compiled data have been recalculated to the basic thermodynamic quantities, $\Delta G_{f,298}^0$, $\Delta H_{f,298}^0$ and S_{298}^0 , the data can be compared and specific values chosen to represent the complexes and to formulate the appropriate reactions and associated thermodynamic quantities for inclusion

TABLE 1. Thermodynamic Data Selected for Basis Species
in the MINTEQ Geochemical Code

Formula	Identification Number	$\Delta G_{f,298}^0$ (a) (-----kcal/mol-----)	$\Delta H_{f,298}^0$ (cal/mol)	S_{298}^0 (cal/mol)	Reference Code (b)
Ag ⁺	020	18.422	25.275	17.538	76C
Al ³⁺	030	-116.900	-126.910	-73.610	78RH
H ₃ AsO ₃ ⁰	060	-152.940	-177.400	46.600	68WE
H ₃ AsO ₄ ⁰	061	-183.100	-215.700	44.000	68WE
H ₃ BO ₃ ⁰	090	-231.560	-256.290	38.800	68WE
Ba ²⁺	100	-134.020	-128.500	2.300	71PW
Br ⁻	130	-24.867	-29.039	19.800	76C
CN ⁻	143(c)	41.2	36.0	22.5	68WE
OCN ⁻	144(c)	-23.3	-34.9	25.5	68WE
Ca ²⁺	150	-132.299	-129.740	-12.690	71PW
Cd ²⁺	160	-18.542	-18.140	-17.500	68WE
Cl ⁻	180	-31.379	-39.933	13.560	76C
ClO ₄ ⁻	181	-2.060	-30.910	43.500	68WE
CO ₃ ²⁻	140	-126.170	-161.840	-13.600	68WE
Cr ²⁺	210	-43.990	-34.300	6.970	84S
CrO ₄ ²⁻	212	-174.810	-210.930	13.780	84S
Cr(OH) ₂ ⁺	211	-153.350	-177.290	-10.030	84S
Cs ⁺	220	-69.722	-61.673	31.750	78RH
Cu ⁺	230	12.000	17.200	9.760	86C
Cu ²⁺	231	15.720	15.700	-23.200	86C
e ⁻	001	0.000	0.000	15.604	76C

TABLE 1. (contd)

Formula	Identification Number	$\Delta G_{f,298}^0$ (-----kcal/mol-----)	$\Delta H_{f,298}^0$ (-----kcal/mol-----)	S_{298}^0 (cal/mol)	Reference Code
F ⁻	270	-67.340	-80.151	-3.150	76C
Fe ²⁺	280	-18.850	-21.300	-32.900	69WE
Fe ³⁺	281	-1.100	-11.600	-75.500	69WE
H ⁺	330	0.000	0.000	0.000	Definition
OH ⁻		-37.605	-54.977	-2.560	76C
H ₂ O	002	-56.690	-68.315	16.718	76C
Hg ₂ ²⁺	360	36.713	39.870	15.660	78C
Hg(OH) ₂ ⁰	361	-65.700	-84.900	34.000	69WE
I ⁻	380	-12.412	-13.599	25.500	76C
K ⁺	410	-67.510	-60.270	24.149	76C
Li ⁺	440	-70.103	-66.561	3.210	81WE
Mg ²⁺	460	-108.700	-111.580	-33.000	71PW
Mn ²⁺	470	-54.500	-52.760	-17.600	69WE
Mn ³⁺	471	-19.600	-27.000	-63.980	76PJ, 52L
MoO ₄ ²⁻	480	-199.900	-238.500	6.500	69WE
Na ⁺	500	-62.590	-57.430	13.960	76C
NH ₄ ⁺	490	-18.991	-31.850	26.570	76C
Ni ²⁺	540	-10.900	-12.900	-30.800	69WE
NO ₂ ⁻	491	-8.900	-25.000	33.500	68WE
NO ₃ ⁻	492	-26.610	-49.560	35.000	68WE
Pb ²⁺	600	-5.830	-0.400	2.500	68WE

TABLE 1. (contd)

Formula	Identification Number	$\Delta G_{f,298}^0$ (-----kcal/mol-----)	$\Delta H_{f,298}^0$ (-----kcal/mol-----)	S_{298}^0 (cal/mol)	Reference Code
PO_4^{3-}	580	-243.500	-305.300	-53.000	68WE
Rb^+	680	-67.784	-60.019	28.791	76C
HS^-	730	2.880	-4.200	15.000	68WE
$S(s)$	731	0.000	0.000	7.600	68WE
$S_2O_3^{2-}$	735	-122.800	-155.900	8.900	74NR
SO_3^{2-}	733	-116.300	-152.400	-8.760	68WE,72CS
SO_4^{2-}	732	-177.970	-217.320	4.800	68WE
$Sb(OH)_3^0$	740(c)	-154.7	-184.9	30.0	74NR
$Sb(OH)_6^-$	741(c)	-288.76	NA(d)	NA(d)	Calculated in Appen- dix D
HSe^-	760	10.500	3.800	19.000	68WE
$HSeO_3^-$	761	-98.360	-122.980	32.300	68WE
SeO_4^{2-}	762	-105.500	-143.200	12.900	68WE
$H_4SiO_4^0$	770	-312.604	-348.948	43.021	78RH
Sr^{2+}	800	-133.481	-130.450	-8.54(e)	71PW
Tl^+	870	-7.740	1.280	30.000	68WE
$Tl(OH)_3^0$	871	-112.300	NA	NA	74NR
U^{3+}	890	-114.900	-116.900	-41.800	76F0,78L
U^{4+}	891	-126.900	-141.300	-98.71(f)	76F0,78L
UO_2^+	892	-231.500	-246.800	-6.000	78L
UO_2^{2+}	893	-227.700	-243.500	-23.200	78L

TABLE 1. (contd)

Formula	Identification Number	$\Delta G_{f,298}^0$ (-----kcal/mol-----)	$\Delta H_{f,298}^0$	S_{298}^0 (cal/mol)	Reference Code
V^{2+}	900	-52.000	-54.000	-31.000	71HM
V^{3+}	901	-57.770	-62.900	-57.100	74NR
VO^{2+}	902	-106.700	-116.300	-32.000	68WE
VO_2^+	903	-140.300	-155.300	-10.100	71WE
Zn^{2+}	950	-35.196	-36.661	-26.190	76C

- (a) Tabulated values were current as of September, 1985.
- (b) The reference code lists in order 1) the last two digits of the year when the reference was published and 2) the first letter of the surnames of the first two authors listed for the reference. See reference list for full citations.
- (c) Basis species added as part of the study described in this report.
- (d) Values indicated by "NA" are not available in the literature.
- (e) S_{298}^0 for Sr^{2+} modified to -8.54 kcal/mol/K from that reported by Deutsch and Krupka (1985) of -7.8 kcal/mol in order to have the self-consistency error to be less than 50 cal.
- (f) S_{298}^0 for U^{4+} modified to -98.71 kcal/mol/K from that reported by Deutsch and Krupka (1985) of -99.0 kcal/mol in order to have the self-consistency error to be less than 50 cal.

in the MINTEQ database. When more than one value has been reported or can be calculated for a complex or solid phase, specific criteria such as the following are used to select among the alternative values:

- the correct reference and standard state for consistency with the existing MINTEQ database
- similarity consistency in the thermodynamic data reported by several researchers using different experimental methods
- data reported at the standard state and not requiring activity or temperature corrections
- data reported in a reputable compilation.

Similarity in the thermodynamic data reported by different researchers for the same reaction is an important criterion. Such similarity suggests that a representative value for the reaction can be determined and allows the user more confidence in the accuracy of the value. However, similarity among the compilations could represent merely an acceptance or reporting of the same data rather than a consensus on the "true" value since much of the review relied on the use of existing thermodynamic compilations.

Often, only one researcher or compilation has reported thermodynamic data for a specific reaction, aqueous complex, or solid phase. In this case, the data were included in the final selection although their reliability was not determined. In the same way, thermodynamic data corrected from high ionic strength to $I = 0$ are also provisionally accepted, with the recognition that errors could arise from the recalculation. Despite the possible errors, these data (single-source data and/or data corrected to $I = 0$) are included in the thermodynamic data to alert the user to the potential presence of the complex or solid phase, with the provision that the thermodynamic data are only approximate. As more data become available, these provisionally accepted data can be evaluated and revised.

In many cases, data for compounds containing cyanide or antimony were not included in the MINTEQ database for the following reasons:

- one or more constituent elements were not in the MINTEQ database
- contained aqueous complexes not in the MINTEQ database

- $\Delta G_{f,298}^{\circ}$ was not available, hence equilibrium constants could not be included in the MINTEQ database.

Reasons for accepting values were as follows:

- In lieu of reasons for contrary selection, the data in NBS documentation were selected (Wagman et al. 1982)
- Energy units were either kilocalories or kilojoules in the respective units of $\Delta G_{f,298}^{\circ}$, $\Delta H_{f,298}^{\circ}$ and S_{298}° . The nomenclature selected to describe these units in the Appendices is "*C" to represent data reported in units of kilocalories. Similarly, "*J" is used to represent data reported in units of kilojoules. The nomenclature "!C" represents data in units of kilocalories calculated from the "*J" data; i.e., !C = *J/4.184
- The data were selected when they were the only data reviewed in this study.
- The database summarized includes any errata revision from earlier National Bureau of Standards publications.

The final step in the data compilation was to assign identification numbers to each aqueous specie and solid phase for which thermodynamic data have been selected. The method used to assign these identification codes is described in Appendix A and is consistent with the procedure currently used to assign identification codes in the MINTEQ thermodynamic database.

DATA CONSISTENCY

An important concern in the development of a thermodynamic database is maintaining internal consistency in the thermodynamic values $\Delta G_{f,298}^{\circ}$, $\Delta H_{f,298}^{\circ}$, and S_{298}° . The data selected should be self-consistent for all aqueous species and solids selected. Also, the data selected should be consistent with prior usage in MINTEQ. If a database is established without ensuring internal consistency in the thermodynamic data, errors that are significant, difficult to quantify, and transparent to the user can occur in the speciation and solubility calculations.

The issue of internal consistency can be addressed in several areas of database development. To ensure optimal internal data consistency, the thermodynamic data should be derived from experimental measurements using the same ancillary data used in the previous thermodynamic database development. Except in the case where an investigator is completing an in-depth, critical review of thermodynamic data for aqueous species and solids containing a particular element, implementation of this particular aspect of internal consistency may be difficult to ensure. To ensure some minimal level of data consistency, we relied primarily on data that were from consistent thermodynamic data sources. The databases from the WATEQ codes (thus, also the MINTEQ code) are derived primarily from sources compatible with NBS publications (Parker, Wagman, and Evans 1971; Wagman et al. 1968, 1969, 1981, 1982) and data compilations from the Committee on Data for Science and Technology (CODATA) of The International Council of Scientific Unions (ICSU) (CODATA Task Group 1972, 1975, 1976, 1977, 1978) and the U.S. Geological Survey (Robie and Waldbaum 1968(a); Robie, Hemingway, and Fisher 1978). When reasons for choosing alternative values are not compelling, our primary selection of data from these references helps to maintain a minimum acceptable level of consistency in the MINTEQ database.

Secondly, the set of $\Delta G_{f,298}^0$, $\Delta H_{f,298}^0$, and S_{298}^0 values accepted for an aqueous species or solid should be internally consistent. This internal consistency check consists of ensuring that the selected $\Delta G_{f,298}^0$ values agree, within the accuracy of the cited data, with those $\Delta G_{f,298}^0$ values calculated from the selected values of $\Delta H_{f,298}^0$ and S_{298}^0 for each species or solid of interest and its constituent elements. Values of $\Delta G_{f,298}^0$ are calculated from $\Delta H_{f,298}^0$ and S_{298}^0 data using the following equation:

$$\Delta G_{f,298}^0 = \Delta H_{f,298}^0 - 298.15 \Delta S_{298}^0. \quad (14)$$

This equation can be expanded by using the definitions of $\Delta H_{f,298}^0$ and ΔS_{298}^0 to obtain the following expression,

-
- (a) Note that the data in Robie, Hemingway, and Fisher (1978) supersede the earlier tabulation of Robie and Waldbaum (1968).

$$\Delta G_{f,298,i}^0 = \Delta H_{f,298,i}^0 - \sum_i \Delta H_{f,298}^0 (\text{elements}) - 298.15 [\Delta S_{298,i}^0 - \sum_i \Delta S_{298}^0 (\text{elements})] \quad (15)$$

where subscript i refers to each aqueous species or solid of interest. Because $\Delta H_{f,298}^0$ for an element in its standard reference state is equal to zero, this equation reduces to

$$\Delta G_{f,298,i}^0 = \Delta H_{f,298,i}^0 - 298.15 [\Delta S_{298,i}^0 - \sum_i \Delta S_{298}^0 (\text{elements})]. \quad (16)$$

Table 2 contains the accepted S_{298}^0 values for the elements in the MINTEQ thermodynamic database.

The equations given previously can also be used to check the internal consistency of the thermodynamic data when all three values of $\Delta G_{f,298}^0$, $\Delta H_{f,298}^0$, and S_{298}^0 are available for a particular aqueous species or solid. When the data required to apply this equation are available, the internal consistency of the $\Delta G_{f,298}^0$ values was determined. A version of the MCRT code (Wolery 1984) modified at the Pacific Northwest Laboratory was used to calculate $\log K_r^0$ and $\Delta H_{r,298}^0$, check for charge and mass balances in the reactions, and prepare the output files for addition to the MINTEQ database. The output of the code also indicates if there is any inconsistency between the selected $\Delta G_{f,298}^0$, $\Delta H_{f,298}^0$, and S_{298}^0 . When an inconsistency in the data is identified, the data was checked for the discordant value.

TABLE 2. Thermodynamic Data Accepted for the Elements for Use with MINTEQ Geochemical Code

Symbol	State(a)	Gram Formula Weight	S_{298}^0 (b) (cal/mol•K)	Reference Code
Ag	c	107.868	10.17	78C
Al	c	26.98154	6.776	78C
Ar	g	39.948	36.982	78C
As	c	74.9216	8.53	73HD
B	c	10.81	1.41	78C
Ba	c	137.33	14.918	73HD
Be	c	9.01218	2.27	78C
Br ₂	l	79.904	36.379	78C
C	c	12.011	1.372	78C
Ca	c	40.08	9.94	78C
Cd	c	112.41	12.38	78C
Ce	c	140.12	16.6	73HD
Cl ₂	g	35.453	53.290	78C
Co	c	58.9332	7.18	73HD
Cr	c	51.996	5.65	73HD
Cs	c	132.9054	20.37	78C
Cu	c	63.546	7.923	78C
Dy	c	162.50	17.90	73HD
e ⁻		0.0000	15.6035	By Definition
Er	c	167.26	17.49	73HD
Eu	c	151.96	19.31	73HD
F ₂	g	18.9984	48.443	78C

(a) The symbols c, g, and l refer to a crystalline, gaseous, or liquid state, respectively, for that element.

(b) Tabulated values are current as of September 1985 (Deutsch and Krupka 1985).

TABLE 2. (contd)

<u>Symbol</u>	<u>State</u>	<u>Gram Formula Weight</u>	<u>S_{298}^0 (cal/mol•K)</u>	<u>Reference Code</u>
Fe	c	55.847	6.52	73HD
Ga	c	69.72	9.758	73HD
Gd	c	157.25	16.24	73HD
Ge	c	72.59	7.431	78C
H ₂	g	1.0079	31.207	78C
He	g	4.0026	30.124	78C
Hf	c	178.49	10.41	73HD
Hg	l	200.59	18.14	78C
Ho	c	164.9304	17.93	73HD
I ₂	c	126.9045	27.758	78C
In	c	114.82	13.820	73HD
Ir	c	192.22	8.486	73HD
K	c	39.0983	15.46	78C
Kr	g	83.80	39.190	78C
La	c	138.9055	13.6	73HD
Li	c	6.941	6.96	78C
Lu	c	174.97	12.18	73HD
Mg	c	24.305	7.811	78C
Mn	c	54.9380	7.65	73HD
Mo	c	95.94	6.85	73HD
N ₂	g	14.0067	45.770	78C
Na	c	22.98977	12.26	78C
Nb	c	92.9064	8.70	73HD
Nd	c	144.24	16.99	73HD
Ne	g	20.179	34.946	78C
Ni	c	58.70	7.14	73HD
O ₂	g	15.9994	49.005	78C
Os	c	190.2	7.80	73HD
P (white)	c	30.97376	9.821	78C

TABLE 2. (contd)

<u>Symbol</u>	<u>State</u>	<u>Gram Formula Weight</u>	<u>S_{298}^0 (cal/mol•K)</u>	<u>Reference Code</u>
Pb	c	207.2	15.49	78C
Pd	c	106.4	9.08	73HD
Pr	c	140.9077	17.67	73HD
Pt	c	195.09	9.95	73HD
Ra	c	226.0254	17.	71PW
Rb	c	85.4678	18.35	78C
Re	c	186.207	8.730	73HD
Rh	c	102.9055	7.530	73HD
Ru	c	101.07	6.82	73HD
S(rhombic)	c	32.06	7.661	78C
Sb	c	121.75	10.88	73HD
Sc	c	44.9559	8.28	73HD
Se	c	78.96	10.10	78RH
Si	c	28.0855	4.496	78C
Sm	c	150.4	16.61	73HD
Sn(white)	c	118.69	12.23	78C
Sr	c	87.62	13.24	78RH
Ta	c	180.9479	9.92	73HD
Tb	c	158.9254	17.52	73HD
U	c	238.029	12.00	78C
V	c	50.9414	6.91	73HD
Zn	c	65.38	9.950	78C

THERMODYNAMIC DATA FOR
AQUEOUS SPECIES AND SOLIDS CONTAINING CYANIDE

The majority of the thermodynamic data tabulated for the aqueous species and solids containing cyanide were taken from the NBS compilation by Wagman et al. (1982), Robie, Hemingway, and Fisher (1978), Smith and Martell (1976) and recent journal articles including Capone et al. (1986), Aruga (1982) and Beck (1987). The article by Beck (1987) describes the results of the critical survey of the stability constants for formation of cyanide complexes conducted by the International Commission on Equilibrium Data of the International Union of Pure and Applied Chemistry and is a significant source of data. The complete summary of the basic thermodynamic data, $\Delta G_{f,298}^{\circ}$, $\Delta H_{f,298}^{\circ}$, and S_{298}° , for aqueous species and solids of cyanide that were compiled from the literature is shown in Appendix B. Data for the gaseous phase of cyanide and for thiocyanide were not included in the review.

The basis species for cyanide are CN^- for cyanide and OCN^- for cyanogen. These species were chosen as the basis species because they predominate in the intermediate pH range. The thermodynamic data chosen to represent these basis species are from Wagman et al. (1982).

Although most of the thermodynamic data was presented in their original citations as $\Delta G_{f,298}^{\circ}$, $\Delta H_{f,298}^{\circ}$ and S_{298}° values, data for 80 reactions involving aqueous species of cyanide with their associated $\log K_r^{\circ}$ and $\Delta H_{r,298}^{\circ}$ values were also reported. These data are given in Table 3. Most of these data were used with the thermodynamic data for the components to calculate the basic thermodynamic data for the cyanide complexes represented in the reactions. These data were also added to the Appendix B except that the data at $I = 3$, i.e., NiCN^+ , ZnCN^+ , HgOH° , $\text{NaFe}(\text{CN})_6^{2-}$, were not included because of potential errors in the ionic strength correction. These species are represented by thermodynamic data from other references (Appendix B).

Basic thermodynamic data are tabulated in Appendix B for 290 aqueous species of cyanide and cyanogen. Most of these data were eliminated from further consideration because the data were reported for a different standard state than that used in the MINTEQ data base. In addition, some of the

TABLE 3. Reported Log K_r and $\Delta H_{r,298}$ Values for Reactions of Aqueous Species of Cyanide and Cyanogen

Reaction	Temperature (°C)	Ionic Strength (M)	Log K_r	ΔH_r	Reference Code
<u>Cyanogen (OCN^-)</u>					
$\text{H}^+ + \text{OCN}^- \leftrightarrow \text{HOCN}^0$	25	0	3.48	-2.0	76SM 28
$\text{Co}^{2+} + 4(\text{OCN}^-) \leftrightarrow \text{Co}(\text{OCN})_4^{2-}$	27	1.5	2.67		76SM 28
$\text{Ag}^+ + 2(\text{OCN}^-) \leftrightarrow \text{Ag}(\text{OCN})_2^-$	30	0	5.00		76SM 28
<u>Cyanide (CN^-)</u>					
$\text{H}^+ + \text{CN}^- \leftrightarrow \text{HCN}^0$	25	0	9.21	-10.43	76SM 26
$\text{H}^+ + \text{CN}^- \leftrightarrow \text{HCN}^0$	25	0	9.21		87B
$\text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{Fe}(\text{CN})_6^{4-}$	25	0	35.4	-85.8	76SM 26
$\text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{Fe}(\text{CN})_6^{4-}$	25	0	36.9		87B
$\text{Co}^{2+} + 5\text{CN}^- \leftrightarrow \text{Co}(\text{CN})_5^{3-}$	25	0		-61.5	76SM 26
$\text{Co}^{2+} + (\text{CN})_5^{2-} + \text{H}^+ \leftrightarrow \text{CoH}(\text{CN})_5^{2-}$	25	0		-32.0	76SM 26
$\text{Ni}^{2+} + \text{CN}^- \leftrightarrow \text{NiCN}^+$	25	3.0	7.03		76SM 26
$\text{Ni}^{2+} + 4\text{CN}^- \leftrightarrow \text{Ni}(\text{CN})_4^{2-}$	25	0	30.22	-43.2	76SM 26

TABLE 3. (contd)

Reaction	Temperature (°C)	Ionic Strength (M)	Log K_r	ΔH_r	Reference Code
$\text{Ni}^{2+} + 2\text{CN}^- \leftrightarrow \text{Ni}(\text{CN})_2^0$	25	0.1	~13.95		87B
$\text{Ni}^{2+} + 3\text{CN}^- \leftrightarrow \text{Ni}(\text{CN})_3^-$	25	0.1	~22.00		87B
$\text{Ni}^{2+} + 4\text{CN}^- \leftrightarrow \text{Ni}(\text{CN})_4^{2-}$	25	0.1	30.5		87B
$\text{Ni}(\text{CN})_4^{2-} + \text{H}^+ \leftrightarrow \text{NiH}(\text{CN})_4^-$	25	0.1	5.4		76SM 26
$\text{NiH}(\text{CN})_4^- + \text{H}^+ \leftrightarrow \text{NiH}_2(\text{CN})_4^0$	25	0.1	4.5		76SM 26
$\text{NiH}_2(\text{CN})_4^0 + \text{H}^+ \leftrightarrow \text{NiH}_3(\text{CN})_4^+$	25	0.1	2.6		76SM 26
$\text{Fe}^{3+} + 6\text{CN}^- \leftrightarrow \text{Fe}(\text{CN})_6^{3-}$	25	0	43.6	-70.1	76SM 26
$\text{Fe}^{3+} + 6\text{CN}^- \leftrightarrow \text{Fe}(\text{CN})_6^{3-}$	25	0	43.9		87B
$\text{Cu}^+ + 2\text{CN}^- \leftrightarrow \text{Cu}(\text{CN})_2^-$	25	0	16.26	-29.1	76SM 26
$\text{Cu}^+ + 3\text{CN}^- \leftrightarrow \text{Cu}(\text{CN})_3^{2-}$	25	0	21.6	-40.2	76SM 26
$\text{Cu}^+ + 4\text{CN}^- \leftrightarrow \text{Cu}(\text{CN})_4^{3-}$	25	0	23.1	-51.4	76SM 26
$\text{Ag}^+ + 2\text{CN}^- \leftrightarrow \text{Ag}(\text{CN})_2^-$	25	0	20.48	-32.9	76SM 26
$\text{Ag}^+ + 3\text{CN}^- \leftrightarrow \text{Ag}(\text{CN})_3^{2-}$	25	0	21.4	-33.5	76SM 26
$\text{Ag}^+ + 4\text{CN}^- \leftrightarrow \text{Ag}(\text{CN})_4^{3-}$	25	1.0	20.8		76SM 26
$\text{Ag}^+ + \text{OH}^- + \text{CN}^- \leftrightarrow \text{AgOHCN}^-$	25	0	13.2		76SM 26

TABLE 3. (contd)

Reaction	Temperature (°C)	Ionic Strength (M)	Log K_r	ΔH_r	Reference Code
$\text{Zn}^{2+} + \text{CN}^- \leftrightarrow \text{ZnCN}^+$	25	3.0	5.3		76SM 26
$\text{Zn}^{2+} + 2\text{CN}^- \leftrightarrow \text{Zn}(\text{CN})_2^0$	25	0	11.07	-11.0	76SM 26
$\text{Zn}^{2+} + 3\text{CN}^- \leftrightarrow \text{Zn}(\text{CN})_3^-$	25	0	16.05	-20.2	76SM 26
$\text{Zn}^{2+} + 4\text{CN}^- \leftrightarrow (\text{CN})_4^{2-}$	25	0	19.62	-27.9	76SM 26
$\text{Cd}^{2+} + \text{CN}^- \leftrightarrow \text{CdCN}^+$	25	0	6.01		76SM 27
$\text{Cd}^{2+} + 2\text{CN}^- \leftrightarrow \text{Cd}(\text{CN})_2^0$	25	0	11.12	-13.0	76SM 27
$\text{Cd}^{2+} + 3\text{CN}^- \leftrightarrow \text{Cd}(\text{CN})_3^-$	25	0	15.65	-21.6	76SM 27
$\text{Cd}^{2+} + 4\text{CN}^- \leftrightarrow \text{Cd}(\text{CN})_4^{2-}$	25	0	17.92	-26.7	76SM 27
$\text{Hg}^{2+} + \text{CN}^- \leftrightarrow \text{HgCN}^+$	25	0	17.00	-23.2	76SM 27
$\text{Hg}^{2+} + 2\text{CN}^- \leftrightarrow \text{Hg}(\text{CN})_2^0$	25	0	32.75	-46.6	76SM 27
$\text{Hg}^{2+} + 3\text{CN}^- \leftrightarrow \text{Hg}(\text{CN})_3^-$	25	0	36.31	-53.4	76SM 27
$\text{Hg}^{2+} + 4\text{CN}^- \leftrightarrow \text{Hg}(\text{CN})_4^{2-}$	25	0	38.97	-59.7	76SM 27
$\text{Hg}^{2+} + \text{OH}^- + \text{CN}^- \leftrightarrow \text{HgOH}(\text{CN})^0$	30	2.0	28.9		76SM 27

TABLE 3. (contd)

Reaction	Temperature (°C)	Ionic Strength (M)	Log K _r	Δ H _r	Reference Code
<u>Hexacyanoferrite (Fe(CN)₆⁴⁻)</u>					
Fe(CN) ₆ ⁴⁻ + H ⁺ ↔ HFe(CN) ₆ ³⁻	25	0	4.30	0.5	76SM 21
Fe(CN) ₆ ⁴⁻ + H ⁺ ↔ HFe(CN) ₆ ³⁻	25	0	4.37	1.6	86CR
Fe(CN) ₆ ⁴⁻ + H ⁺ ↔ HFe(CN) ₆ ³⁻	25	0	4.17		87B
HFe(CN) ₆ ³⁻ + H ⁺ ↔ H ₂ Fe(CN) ₆ ²⁻	25	0	2.6	1.0	76SM 21
K ⁺ + Fe(CN) ₆ ⁴⁻ ↔ KFe(CN) ₆ ³⁻	25	0	2.34	1.0	76SM 21
Mg ²⁺ + Fe(CN) ₆ ⁴⁻ ↔ MgFe(CN) ₆ ²⁻	25	0	3.8		76SM 21
Ca ²⁺ + Fe(CN) ₆ ⁴⁻ ↔ CaFe(CN) ₆ ²⁻	25	0	3.8	2.1(a)	76SM 21
Ca ²⁺ + Fe(CN) ₆ ⁴⁻ ↔ CaFe(CN) ₆ ²⁻	25	0	4.06	2.7	86CR
CaFe(CN) ₆ ²⁻ + Ca ²⁺ ↔ Ca ₂ Fe(CN) ₆ ⁰	25	0	1.4		76SM 21
Ba ²⁺ + Fe(CN) ₆ ⁴⁻ ↔ BaFe(CN) ₆ ²⁻	25	0	3.8		76SM 21
2H ⁺ + Fe(CN) ₆ ⁴⁻ ↔ H ₂ Fe(CN) ₆ ²⁻	25	0	6.79	2.7	86CR
HFe(CN) ₆ ³⁻ + H ⁺ ↔ H ₂ Fe(CN) ₆ ²⁻	25	0	2.2		87B
Li ⁺ + Fe(CN) ₆ ⁴⁻ ↔ LiFe(CN) ₆ ³⁻	25	0	2.06	5.6	86CR
2Li ⁺ + Fe(CN) ₆ ⁴⁻ ↔ Li ₂ Fe(CN) ₆ ²⁻	25	0	2.90	2.3	86CR

(a) 26⁰, I = 0.1M

TABLE 3. (contd)

Reaction	Temperature (°C)	Ionic Strength (M)	Log K_r	ΔH_r	Reference Code
$\text{Li}^+ + \text{H}^+ + \text{Fe}(\text{CN})_6^{4-} \leftrightarrow \text{LiHFe}(\text{CN})_6^{2-}$	25	0	5.59	4.8	86CR
$\text{Na}^+ + \text{Fe}(\text{CN})_6^{4-} \leftrightarrow \text{NaFe}(\text{CN})_6^{3-}$	25	0	2.36	0.9	86CR
$2\text{Na}^+ + \text{Fe}(\text{CN})_6^{4-} \leftrightarrow \text{Na}_2\text{Fe}(\text{CN})_6^{2-}$	25	0	3.11	0.8	86CR
$\text{Na}^+ + \text{H}^+ + \text{Fe}(\text{CN})_6^{4-} \leftrightarrow \text{NaHFe}(\text{CN})_6^{2-}$	25	0	5.80	0.2	86CR
$\text{K}^+ + \text{Fe}(\text{CN})_6^{4-} \leftrightarrow \text{KFe}(\text{CN})_6^{3-}$	25	0	2.49	1.8	86CR
$\text{K}^+ + \text{Fe}(\text{CN})_6^{4-} \leftrightarrow \text{KFe}(\text{CN})_6^{3-}$	25	0	2.35		87B
$2\text{K}^+ + \text{Fe}(\text{CN})_6^{4-} \leftrightarrow \text{K}_2\text{Fe}(\text{CN})_6^{2-}$	25	0	3.35	8.5	86CR
$\text{K}^+ + \text{H}^+ + \text{Fe}(\text{CN})_6^{4-} \leftrightarrow \text{KHFe}(\text{CN})_6^{2-}$	25	0	5.84	7.7	86CR
$\text{NH}_4^+ + \text{Fe}(\text{CN})_6^{4-} \leftrightarrow \text{NH}_4\text{Fe}(\text{CN})_6^{3-}$	25	0	2.44	1.3	86CR
$2\text{NH}_4^+ + \text{Fe}(\text{CN})_6^{4-} \leftrightarrow (\text{NH}_4)_2\text{Fe}(\text{CN})_6^{2-}$	25	0	3.24	2.8	86CR
$\text{NH}_4^+ + \text{H}^+ + \text{Fe}(\text{CN})_6^{4-} \leftrightarrow \text{NH}_5\text{Fe}(\text{CN})_6^{2-}$	25	0	5.77	1.9	86CR
$\text{Ca}^{2+} + \text{Fe}(\text{CN})_6^{4-} \leftrightarrow \text{CaFe}(\text{CN})_6^{2-}$	25	0	4.06	2.7	86CR
$2\text{Ca}^{2+} + \text{Fe}(\text{CN})_6^{4-} \leftrightarrow \text{Ca}_2\text{Fe}(\text{CN})_6^0$	25	0	5.37	2.1	86CR
$\text{Ca}^{2+} + \text{H}^+ + \text{Fe}(\text{CN})_6^{4-} \leftrightarrow \text{CaHFe}(\text{CN})_6^0$	25	0	7.08	3.8	86CR

TABLE 3. (contd)

Reaction	Temperature (°C)	Ionic Strength (M)	Log K_r	ΔH_r	Reference Code
<u>Hexacyanoferrate ($\text{Fe}(\text{CN})_6^{3-}$)</u>					
$\text{Na}^+ + \text{Fe}(\text{CN})_6^{3-} \leftrightarrow \text{NaFe}(\text{CN})_6^{2-}$	25	3.0	-0.3		76SM 22
$\text{K}^+ + \text{Fe}(\text{CN})_6^{3-} \leftrightarrow \text{KFe}(\text{CN})_6^{2-}$	25	0	1.43		76SM 22
$\text{Cs}^+ + \text{Fe}(\text{CN})_6^{3-} \leftrightarrow \text{CsFe}(\text{CN})_6^{2-}$	25	3.0	0.52		76SM 22
$\text{Mg}^{2+} + \text{Fe}(\text{CN})_6^{3-} \leftrightarrow \text{MgFe}(\text{CN})_6^{-}$	25	0	2.79		76SM 22
$\text{Mg}^{2+} + \text{Fe}(\text{CN})_6^{3-} \leftrightarrow \text{MgFe}(\text{CN})_6^{-}$	25	0.1	1.44		82A
$\text{Ca}^{2+} + \text{Fe}(\text{CN})_6^{3-} \leftrightarrow \text{CaFe}(\text{CN})_6^{-}$	25	0	2.83	1.6(a)	76SM 22
$\text{Ca}^{2+} + \text{Fe}(\text{CN})_6^{3-} \leftrightarrow \text{CaFe}(\text{CN})_6^{-}$	25	0.1	1.48		82A
$\text{Sr}^{2+} + \text{Fe}(\text{CN})_6^{3-} \leftrightarrow \text{SrFe}(\text{CN})_6^{-}$	25	0	2.85		76SM 22
$\text{Sr}^{2+} + \text{Fe}(\text{CN})_6^{3-} \leftrightarrow \text{SrFe}(\text{CN})_6^{-}$	25	0.1	1.5		82A
$\text{Ba}^{2+} + \text{Fe}(\text{CN})_6^{3-} \leftrightarrow \text{BaFe}(\text{CN})_6^{-}$	25	0	2.88		76SM 22
$\text{Ba}^{2+} + \text{Fe}(\text{CN})_6^{3-} \leftrightarrow \text{BaFe}(\text{CN})_6^{-}$	25	0.1	1.53		82A
$\text{Fe}^{3+} + \text{Fe}(\text{CN})_6^{3-} \leftrightarrow \text{Fe}_2(\text{CN})_6^0$	25	0.5	1.55		76SM 22

(a) 25°C, 1 = 0.1M.

species were removed from additional consideration because no $\Delta G_{f,298}^{\circ}$ values were reported for the species. After eliminating all those species, 62 species and two components remained.

The final thermodynamic data for these 64 aqueous species are presented in Table 4. These data for most of the species were chosen, if alternatives were presented, from the values given in Wagman et al. (1982) or related NBS publications. The only major exception to this rule was the selection of the data calculated from Capone et al. (1986) for those species contained in that report. If no data from either of these publications were available, then the data in other accepted compilations or the most recent publications were chosen. All chosen data agree with that chosen in the review by Beck (1987); however, the number of aqueous species reported here is substantially larger than that reported in Beck (1987). For all of the final aqueous species, differences between the reported thermodynamic data were usually on the order of a few kilocalories, which would translate into an uncertainty in the log K_r° value of a few tenths of a log unit. Thus, even if alternative values were chosen, the resulting effect on the speciation would be minor. The calculated log K_r° and $\Delta H_{r,298}^{\circ}$ values for the formation of these species using the basis species, CN^- and OCN^- , are given in Table 5.

Reaction data and associated log K_r values were also found in the literature for eight solids containing cyanide or cyanogen (Table 6). The data for $\text{Zn}(\text{CN})_2$ could not be used because of the high ionic strength ($I = 3$) at which these data were determined. The log K_r° values for the other reactions were used to calculate $\Delta G_{f,298}^{\circ}$ values for the solid phases. These data are given in Appendix C. Of the 121 solids for which basic thermodynamic data were tabulated, log K_r° values could not be calculated for most of these solids because either $\Delta G_{f,298}^{\circ}$ data was missing and/or one of the components is not currently included in the MINTEQ database. The chosen basic thermodynamic data for the remaining 27 solids is presented in Table 7. These data were chosen from Wagman et al. (1982). As with the aqueous species, there was very little discrepancy among different reported thermodynamic data. The reaction and associated log K_r° and $\Delta H_{r,298}^{\circ}$ values for the formation of the cyanide and cyanogen solid phases are given in Table 8.

The MINTEQ files for cyanide are given in Appendix E.

TABLE 4. Thermodynamic Data Selected for Aqueous Species Containing Cyanide

Formula	Identification Number	$\Delta G_{f,298}^0$ (-----kcal/mol-----)	$\Delta H_{f,298}^0$	S_{298}^0 (cal/mol•K)	Reference Code
CN^-	143(a)	41.2	36.0	22.5	82WE 2-89
OCN^-	144(a)	-23.3	-34.9	25.5	82WE 2-89
$\text{Ag}(\text{CN})\text{OH}^-$	0201431	3.70	NA ^(b)	NA	82WE 2-163
$\text{Ag}(\text{CN})_2^-$	0201432	73.02	64.60	45.9	82WE 2-163
$\text{Ag}(\text{CN})_3^{2-}$	0201433	112.83	99.78	70.58	76SM 26
$\text{Ag}(\text{OCN})_2^-$	0201440	-35.0	NA	NA	76SM 28
$\text{BaFe}(\text{CN})_6^-$	1001431	36.45	6.22	81.15	82A
$\text{BaFe}(\text{CN})_6^{2-}$	1001430	20.93	NA	NA	76SM 21
$\text{CaFe}(\text{CN})_6^-$	1501431	38.12	5.16	67.06	82WE 2-274; 82A
$\text{CaFe}(\text{CN})_6^{2-}$	1501432	28.26	-18.14	37.65	86CR
$\text{Ca}_2\text{Fe}(\text{CN})_6^0$	1501433	-105.82	-148.48	28.91	86CR
$\text{CaHFe}(\text{CN})_6^{2-}$	1501434	24.14	-17.04	70.70	86CR
CdCN^+	1601431	15.4	NA	NA	82WE 2-148
$\text{Cd}(\text{CN})_2^0$	1601432	49.7	40.86	34.78	82WE 2-148; 76SM 27
$\text{Cd}(\text{CN})_3^-$	1601433	84.82	68.26	49.16	82WE 2-148; 76SM 27
$\text{Cd}(\text{CN})_4^{2-}$	1601434	121.3	102.3	77.7	82WE 2-148
$\text{Cu}(\text{CN})_4^{3-}$	2301431	135.4	109.8	32.05	82WE 2-158; 76SM 26
$\text{Cu}(\text{CN})_2^-$	2301432	61.62	60.1	31.55	82WE 2-158; 76SM 26
$\text{Cu}(\text{CN})_3^{2-}$	2301433	96.51	85.0	41.24	82WE 2-158; 76SM 26

TABLE 4. (contd)

Formula	Identification Number	$\Delta G_{f,298}^0$ (-----kcal/mol-----)	$\Delta H_{f,298}^0$	S_{298}^0 (cal/mol•K)	Reference Code
$\text{Fe}(\text{CN})_6^{4-}$	2801431	160.13	110.5	48.1	86CR
$\text{HFe}(\text{CN})_6^{3-}$	2801432	160.14	110.54	48.06	86CR
$\text{H}_2\text{Fe}(\text{CN})_6^{2-}$	2801433	156.8	111.6	62.85	86CR
$\text{Fe}(\text{CN})_6^{3-}$	2811431	174.3	134.3	64.60	82WE 2-181; 76SM 26
$\text{Fe}_2(\text{CN})_6^0$	2811432	167.26	NA	NA	
HCN^0	3301431	28.6	25.6	29.8	82WE 2-89
HOCN^0	3301441	-28.0	-36.9	34.6	82WE 2-90
HgCN^+	3611431	55.9	53.9	20.09	82WE 2-153
$\text{Hg}(\text{CN})_2^0$	3611432	74.62	66.49	39.51	82WE 2-153
$\text{Hg}(\text{CN})_3^-$	3611433	110.7	94.9	53.52	82WE 2-153
$\text{Hg}(\text{CN})_4^{2-}$	3611434	147.8	125.8	72.59	82WE 2-153
$\text{Hg}(\text{CN})_2\text{Cl}^-$	3611435	43.62	NA	NA	82WE 2-153
$\text{Hg}(\text{CN})_3\text{Cl}^{2-}$	3611436	80.1	NA	NA	82WE 2-153
$\text{Hg}(\text{CN})_3\text{Br}^{2-}$	3611437	85.1	NA	NA	82WE 2-153
I_2CN^-	3801432	32.54	NA	NA	82WE 2-92
$\text{I}(\text{CN})_2^-$	3801433	85.62	NA	NA	82WE 2-108
$\text{K}_2\text{H}_2\text{Fe}(\text{CN})_6^0$	4101431	21.97	-11.7	101.26	76WE 59
$\text{K}_3\text{HFe}(\text{CN})_6^0$	4101432	-42.70	-72.1	115.43	76WE 59
$\text{KFe}(\text{CN})_6^{2-}$	4101430	104.84	NA	NA	76SM 22
$\text{KFe}(\text{CN})_6^{3-}$	4101433	95.19	50.43	64.29	86CR
$\text{K}_2\text{Fe}(\text{CN})_6^{2-}$	4101434	26.51	-3.14	114.79	86CR

TABLE 4. (contd)

Formula	Identification Number	$\Delta G_{f,298}^{\circ}$ (-----kcal/mol-----)	$\Delta H_{f,298}^{\circ}$	S_{298}° (cal/mol·K)	Reference Code
$\text{KFe}(\text{CN})_6^{2-}$	4101435	90.62	56.33	99.41	86CR
$\text{LiFe}(\text{CN})_6^{3-}$	4401431	93.19	47.99	54.12	86CR
$\text{Li}_2\text{Fe}(\text{CN})_6^{2-}$	4401432	21.93	-21.92	50.12	86CR
$\text{LiHFe}(\text{CN})_6^{2-}$	4401433	88.37	47.14	67.60	86CR
$\text{MgFe}(\text{CN})_6^{-}$	4601431	61.83	23.51	46.69	82WE 2-265; 82A
$\text{MgFe}(\text{CN})_6^{2-}$	4601432	52.22	NA	NA	82WE 2-265
$\text{NH}_4\text{Fe}(\text{CN})_6^{3-}$	4901431	143.78	78.35	202.03	86CR
$(\text{NH}_4)_2\text{Fe}(\text{CN})_6^{2-}$	4901432	123.70	48.00	100.06	86CR
$\text{NH}_5\text{Fe}(\text{CN})_6^{2-}$	4901433	139.23	78.95	219.30	86CR
$\text{NaFe}(\text{CN})_6^{3-}$	5001431	100.29	52.37	50.48	86CR
$\text{Na}_2\text{Fe}(\text{CN})_6^{2-}$	5001432	36.67	-5.16	67.56	86CR
$\text{NaHFe}(\text{CN})_6^{2-}$	5001433	95.59	51.67	63.89	86CR
$\text{Ni}(\text{CN})_4^{2-}$	5401431	112.8	87.91	52.1	82WE 2-169
$\text{NiH}(\text{CN})_4^{-}$	5401432	103.765	NA	NA	76SM 26
$\text{NiH}_2(\text{CN})_4^0$	5401433	97.34	NA	NA	76SM 26
$\text{NiH}_3(\text{CN})_4^{+}$	5401434	93.94	NA	NA	76SM 26
$\text{Ni}(\text{CN})_2^0$	5401435	51.60	NA	NA	76SM 26
$\text{Ni}(\text{CN})_3^{-}$	5401436	81.82	NA	NA	76SM 26
$\text{SrFe}(\text{CN})_6^{-}$	8001431	36.74	4.12	70.89	82WE 2-281; (82A)
$\text{Tl}(\text{CN})_4^{-}$	8701431	168.0	NA	NA	82WE 2-137
$\text{TlFe}(\text{CN})_6^{3-}$	8701432	154.1	111.1	70.0	69WE 88; 82WE 2-181

TABLE 4. (contd)

Formula	Identification Number	$\Delta G_{f,298}^0$ (-----kcal/mol-----)	$\Delta H_{f,298}^0$	S_{298}^0 (cal/mol•K)	Reference Code
$\text{Zn}(\text{CN})_2^0$	9501430	32.1	24.34	32.56	76SM 26
$\text{Zn}(\text{CN})_4^{2-}$	9501431	106.8	81.8	54.33	82WE 2-143
$\text{Zn}(\text{CN})_3^-$	9501432	66.51	51.14	46.98	76SM 26

(a) Basis species.

(b) Values indicated by NA are not available in the literature reviewed in this study.

TABLE 5. Equilibrium Constants and Enthalpies of Reaction at 298 K and 1 Atm for Reactions Containing Aqueous Species of Cyanide

Identification Number	Reactions	Log $K_{r,298}^0$	$\Delta H_{r,298}^0$ (-----kcal-----)
0201440	$2(\text{OCN}^-) + \text{Ag}^+ \leftrightarrow \text{Ag}(\text{OCN})_2^-$	5.0034	
0201431	$\text{CN}^- + \text{Ag}^+ + \text{H}_2\text{O} \leftrightarrow \text{Ag}(\text{CN})\text{OH}^- + \text{H}^+$	-0.5600	
0201433	$3\text{CN}^- + \text{Ag}^+ \leftrightarrow \text{Ag}(\text{CN})_3^{2-}$	21.4002	-33.4950
0201432	$2\text{CN}^- + \text{Ag}^+ \leftrightarrow \text{Ag}(\text{CN})_2^-$	20.3814	-32.6750
1001430	$\text{Ba}^{2+} + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{BaFe}(\text{CN})_6^{2-}$	49.4032	
1001431	$\text{Ba}^{2+} + \text{Fe}^{3+} + 6\text{CN}^- \leftrightarrow \text{BaFe}(\text{CN})_6^-$	55.4356	-69.6800
1501431	$6\text{CN}^- + \text{Ca}^{2+} + \text{Fe}^{3+} \leftrightarrow \text{CaFe}(\text{CN})_6^-$	55.4730	-69.5000
1501432	$6\text{CN}^- + \text{Ca}^{2+} + \text{Fe}^{2+} \leftrightarrow \text{CaFe}(\text{CN})_6^{2-}$	49.6898	-83.1000
1501433	$6\text{CN}^- + 2\text{Ca}^{2+} + \text{Fe}^{2+} \leftrightarrow \text{Ca}_2\text{Fe}(\text{CN})_6^0$	50.9952	-83.7000
1501434	$\text{Ca}^{2+} + \text{H}^+ + \text{Fe}^{2+} + 6\text{CN}^- + \text{e}^- \leftrightarrow \text{CaHFe}(\text{CN})_6^{2-}$	52.7097	-82.00
1601431	$\text{CN}^- + \text{Cd}^{2+} \leftrightarrow \text{CdCN}^+$	5.3200	
1601432	$2\text{CN}^- + \text{Cd}^{2+} \leftrightarrow \text{Cd}(\text{CN})_2^0$	10.3703	-13.000
1601433	$3\text{CN}^- + \text{Cd}^{2+} \leftrightarrow \text{Cd}(\text{CN})_3^-$	14.8341	-21.6000
1601434	$4\text{CN}^- + \text{Cd}^{2+} \leftrightarrow \text{Cd}(\text{CN})_4^{2-}$	18.2938	-23.5600
2301431	$4\text{CN}^- + \text{Cu}^+ \leftrightarrow \text{Cu}(\text{CN})_4^{3-}$	30.3456	-51.400
2301432	$2\text{CN}^- + \text{Cu}^+ \leftrightarrow \text{Cu}(\text{CN})_2^-$	24.0272	-29.1000
2301433	$3\text{CN}^- + \text{Cu}^+ \leftrightarrow \text{Cu}(\text{CN})_3^{2-}$	28.6524	-40.2000
2801431	$6\text{CN}^- + \text{Fe}^{2+} \leftrightarrow \text{Fe}(\text{CN})_6^{4-}$	45.6063	-85.8000
2801432	$6\text{CN}^- + \text{Fe}^{2+} + \text{H}^+ \leftrightarrow \text{HFe}(\text{CN})_6^{3-}$	49.9969	-84.1600
2801433	$6\text{CN}^- + 2\text{H}^+ + \text{Fe}^{2+} \leftrightarrow \text{H}_2\text{Fe}(\text{CN})_6^{2-}$	52.4450	-83.1000

TABLE 5. (contd)

Identi- fication Number	Reactions	Log $K_{r,298}^0$ (-----kcal-----)	$\Delta H_{r,298}^0$
2811431	$6\text{CN}^- + \text{Fe}^{3+} \leftrightarrow \text{Fe}(\text{CN})_6^{3-}$	52.6283	-70.1000
2811432	$6\text{CN}^- + 2\text{Fe}^{3+} \leftrightarrow \text{Fe}_2(\text{CN})_6^0$	56.9822	
3301431	$\text{CN}^- + \text{H}^+ \leftrightarrow \text{HCN}^0$	9.2356	-10.400
3301441	$\text{OCN}^- + \text{H}^+ \leftrightarrow \text{HOCN}^0$	3.4450	-2.000
3611431	$\text{CN}^- + \text{Hg}(\text{OH})_2^0 + 2\text{H}^+ \leftrightarrow \text{HgCN}^+ + 2\text{H}_2\text{O}$	24.1738	-33.8300
3611432	$2\text{CN}^- + \text{Hg}(\text{OH})_2^0 + 2\text{H}^+ \leftrightarrow \text{Hg}(\text{CN})_2^0 + 2\text{H}_2\text{O}$	40.6513	-57.2400
3611433	$3\text{CN}^- + \text{Hg}(\text{OH})_2^0 + 2\text{H}^+ \leftrightarrow \text{Hg}(\text{CN})_3^- + 2\text{H}_2\text{O}$	44.4042	-64.8300
3611434	$4\text{CN}^- + \text{Hg}(\text{OH})_2^0 + 2\text{H}^+ \leftrightarrow \text{Hg}(\text{CN})_4^{2-} + 2\text{H}_2\text{O}$	47.4094	-69.9300
3611435	$\text{Cl}^- + 2\text{CN}^- + \text{Hg}(\text{OH})_2^0 + 2\text{H}^+ \leftrightarrow \text{Hg}(\text{CN})_2\text{Cl}^- + 2\text{H}_2\text{O}$	40.3735	
3611436	$\text{Cl}^- + 3\text{CN}^- + \text{Hg}(\text{OH})_2^0 + 2\text{H}^+ \leftrightarrow \text{Hg}(\text{CN})_3\text{Cl}^{2-} + 2\text{H}_2\text{O}$	43.8332	
3611437	$\text{Br}^- + 3\text{CN}^- + \text{Hg}(\text{OH})_2^0 + 2\text{H}^+ \leftrightarrow \text{Hg}(\text{CN})_3\text{Br}^{2-} + 2\text{H}_2\text{O}$	44.9415	
3801432	$\text{CN}^- + 2\text{I}^- \leftrightarrow \text{I}_2\text{CN}^- + 2\text{e}^-$	-11.8480	
3801433	$2\text{CN}^- + \text{I}^- \leftrightarrow \text{I}(\text{CN})_2^- + 2\text{e}^-$	-11.4580	
4101431	$6\text{CN}^- + 2\text{K}^+ + 2\text{H}^+ + \text{Fe}^{2+} \leftrightarrow \text{K}_2\text{H}_2\text{Fe}(\text{CN})_6^0$	52.3058	-85.8600
4101432	$6\text{CN}^- + 3\text{K}^+ + \text{H}^+ + \text{Fe}^{2+} \leftrightarrow \text{K}_3\text{HFe}(\text{CN})_6^0$	50.2241	-85.9900
4101433	$\text{K}^+ + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{KFe}(\text{CN})_6^{3-}$	48.1204	-84.000
4101434	$2\text{K}^+ + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{K}_2\text{Fe}(\text{CN})_6^{2-}$	48.9780	-77.300
4101435	$\text{K}^+ + \text{H}^+ + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{KHFe}(\text{CN})_6^{2-}$	51.4702	-78.100

TABLE 5. (contd)

Identi- fication Number	Reactions	Log $K_{r,298}^0$ (-----kcal-----)	$\Delta H_{r,298}^0$
4401431	$6\text{CN}^- + \text{Li}^+ + \text{Fe}^{2+} \leftrightarrow \text{LiFe}(\text{CN})_6^{3-}$	47.6858	-80.1490
4401432	$2\text{Li}^+ + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{Li}_2\text{Fe}(\text{CN})_6^{2-}$	48.5338	-93.4980
4401433	$\text{Li}^+ + \text{H}^+ + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{LiHFe}(\text{CN})_6^{2-}$	51.2188	-80.9990
4601431	$6\text{CN}^- + \text{Mg}^{2+} + \text{Fe}^{3+} \leftrightarrow \text{MgFe}(\text{CN})_6^-$	55.3916	-69.3100
4601432	$6\text{CN}^- + \text{Mg}^{2+} + \text{Fe}^{2+} \leftrightarrow \text{MgFe}(\text{CN})_6^{2-}$	49.4251	
4901431	$\text{NH}_4^+ + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{NH}_4\text{Fe}(\text{CN})_6^{3-}$	48.0684	-84.500
4901432	$2\text{NH}_4^+ + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow (\text{NH}_4)_2\text{Fe}(\text{CN})_6^{2-}$	48.8666	-83.000
4901433	$\text{NH}_4^+ + \text{H}^+ + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{NH}_5\text{Fe}(\text{CN})_6^{2-}$	51.4035	-83.900
5001431	$\text{Na}^+ + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{NaFe}(\text{CN})_6^{3-}$	47.9885	-84.900
5001432	$2\text{Na}^+ + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{Na}_2\text{Fe}(\text{CN})_6^{2-}$	48.7435	-85.000
5001433	$\text{Na}^+ + \text{H}^+ + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{NaHFe}(\text{CN})_6^{2-}$	51.4335	-85.600
5401431	$4\text{CN}^- + \text{Ni}^{2+} \leftrightarrow \text{Ni}(\text{CN})_4^{2-}$	30.1257	-43.1900
5401432	$4\text{CN}^- + \text{H}^+ + \text{Ni}^{2+} \leftrightarrow \text{NiH}(\text{CN})_4^-$	36.7482	
5401433	$4\text{CN}^- + 2\text{H}^+ + \text{Ni}^{2+} \leftrightarrow \text{NiH}_2(\text{CN})_4^0$	41.4576	
5401434	$4\text{CN}^- + 3\text{H}^+ + \text{Ni}^{2+} \leftrightarrow \text{NiH}_3(\text{CN})_4^+$	43.9498	
5401435	$2\text{CN}^- + \text{Ni}^{2+} \leftrightarrow \text{Ni}(\text{CN})_2^0$	14.5864	
5401436	$3\text{CN}^- + \text{Ni}^{2+} \leftrightarrow \text{Ni}(\text{CN})_3^-$	22.6346	
8001431	$\text{Sr}^{2+} + \text{Fe}^{3+} + 6\text{CN}^- \leftrightarrow \text{SrFe}(\text{CN})_6^-$	55.6181	-69.8300
8701431	$4\text{CN}^- + \text{Tl}^+ \leftrightarrow \text{Tl}(\text{CN})_4^- + 2\text{e}^-$	-8.0189	
8701432	$6\text{CN}^- + \text{Tl}^+ + \text{Fe}^{2+} \leftrightarrow \text{TlFe}(\text{CN})_6^{3-}$	48.7508	-84.8800
9501430	$2\text{CN}^- + \text{Zn}^{2+} \leftrightarrow \text{Zn}(\text{CN})_2^0$	11.0710	-10.9990
9501431	$4\text{CN}^- + \text{Zn}^{2+} \leftrightarrow \text{Zn}(\text{CN})_4^{2-}$	16.7150	-25.5390
9501432	$3\text{CN}^- + \text{Zn}^{2+} \leftrightarrow \text{Zn}(\text{CN})_3^-$	16.0480	-20.1990

TABLE 6. Reported Log K_r Values for Reactions of Solid Phases of Cyanide

Reaction	Temperature (°C)	Ionic Strength (M)	Log K_r	Reference Code
$\text{Hg}(\text{CN})_2 \leftrightarrow \text{Hg}^{2+} + 2\text{CN}^-$	25	0	-39.3	76SM 26
$\text{AgCN} \leftrightarrow \text{Ag}^+ + \text{CN}^-$	25	0	-15.66	76SM 26
$\text{Zn}(\text{CN})_2 \leftrightarrow \text{Zn}^{2+} + 2\text{CN}^-$	25	3.0	15.5	76SM 26
$\text{AgOCN} \leftrightarrow \text{Ag}^+ + \text{OCN}^-$	19	0	-6.64	76SM 28
$\text{Ag}_4\text{Fe}(\text{CN})_6 \leftrightarrow 4\text{Ag}^+ + \text{Fe}(\text{CN})_6^{4-}$	25	0	-44.07	76SM 21
$\text{Zn}_2\text{Fe}(\text{CN})_6 \leftrightarrow 2\text{Zn}^{2+} + \text{Fe}(\text{CN})_6^{4-}$	25	0	-15.68	76SM 21
$\text{Cd}_2\text{Fe}(\text{CN})_6 \leftrightarrow 2\text{Cd}^{2+} + \text{Fe}(\text{CN})_6^{4-}$	25	0	-17.38	76SM 21
$\text{Pb}_2\text{Fe}(\text{CN})_6 \leftrightarrow 2\text{Pb}^{2+} + \text{Fe}(\text{CN})_6^{4-}$	25	0	-18.02	76SM 21

TABLE 7. Thermodynamic Data Selected for Solid Phases Containing Cyanide

Formula	Identification Number	$\Delta G_{f,298}^{\circ}$ (-----kcal/mol-----)	$\Delta H_{f,298}^{\circ}$	S_{298}° (cal/mol•K)	Reference Code
$\text{Ag}_4\text{Fe}(\text{CN})_6 \cdot \text{H}_2\text{O}$	1102001	123.0	NA(a)	NA	82WE 2-181
AgCN	1102002	37.50	34.89	25.19	82WE 2-163
$\text{Cd}_2\text{Fe}(\text{CN})_6 \cdot 7\text{H}_2\text{O}$	1116001	-291.49	NA	NA	82WE 2-181
CrCN	1121001	29.80	NA	NA	82WE 2-198
Cr_2CN	1121002	30.50	NA	NA	82WE 2-198
CuCN	1123001	26.60	23.0	20.2	82WE 2-158
$\text{Cu}_2\text{Fe}(\text{CN})_6$	1123102	176.0	NA	NA	82WE 2-181
CNI	1138001	44.22	39.71	23.0	82WE 2-92
$\text{K}_{12}\text{Ni}_8(\text{Fe}(\text{CN})_6)_7$	1141001	113.0	NA	NA	82WE 2-348
KCN	1141002	-24.45	-27.01	30.71	82WE 2-342
$\text{K}_2\text{CdFe}(\text{CN})_6$	1141003	-11.2	NA	NA	82WE 2-348
$\text{K}_4\text{Ni}_4(\text{Fe}(\text{CN})_6)_3$	1141004	121.0	NA	NA	82WE 2-348
$\text{K}_4\text{Fe}(\text{CN})_6$	1141005	-108.3	-142.0	100.87	82WE 2-347
$\text{K}_2\text{Mn}_3(\text{Fe}(\text{CN})_6)_2$	1141006	-6.9	NA	NA	82WE 2-350
$\text{K}_2\text{Ni}_3(\text{Fe}(\text{CN})_6)_2$	1141007	121.0	NA	NA	82WE 2-348
$\text{K}_4\text{Fe}(\text{CN})_6 \cdot 3\text{H}_2\text{O}$	1141008	-274.35	-350.50	141.9	82WE 2-348
$\text{K}_{12}\text{Cd}_8(\text{Fe}(\text{CN})_6)_7$	1141009	37.0	NA	NA	82WE 2-348
$\text{KZn}_{1.5}\text{Fe}(\text{CN})_6$	1141010	16.9	NA	NA	82WE 2-348
$\text{K}_3\text{Fe}(\text{CN})_6$	1141011	-30.98	-59.7	101.82	82WE 2-347
$\text{K}_8\text{Mn}_6(\text{Fe}(\text{CN})_6)_5$	1141012	-126.0	NA	NA	82WE 2-350
$\text{K}_2\text{Cu}_2\text{Fe}(\text{CN})_6$	1141013	18.4	NA	NA	82WE 2-348
$\text{Mn}_2\text{Fe}(\text{CN})_6$	1147014	38.82	NA	NA	82WE 2-194

TABLE 7. (contd)

Formula	Identification Number	$\Delta G_{f,298}^0$ (-----kcal/mol-----)	$\Delta H_{f,298}^0$	S_{298}^0 (cal/mol·K)	Reference Code
NaCN (cr, I, cubic) (b)	1150001	-18.27	-20.91	27.63	82WE 2-316
Pb ₂ Fe(CN) ₆ ·3H ₂ O	1160001	-40.15	NA	NA	82WE 2-181
Tl ₄ Fe(CN) ₆ ·2H ₂ O	1187001	6.36	NA	NA	82WE 2-181
Zn ₂ Fe(CN) ₆ ·2H ₂ O	1195001	-38.96	NA	NA	82WE 2-181
AgOCN	7714401	-13.9	-22.8	28.08	82WE 2-163

(a) Values indicated by NA are not available in the literature reviewed in this study.

(b) See Wagman et al. (1982).

TABLE 8. Equilibrium Constants and Enthalpies of Reaction at 298 K and 1 Atm for Reactions Containing Solid Phases of Cyanide

Identification Number	Reactions	Log $K_{r,298}^0$ (-----kcal-----)	$\Delta H_{r,298}^0$
1102001	$6\text{CN}^- + 4\text{Ag}^+ + \text{Fe}^{2+} + \text{H}_2\text{O} \leftrightarrow \text{Ag}_4\text{Fe}(\text{CN})_6 \cdot \text{H}_2\text{O}$	89.6909	
1102002	$\text{CN}^- + \text{Ag}^+ \leftrightarrow \text{AgCN}$	16.2180	-26.385
1102003	$4\text{Ag}^+ + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{Ag}_4\text{Fe}(\text{CN})_6$	193.914	-260.91
1116001	$6\text{CN}^- + 2\text{Cd}^{2+} + \text{Fe}^{2+} + 7\text{H}_2\text{O} \leftrightarrow \text{Cd}_2\text{Fe}(\text{CN})_6 \cdot 7\text{H}_2\text{O}$	62.9824	
1116002	$2\text{CO}^{2+} + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{Cd}_2\text{Fe}(\text{CN})_6$	28.2243	
1121001	$\text{CN}^- + \text{Cr}^{2+} + \text{e}^- \leftrightarrow \text{CrCN}$	-23.8880	
1121002	$\text{CN}^- + 2\text{Cr}^{2+} + 3\text{e}^- \leftrightarrow \text{Cr}_2\text{CN}$	-56.6450	
1123001	$\text{CN}^- + \text{Cu}^+ \leftrightarrow \text{CuCN}$	19.4974	-30.200
1123102	$6\text{CN}^- + 2\text{Cu}^{2+} + \text{Fe}^{2+} \leftrightarrow \text{Cu}_2\text{Fe}(\text{CN})_6$	61.4168	
1136100	$\text{Hg}(\text{OH})_2 + 2\text{CN}^- + 2\text{H}^+ \leftrightarrow \text{Hg}(\text{CN})_2 + 2\text{H}_2\text{O}$	45.3791	-60.73
1138001	$\text{CN}^- + \text{I}^- \leftrightarrow \text{CNI} + 2\text{e}^-$	-11.3114	17.3090
1141001	$42\text{CN}^- + 12\text{K}^+ + 8\text{Ni}^{2+} + 7\text{Fe}^{2+} \leftrightarrow \text{K}_{12}\text{Ni}_8(\text{Fe}(\text{CN})_6)_7$	431.0902	
1141002	$\text{CN}^- + \text{K}^+ \leftrightarrow \text{KCN}$	-1.4403	-2.7400
1141003	$6\text{CN}^- + 2\text{K}^+ + \text{Cd}^{2+} + \text{Fe}^{2+} \leftrightarrow \text{K}_2\text{CdFe}(\text{CN})_6$	63.0279	
1141004	$18\text{CN}^- + 4\text{K}^+ + 4\text{Ni}^{2+} + 3\text{Fe}^{2+} \leftrightarrow \text{K}_4\text{Ni}_4(\text{Fe}(\text{CN})_6)_3$	183.5467	
1141005	$6\text{CN}^- + 4\text{K}^+ + \text{Fe}^{2+} \leftrightarrow \text{K}_4\text{Fe}(\text{CN})_6$	48.8241	-95.6200

TABLE 8. (contd)

Identification Number	Reactions	Log $K_{r,298}^0$	$\Delta H_{r,298}^0$ (-----cal-----)
1141006	$12\text{CN}^- + 2\text{K}^+ + 3\text{Mn}^{2+} + 2\text{Fe}^{2+} \leftrightarrow \text{K}_2\text{Mn}_3(\text{Fe}(\text{CN})_6)_2$	121.0011	
1141007	$12\text{CN}^- + 2\text{K}^+ + 3\text{Ni}^{2+} + 2\text{Fe}^{2+} \leftrightarrow \text{K}_2\text{Ni}_3(\text{Fe}(\text{CN})_6)_2$	123.1267	
1141008	$6\text{CN}^- + 4\text{K}^+ + \text{Fe}^{2+} + 3\text{H}_2\text{O} \leftrightarrow \text{K}_4\text{Fe}(\text{CN})_6 \cdot 3\text{H}_2\text{O}$	49.5424	-99.1750
1141009	$42\text{CN}^- + 12\text{K}^+ + 8\text{Cd}^{2+} + 7\text{Fe}^{2+} \leftrightarrow \text{K}_{12}\text{Cd}_8(\text{Fe}(\text{CN})_6)_7$	441.9853	
1141010	$6\text{CN}^- + \text{K}^+ + 1.5\text{Zn}^{2+} + \text{Fe}^{2+} \leftrightarrow \text{KZn}_{1.5}\text{Fe}(\text{CN})_6$	66.8086	
1141011	$6\text{CN}^- + 3\text{K}^+ + \text{Fe}^{3+} \leftrightarrow \text{K}_3\text{Fe}(\text{CN})_6$	54.6440	-83.2900
1141012	$30\text{CN}^- + 8\text{K}^+ + 6\text{Mn}^{2+} + 5\text{Fe}^{2+} \leftrightarrow \text{K}_8\text{Mn}_6(\text{Fe}(\text{CN})_6)_5$	293.6849	
1141013	$6\text{CN}^- + 2\text{K}^+ + 2\text{Cu}^+ + \text{Fe}^{2+} \leftrightarrow \text{K}_2\text{Cu}_2\text{Fe}(\text{CN})_6$	72.5142	
1147014	$6\text{CN}^- + 2\text{Mn}^{2+} + \text{Fe}^{2+} \leftrightarrow \text{Mn}_2\text{Fe}(\text{CN})_6$	59.0272	
1150001	$\text{CN}^- + \text{Na}^+ \leftrightarrow \text{NaCN}$	-2.2869	0.5200
1160001	$6\text{CN}^- + 2\text{Pb}^{2+} + \text{Fe}^{2+} + 3\text{H}_2\text{O} \leftrightarrow \text{Pb}_2\text{Fe}(\text{CN})_6 \cdot 3\text{H}_2\text{O}$	63.6011	
1160002	$2\text{Pb}^{2+} + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{Pb}_2\text{Fe}(\text{CN})_6$	27.5895	
1187001	$6\text{CN}^- + 4\text{Tl}^+ + \text{Fe}^{2+} + 2\text{H}_2\text{O} \leftrightarrow \text{Tl}_4\text{Fe}(\text{CN})_6 \cdot 2\text{H}_2\text{O}$	56.9162	
1195001	$6\text{CN}^- + 2\text{Zn}^{2+} + \text{Fe}^{2+} + 2\text{H}_2\text{O} \leftrightarrow \text{Zn}_2\text{Fe}(\text{CN})_6 \cdot 2\text{H}_2\text{O}$	61.2321	
1195002	$2\text{Zn}^{2+} + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{Zn}_2\text{Fe}(\text{CN})_6$	29.9263	
7714401	$\text{OCN}^- + \text{Ag}^+ \leftrightarrow \text{AgOCN}$	6.6159	-13.1750

THERMODYNAMIC DATA FOR
AQUEOUS SPECIES AND SOLIDS CONTAINING ANTIMONY

The majority of the thermodynamic data tabulated for the aqueous species and solids containing antimony were taken from the NBS compilation by Wagman et al. (1982). Some data were also found in Robie, Hemingway, and Fisher (1978), Sillen and Martell (1976), Baes and Mesmer (1976), and recent journal articles including Itagaki and Nishimura (1986). Appendix C gives the complete summary of the basic thermodynamic data, $\Delta G_{f,298}^{\circ}$, $\Delta H_{f,298}^{\circ}$ and S_{298}° , for aqueous species and solids of antimony that was compiled from the literature. High-temperature data were reported in Pankajavalli and Sreedharan (1987) for Sb_2O_4 , and Azad, Pankajavalli, and Sreedharan (1986) and Hahn and Stevenson (1979) for Sb_2O_3 . These data were not included in the review.

The basis or parent species for antimony are $Sb(OH)_3^0$ for the Sb[III] oxidation state and $Sb(OH)_6^-$ for the Sb[V] oxidation state because these are the dominant aqueous species for these oxidation states in waters of neutral pH. These basis species are consistent with the basis species used in the compilation of Deutsch and Krupka (1985)(a). The thermodynamic data chosen to represent these basis species are also consistent with that publication.

Although most of the thermodynamic data was presented in the original citations as $\Delta G_{f,298}^{\circ}$, $\Delta H_{f,298}^{\circ}$, and S_{298}° values, data for reactions with 21 aqueous species of antimony and their associated $\log K_r$ values were also reported. These data are given in Table 9. The reactions with the $Sb(OH)_2^+$ and $Sb(OH)_4^-$ species from Sillen and Martell (1976) and Baes and Mesmer (1976) were used with the thermodynamic data for the components to estimate the $\Delta G_{f,298}^{\circ}$ for these species. The $\Delta G_{f,298}^{\circ}$ values for $Sb(OH)_2^+$ are -99.05 and -99.333 for Sillen and Martell (1976) and Baes and Mesmer (1976) data, respectively, and the $\Delta G_{f,298}^{\circ}$ values for $Sb(OH)_4^-$ are -194.695 and -194.668 for Sillen and Martell (1976) and Baes and Mesmer (1976) data, respectively.

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- (a) Deutsch, W. J., and K. M. Krupka. 1985. MINTEQ Geochemical Code: Compilation of Thermodynamic Database for the Aqueous Species, Gasses and Solids Containing Chromium, Mercury, Selenium, and Thallium. Draft report submitted to the Environmental Protection Agency, Athens, Georgia. Unpublished.

TABLE 9. Reported Log K_r Values for Reactions of Aqueous Species of Antimony

Reaction	Temperature (°C)	Ionic Strength (M)	Log K_r	Reference Code
<u>Aqueous Species</u>				
$\text{Sb}(\text{OH})_2^+ \leftrightarrow \text{SbOH}^{2+} + \text{OH}^-$	25	5.0	-15.5 ^(a)	76SM-12
$\text{Sb}(\text{OH})_3^0 \leftrightarrow \text{Sb}(\text{OH})_2^+ + \text{OH}^-$	25	0	-12.8	76SM-12
$\text{Sb}(\text{OH})_4^- \leftrightarrow \text{Sb}(\text{OH})_3^0 + \text{OH}^-$	25	0	2.2	76SM-12
$\text{Sb}_2(\text{OH})_2^{4+} + \text{H}_2\text{O} \leftrightarrow 2\text{Sb}(\text{OH})_2^+ + 2\text{H}^+$	25	5.0	-0.7 ^(a)	76SM-12
$\text{Sb}(\text{OH})_5^0 + \text{H}_2\text{O} \leftrightarrow \text{Sb}(\text{OH})_6^- + \text{H}^+$	25	0	2.72	76SM-133, 76BM-375
$\text{Sb}_{12}(\text{OH})_{64}^0 + 4\text{H}^+ \leftrightarrow 12\text{Sb}(\text{OH})_5^0 + 4\text{H}_2\text{O}$	25	0	-20.34	76SM-133
$\text{Sb}_{12}(\text{OH})_{64}^0 + \text{H}_2\text{O} \leftrightarrow \text{Sb}_{12}(\text{OH})_{65}^- + \text{H}^+$	25	0	-3.62	76SM-133
$\text{Sb}_{12}(\text{OH})_{65}^0 + \text{H}_2\text{O} \leftrightarrow \text{Sb}_{12}(\text{OH})_{66}^{2-} + \text{H}^+$	25	0	-4.83	76SM-133
$\text{Sb}_{12}(\text{OH})_{66}^{2-} + \text{H}_2\text{O} \leftrightarrow \text{Sb}(\text{OH})_{66}^{3-} + \text{H}^+$	25	0	-5.82	76SM-133
$\text{Sb}(\text{OH})_3^0 + \text{H}^+ \leftrightarrow \text{Sb}(\text{OH})_2^+ + \text{H}_2\text{O}$	25	0	1.41	76BM 375
$\text{Sb}(\text{OH})_3^0 + \text{H}_2\text{O} \leftrightarrow \text{Sb}(\text{OH})_4^- + \text{H}^+$	25	0	11.82	76BM 375

TABLE 9. (contd)

Reaction	Temperature (°C)	Ionic Strength (M)	Log K_r	Reference Code
$\text{Sb}^{3+} + 2\text{Cl}^- \leftrightarrow \text{SbCl}_2^+$	25	4.0	2.3	76SM 110
$\text{Sb}^{3+} + 2\text{Cl}^- \leftrightarrow \text{SbCl}_2^+$	25	4.0	3.5	76SM 110
$\text{Sb}^{3+} + 3\text{Cl}^- \leftrightarrow \text{SbCl}_3^0$	25	4.0	4.2	76SM 110
$\text{Sb}^{3+} + 4\text{Cl}^- \leftrightarrow \text{SbCl}_4^-$	25	4.0	4.7	76SM 110
$\text{Sb}^{3+} + 5\text{Cl}^- \leftrightarrow \text{SbCl}_5^{2-}$	25	4.0	4.7	76SM 110
$\text{Sb}^{3+} + 6\text{Cl}^- \leftrightarrow \text{SbCl}_6^{3-}$	25	4.0	4.1	76SM 110
$\text{Sb}^{3+} + \text{F}^- \leftrightarrow \text{SbF}_2^+$	30	2.0	3.0	76SM 102
$\text{Sb}^{3+} + 2\text{F}^- \leftrightarrow \text{SbF}_2^+$	30	2.0	5.7	76SM 102
$\text{Sb}^{3+} + 3\text{F}^- \leftrightarrow \text{SbF}_3^0$	30	2.0	8.3	76SM 102
$\text{Sb}^{3+} + 4\text{F}^- \leftrightarrow \text{SbF}_4^-$	30	2.0	10.9	76SM 102

(a) Assuming $\text{SbOH}^+ \leftrightarrow \text{Sb}^{3+} + \text{OH}^-$, $\text{Log } K_r = 14.0$.

The $\Delta G_{f,298}^0$ values for Sb(OH)_6^- and Sb(OH)_5^0 were also calculated from thermodynamic reaction data given in Sillen and Martell (1976). These calculations are described in Appendix D. The $\Delta G_{f,298}^0$ values for these species are -288.76 and -235.78 for Sb(OH)_6^- and Sb(OH)_5^0 , respectively. The calculated $\Delta G_{f,298}^0$ values for these species are also reported in Appendix C. The other aqueous species in Table 9 were eliminated from further consideration because of the very high ionic strength at which the measurements were made (e.g., $\text{Sb}_2(\text{OH})_2^{4+}$) or because thermodynamic data for one or more of the components in the reaction were not available (e.g., chloride and fluoride species). Alternative data were available for some, but not all, of these aqueous species that were eliminated from consideration. The polynuclear species were not included in the thermodynamic data for two reasons. First, because the thermodynamic data for Sb(OH)_5^0 , which is one of the species in the reactions, was estimated based on several assumptions, confidence in this value is limited. Second, polynuclear species will only be important at high antimony concentrations; therefore, elimination of these species should result in insignificant error in the speciation calculations at environmentally relevant antimony concentrations. If desired, these species could be added to a provisional data base using the $\log K_r^0$ values given in Table 9.

Of the 33 aqueous species for which basic thermodynamic data are tabulated in Appendix C, $\log K_r^0$ values and $\Delta H_{r,298}^0$ values for reactions with eight of these species could not be calculated because no $\Delta G_{f,298}^0$ values were reported for these species. Also, the thermodynamic data for an additional 12 species were reported for a different standard state than that used of the MINTEQ data base; therefore, these species were also eliminated from further consideration.

The final thermodynamic data for the remaining 13 species were chosen, if alternatives were presented, as equal to the values given in Wagman et al. (1982) or related NBS publications. If no data from these publications were available, then the data in other accepted compilations or the most recent tabulations were chosen. For all of the final aqueous species, differences among the reported thermodynamic data were usually on the order of a few kilocalories, which would translate into an uncertainty in the $\log K_r^0$ value of a few tenths of a log unit. Thus, even if alternative values were chosen,

the resulting effect on the speciation would be minor. The final basic thermodynamic data for the aqueous species of Sb are given in Table 10. The calculated $\log K_r^0$ and $\Delta H_{r,298}^0$ values for the formation of these species, using the basis species Sb(OH)_3^- and Sb(OH)_6^- , are given in Table 11.

Reaction data and associated $\log K_r$ values were also found in the literature for three solids (Table 12). The data for $\text{Sb}_2\text{O}_3(\text{s,cubic})$ and $\text{Sb}_2\text{O}_3(\text{c})$ could not be used because of the high ionic strength ($I = 5$ and $I = 4$, respectively) at which these data were determined. The $\log K_r^0$ values for the other reactions were used to calculate $\Delta G_{f,298}^0$ values for the solid phases, $\text{Sb}_2\text{O}_3(\text{s,orthorhombic})$ and $\text{Sb}_2\text{S}_3(\text{s})$. These data are given in Appendix C. Of the 74 solids for which basic thermodynamic data were tabulated, $\log K_r^0$ values could not be calculated for 43 of these solids because either $\Delta G_{f,298}^0$ data were missing and/or one of the components is not currently included in the MINTEQ database. The chosen basic thermodynamic data for the remaining 31 solids are presented in Table 13. These data were chosen predominantly from the data given in Wagman et al. (1982) though other important sources were Itagaki and Nishimura (1986), Bard, Parsons, and Jordan (1985), Barner and Scheuerman (1978), and Naumov, Ryzhenk, and Khodakovskiy (1974). As with the aqueous species, there was very little discrepancy among different reported thermodynamic data. The reaction and associated $\log K_r^0$ and $\Delta H_{r,298}^0$ values for the formation of the antimony solid phases are given in Table 14.

The MINTEQ files for antimony are given in Appendix F.

TABLE 10. Thermodynamic Data Selected for Aqueous Species Containing Antimony

Formula	Identification Number	$\Delta G_{f,298}^{\circ}$ (-----kcal/mol-----)	$\Delta H_{f,298}^{\circ}$	S_{298}° (cal/mol·K)	Reference Code
Sb(OH)_3°	Basis Species 740	-154.1	-184.9	27.8	82WE 2-79, 68WE 100
Sb(OH)_6^{-}	Basis Species 741	-288.76	NA(a)	NA	88SC 7, 76BM
Sb(OH)_5°	7410020	-235.78	NA	NA	76SM 133
Sb(OH)_4^{-}	7400020	-194.36	-236.52	45.51	85BP 174
HSbO_2°	7400021	-97.40	-116.6	11.1	82WE 2-79
SbOF°	7402700	-116.5	NA	NA	82WE 2-79
$\text{Sb(OH)}_2\text{F}^{\circ}$	7402702	-173.2	NA	NA	82WE 2-79
SbO^{+}	7403300	-41.979	-46.30	5.34	85BP 173, 82WE 2-79
SbO_2^{-}	7403301	-81.31	-99.81	13.2	85BP 173, 82WE 2-79
Sb(OH)_2^{+}	7403302	-99.3	NA	NA	76BM-375
$\text{Sb}_2\text{S}_4^{2-}$	7407300	-23.8	-52.39	-12.23	82WE 2-80
SbO_3^{-}	7410021	-122.93	NA	NA	74P 525, 86IN 40
SbO_2^{+}	7413300	-65.50	NA	NA	74P 525, 86IN 40

(a) Values indicated by NA are not available in the literature reviewed in this study.

TABLE 11. Equilibrium Constants and Enthalpies of Reaction at 298 K and 1 Atm for Reactions Containing Aqueous Species of Antimony

Identification Number	Reactions	Log $K_{r,298}^0$	$\Delta H_{r,298}^0$ (-----kcal-----)
<u>Redox Couple</u>			
7407410	$\text{Sb(OH)}_6^- + 3\text{H}^+ + 2\text{e}^- \leftrightarrow \text{Sb(OH)}_3^0 + 3\text{H}_2\text{O}$	25.7791	
<u>Antimony [III]</u>			
7400020	$\text{Sb(OH)}_3^0 + \text{H}_2\text{O} \leftrightarrow \text{Sb(OH)}_4^- + \text{H}^+$	-12.0429	16.6950
7400021	$\text{Sb(OH)}_3^0 \leftrightarrow \text{HSbO}_2^0 + \text{H}_2\text{O}$	-0.0073	-0.0150
7402700	$\text{Sb(OH)}_3^0 + \text{F}^- + \text{H}^+ \leftrightarrow \text{SbOF}^0 + 2\text{H}_2\text{O}$	6.1864	
7402702	$\text{Sb(OH)}_3^0 + \text{F}^- + \text{H}^+ \leftrightarrow \text{Sb(OH)}_2\text{F}^0 + \text{H}_2\text{O}$	6.1937	
7403300	$\text{Sb(OH)}_3^0 + \text{H}^+ \leftrightarrow \text{SbO}^+ + 2\text{H}_2\text{O}$	0.9228	1.9700
7403301	$\text{Sb(OH)}_3^0 \leftrightarrow \text{SbO}_2^- + \text{H}_2\text{O} + \text{H}^+$	-11.8011	16.7750
7403302	$\text{Sb(OH)}_3^0 + \text{H}^+ \leftrightarrow \text{Sb(OH)}_2^+ + \text{H}_2\text{O}$	1.3853	
7407300	$2\text{Sb(OH)}_3^0 + 4\text{HS}^- + 2\text{H}^+ \leftrightarrow \text{Sb}_2\text{S}_4^{2-} + 6\text{H}_2\text{O}$	49.3005	-75.6800
<u>Antimony [IV]</u>			
7410021	$\text{Sb(OH)}_6^- \leftrightarrow \text{SbO}_3^- + 3\text{H}_2\text{O}$	2.9319	
7413300	$\text{Sb(OH)}_6^- + 2\text{H}^+ \leftrightarrow \text{SbO}_2^+ + 4\text{H}_2\text{O}$	2.3895	

TABLE 12. Reported Log K_r Values for Reactions of Solids of Antimony

Reaction	Temperature (°C)	Ionic Strength (M)	Log K_r	Reference Code
$\text{Sb(OH)}_2 \leftrightarrow \text{H}^+ + \frac{1}{2}\text{H}_2\text{O} + \frac{1}{2}\text{Sb}_2\text{O}_3$ (s, orthorhombic)	25	0	3.09	76SM 12
$\text{Sb(OH)}_2 \leftrightarrow \text{H}^+ + \frac{1}{2}\text{H}_2\text{O} + \frac{1}{2}\text{Sb}_2\text{O}_3$ (s, cubic)	25	5.0	3.18 ^(a)	76SM 12
$\text{Sb(OH)}_3^+ \leftrightarrow \frac{1}{2}\text{Sb}_2\text{O}_3 + \frac{3}{2}\text{H}_2\text{O}$	25	4.0	2.3	76SM 110
$\text{Sb}_2\text{S}_3(\text{s}) \leftrightarrow 2\text{Sb(OH)}_2 + 3\text{S}^{2-} + 4\text{H}^+ + 4\text{H}_2\text{O}$	25	0	-90.8	76SM 77

(a) Assuming $\text{H}^+ + \text{OH}^- \leftrightarrow \text{H}_2\text{O}$, $\log K = 14.6$.

TABLE 13. Thermodynamic Data Selected for Solid Phases Containing Antimony

Formula	Identification Number	$\Delta G_{f,298}^0$ (-----kcal/mol-----)	$\Delta H_{f,298}^0$	S_{298}^0 (cal/mol·K)	Reference Code
Sb[III](s)	0074001	0.0	0.0	10.92	82WE 2-79
Sb ₂ S ₃ (black, stibnite)	1074000	-41.49	-41.80	43.82	82WE 2-79
Sb ₂ Se ₃	1274000	-29.0	-30.5	47.1	74NR 63
NiSb(breithauptite)	1474001	-20.2	-15.8	calc	74NR 64
ZnSb	1474002	-4.2	-3.5	calc	86IN (from 77BK), 68WE 245
AlSb	1474003	-11.4	NA(a)	NA	86IN 40 (from 77BK)
CdSb	1474004	-3.11	-3.44	22.2	82WE 2-148
Mg ₂ Sb ₃	1474005	-67.6	NA	NA	86IN 40 from 77BK
Ag ₃ Sb	1474006	-5.4	NA	NA	86IN 40 (from 77BK)
Na ₃ Sb	1474007	-43.0	-49.0	37.58	82WE 2-313
NaSb	1474008	-15.0	-15.0	23.18	82WE 2-313
Mn ₂ Sb	1474009	-9.7	NA	NA	86IN 40 (from 77BK)

TABLE 13. (contd)

Formula	Identification Number	$\Delta G_{f,298}^{\circ}$ (-----kcal/mol-----)	$\Delta H_{f,298}^{\circ}$	S_{298}° (cal/mol•K)	Reference Code
Ca_3Sb_2	1474010	-169.9	-174.0	calc	86IN 40, 82WE 2-272
USb_2	1474011	-42.1	-42.1	33.81	82WE 2-250
Cu_2Sb	1474012	-3.9	-2.8	calc	86IN 40 (from 77BK); 69WE 23
MnSb	1474013	-7.6	-12.0	calc	86IN 40, 82WE 2-193
Cu_3Sb	1474014	-6.14	-2.0	calc	86IN (from 79LS), 69WE 23
U_3Sb_4	1474015	-109.0	-108.0	83.03	82WE 2-250
Sb_2O_4	2074001	-190.1	-216.9	39.96	82WE 2-79
Sb_4O_6 (11, cubic)	2074002	-303.08	-344.31	52.80	82WE 2-79
Sb_4O_6 (I, orthorhombic)	2074003	-299.50	-338.70	58.80	82WE 2-79
$\text{Sb}(\text{OH})_3$	2074004	-163.8	-192.1	calc	82WE 2-79, 74NR 60
$\text{Cu}(\text{SbO}_3)_2$	2074005	-230.8	NA	NA	86IN 40 (from 79LS)
Sb_2O_3 (senarmontite, cubic)	2074006	-155.0	-172.18	37.73	74NR 58

TABLE 13. (contd)

Formula	Identification Number	$\Delta G_{f,298}^{\circ}$ (-----kcal/mol-----)	$\Delta H_{f,298}^{\circ}$	S_{298}° (cal/mol•K)	Reference Code
Sb_2O_3 (valentinite, orthorhombic)	2074007	-149.7	-169.4	29.4	79RM 21
Sb_2O_5	2074100	-198.2	-232.3	29.9	68WE 99, 82WE 2-79
SbO_2	2074102	-100.2	-113.5	15.2	78BS 79 (from 71CR)
$SbBr_3$	4074000	-57.19	-62.0	49.5	82WE 2-79
$SbCl_3$	4174000	-77.36	-91.34	44.0	82WE 2-79
SbF_3	4274000	-200.0	-218.8	20.53	85BP 174
SbI_3	4374000	-22.0	-24.0	45.84	85BP 175, 82WE 2-79

(a) Values indicated by NA are not available in the literature reviewed in this study.

TABLE 14. Equilibrium Constants and Enthalpies of Reaction at 298 K and 1 Atm for Reactions Containing Solid Phases of Antimony

Identification Number	Reactions	Log $K_{r,298}^0$ (-----kcal-----)	$\Delta H_{r,298}^0$
0074001	$\text{Sb(OH)}_3^0 + 3\text{H}^+ + 3\text{e}^- \leftrightarrow \text{Sb} + 3\text{H}_2\text{O}$	11.7058	-20.0450
1074000	$2\text{Sb(OH)}_3^0 + 3\text{HS}^- + 3\text{H}^+ \leftrightarrow \text{Sb}_2\text{S}_3 + 6\text{H}_2\text{O}$	60.156	-69.2900
1274000	$2\text{Sb(OH)}_3^0 + 3\text{HSe}^- + 3\text{H}^+ \leftrightarrow \text{Sb}_2\text{Se}_3 + 6\text{H}_2\text{O}$	67.7571	-81.9900
1474001	$\text{Sb(OH)}_3^0 + 5\text{e}^- + 3\text{H}^+ + \text{Ni}^{2+} \leftrightarrow \text{NiSb} + 3\text{H}_2\text{O}$	18.5225	-22.9450
1474002	$\text{Sb(OH)}_3^0 + 5\text{e}^- + \text{Zn}^{2+} + 3\text{H}^+ \leftrightarrow \text{ZnSb} + 3\text{H}_2\text{O}$	-11.0138	13.1160
1474003	$\text{Sb(OH)}_3^0 + 6\text{e}^- + \text{Al}^{3+} + 3\text{H}^+ \leftrightarrow \text{AlSb} + 3\text{H}_2\text{O}$	-65.6241	
1474004	$\text{Sb(OH)}_3^0 + 5\text{e}^- + \text{Cd}^{2+} + 3\text{H}^+ \leftrightarrow \text{CdSb} + 3\text{H}_2\text{O}$	0.3943	-5.3450
1474005	$2\text{Mg}^{2+} + 3\text{Sb(OH)}_3^0 + 9\text{H}^+ + 13\text{e}^- \leftrightarrow \text{Mg}_2\text{Sb}_3 + 9\text{H}_2\text{O}$	-74.6838	
1474006	$\text{Sb(OH)}_3^0 + 6\text{e}^- + 3\text{Ag}^+ + 3\text{H}^+ \leftrightarrow \text{Ag}_3\text{Sb} + 3\text{H}_2\text{O}$	56.1818	
1474007	$3\text{Na}^+ + \text{Sb(OH)}_3^0 + 3\text{H}^+ + 6\text{e}^- \leftrightarrow \text{Na}_3\text{Sb} + 3\text{H}_2\text{O}$	-94.4084	103.2450
1474008	$\text{Na}^+ + \text{Sb(OH)}_3^0 + 3\text{H}^+ + 4\text{e}^- \leftrightarrow \text{NaSb} + 3\text{H}_2\text{O}$	-23.1770	22.3850
1474009	$2\text{Mn}^{2+} + \text{Sb(OH)}_3^0 + 7\text{e}^- + 3\text{H}^+ \leftrightarrow \text{Mn}_2\text{Sb} + 3\text{H}_2\text{O}$	-61.0796	
1474010	$3\text{Ca}^{2+} + 2\text{Sb(OH)}_3^0 + 6\text{H}^+ + 12\text{e}^- \leftrightarrow \text{Ca}_3\text{Sb}_2 + 6\text{H}_2\text{O}$	-142.9738	175.1300

TABLE 14. (contd)

Identification Number	Reactions	Log $K_{r,298}^0$ (-----kcal-----)	$\Delta H_{r,298}^0$
1474011	$UO_2^{2+} + 2Sb(OH)_3^0 + 12e^- + 10H^+ \leftrightarrow USb_2 + 8H_2O$	-29.5246	24.6800
1474012	$Sb(OH)_3^0 + 6e^- + 3H^+ + Cu^{2+} + Cu^+ \leftrightarrow Cu_2Sb + 3H_2O$	34.8827	-55.7450
1474013	$Mn^{3+} + Sb(OH)_3^0 + 6e^- + 3H^+ \leftrightarrow MnSb + 3H_2O$	2.9099	-5.0450
1474014	$Sb(OH)_3^0 + 6e^- + 3H^+ + 3Cu^+ \leftrightarrow Cu_3Sb + 3H_2O$	42.5937	-73.6450
1474015	$3U^{4+} + 4Sb(OH)_3^0 + 24e^- + 12H^+ \leftrightarrow U_3Sb_4 + 12H_2O$	-152.3288	235.72
2074001	$2Sb(OH)_3^0 \leftrightarrow Sb_2O_4 + 2H_2O + 2H^+ + 2e^-$	-3.4597	16.2700
2074002	$4Sb(OH)_3^0 \leftrightarrow Sb_4O_6 + 6H_2O$ (II, cubic) (a)	19.6586	-14.600
2074003	$4Sb(OH)_3^0 \leftrightarrow Sb_4O_6 + 6H_2O$ (I, orthorhombic) (a)	17.0346	-8.9900
2074004	$Sb(OH)_3^0 \leftrightarrow Sb(OH)_3(s)$	7.1099	-7.200
2074005	$2Sb(OH)_3^0 + Cu^{2+} \leftrightarrow Cu(SbO_3)_2 + 6H^+ + 4e^-$	-45.2105	
2074006	$2Sb(OH)_3^0 \leftrightarrow Sb_2O_3 + 3H_2O$ (senarmonite, cubic)	12.3654	-7.3250
2074007	$2Sb(OH)_3^0 \leftrightarrow Sb_2O_3 + 3H_2O$ (valentinite, orthorhombic)	8.4806	-4.5450
2074100	$2Sb(OH)_6^- + 2H^+ \leftrightarrow Sb_2O_5 + 7H_2O$	12.4827	

(a) See Wagman et al. (1982).

CONCLUSIONS

This literature review found thermodynamic data for 290 aqueous species of cyanide and cyanogen, 121 solid phases containing cyanide or cyanogen, 33 aqueous species of antimony and 74 solid phases containing antimony. Much of these data, however, were reported for a standard state that was not consistent with that used in MINTEQ or was incomplete. Thus, basic thermodynamic data could be chosen for only 62 aqueous species, 2 components, and 33 solid phases of cyanide and cyanogen, as well as for 11 aqueous species, 2 components and 31 solid phases of antimony. Most of the chosen data was from the compilations of Wagman et al. (1982); however, the data from several recent papers and other compilations allowed for inclusion of additional aqueous species and solid phases for both cyanide and antimony that were not included in that source.

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APPENDIX A

IDENTIFICATION CODES

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IDENTIFICATION CODES

All compounds summarized in this review are described by identification codes currently used in the MINTEQ database or additions for antimony and cyanide. Identification codes are described for three types of materials: 1) "basis species" or "components," 2) aqueous complexes of components, and 3) solid components. The identification codes are seven digits long, each consisting of three subcodes.

The subcodes are different for solids and aqueous complexes. For solids, the first two digits represent mineral groups. For instance, cyanides are represented by the two digits 11, cyanogenates are represented by 77, and antimonides are represented by 14. The next three digits represent the leading cation component. The last two digits are arbitrary and represent the sequence of compounds tabulated. For aqueous species, on the other hand, the first three digits of the identification number represent the cationic component, the next three digits represent the anionic component, and the last digit represents the arbitrary sequence.

Reactions in the MINTEQ thermodynamic database are formulated as association reactions of the aqueous species or solids of interest. For antimony, the species Sb(OH)_3^0 and Sb(OH)_6^- were selected as the basis species for the reactions compiled in this study. These species are defined as component 740 in MINTEQ for Sb(OH)_3^0 and component 741 for Sb(OH)_6^- . For cyanides, the species CN^- and OCN^- were selected as the basis species for aqueous components and solids, respectively. These are defined as components 143 and 144 for CN^- and OCN^- , respectively.

COMPONENTS

Chemical reaction equations in the MINTEQ thermodynamic database are written in terms of components. Several components are required to describe the compounds and oxidation states for each element included in MINTEQ. For instance, redox elements have a component for each oxidation state: iron has

two components, Fe[II] and Fe[III], to represent its +2 and +3 oxidation states. These particular components (Fe[II] and Fe[III]) are represented by the subcode numbers 280 and 281, respectively. In each case, the leading digits 28 represent iron, and the last digit (0 and 1) is an arbitrary number to distinguish between the oxidation states.

The leading two digits for iron in the subcode, 28, correspond to the alphabetical order of chemical symbols of the 96 elements in MINTEQ. The elements and their MINTEQ numbers are shown in Table A.1.(a)

Selected components in MINTEQ are summarized in Table A.2 (Peterson et al. 1987). Each component is represented by a three-digit subcode or identification (ID) number. For instance, components introduced for this review, noted by an asterisk in Table A.2, include identification numbers 740 and 742 for antimony and 143 for cyanide. The identification number 740 was selected for $\text{Sb}(\text{OH})_3^0$ because antimony is the 74th element listed in Table A.1, and "0" is the arbitrary digit representing the III oxidation state of antimony. The identification number 741 was selected for $\text{Sb}(\text{OH})_6^-$ to represent the V oxidation states of antimony.

The arbitrary identification number 143 was selected for CN^- because cyanide is considered as a compound of carbon since "C" is written first in the chemical symbol CN^- . Also, the identification numbers 140, 141, and 142 for carbon have been used in the MINTEQ database for CO_3^{2-} , fulvate and humate, respectively. The identification number 144 was selected to represent OCN^- .

Identification numbers greater than or equal to 990 are arbitrary and do not refer to a single element. Those beginning with 990 are a function of adsorption algorithms (Peterson et al. 1987).

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- (a) Also shown is the order of elements listed in the National Bureau of Standards Tables of Chemical Thermodynamic Properties (Wagman et al. 1982), which is used as a basis of ordering the thermodynamic data reviewed in this report. The NBS and MINTEQ numbering systems are different. The elements Bk, Cf, Es, Fm, Lw, Md and No are not in MINTEQ but are in the NBS document, and hence are not included in the numbering of the alphabetical order in MINTEQ.

TABLE A.1. Identification Numbers for Elements

Element	Symbol	MINTEQ Number	NBS Order	Element	Symbol	MINTEQ Number	NBS Order
Actinium	Ac	1	91	Nitrogen	N	49	18
Silver	Ag	2	37	Sodium	Na	50	99
Aluminum	Al	3	29	Niobium	Nb	51	55
Americium	Am	4	85	Neodymium	Nd	52	73
Argon	Ar	5	5	Neon	Ne	53	4
Arsenic	As	6	20	Nickel	Ni	54	39
Astatine	At	7	13	Neptunium	Np	55	87
Gold	Au	8	38	Oxygen	O	56	1
Boron	B	9	28	Osmium	Os	57	47
Barium	Ba	10	96	Phosphorus	P	58	19
Beryllium	Be	11	92	Protactinium	Pa	59	89
Bismuth	Bi	12	22	Lead	Pb	60	27
Bromine	Br	13	11	Palladium	Pd	61	42
Carbon	C	14	23	Promethium	Pm	62	72
Calcium	Ca	15	94	Polonium	Po	63	17
Cadmium	Cd	16	34	Praseodymium	Pr	64	74
Cerium	Ce	17	75	Platinum	Pt	65	45
Chlorine	Cl	18	10	Plutonium	Pu	66	86
Curium	Cm	19	84	Radium	Ra	67	97
Cobalt	Co	20	40	Rubidium	Rb	68	101
Chromium	Cr	21	51	Rhenium	Re	69	50
Cesium	Cs	22	102	Rhodium	Rh	70	43
Copper	Cu	23	36	Radon	Rn	71	8
Dysprosium	Dy	24	67	Ruthenium	Ru	72	44
Erbium	Er	25	65	Sulfur	S	73	14
Europium	Eu	26	70	Antimony	Sb	74	21
Fluorine	F	27	9	Scandium	Sc	75	60
Iron	Fe	28	41	Selenium	Se	76	15
Francium	Fr	29	103	Silicon	Si	77	24
Gallium	Ga	30	30	Samarium	Sm	78	71
Gadolinium	Gd	31	69	Tin	Sn	79	26
Germanium	Ge	32	25	Strontium	Sr	80	95
Hydrogen	H	33	2	Tantalum	Ta	81	56
Helium	He	34	3	Terbium	Tb	82	68
Hafnium	Hf	35	59	Technetium	Tc	83	49
Mercury	Hg	36	35	Tellurium	Te	84	16
Holmium	Ho	37	66	Thorium	Th	85	90
Iodine	I	38	12	Titanium	Ti	86	57
Indium	In	39	31	Thallium	Tl	87	32
Iridium	Ir	40	46	Thulium	Tm	88	64
Potassium	K	41	100	Uranium	U	89	88
Krypton	Kr	42	6	Vanadium	V	90	54
Lanthanum	La	43	76	Tungsten	W	91	53
Lithium	Li	44	98	Xenon	Xe	92	7
Lutetium	Lu	45	62	Yttrium	Y	93	61
Magnesium	Mg	46	93	Ytterbium	Yb	94	63
Manganese	Mn	47	48	Zinc	Zn	95	33
Molybdenum	Mo	48	52	Zirconium	Zr	96	58

TABLE A.2. Components in MINTEQ (Peterson et al. 1987)

ID Number	Component	ID Number	Component	ID Number	Component
001	E	281	Fe ³⁺	742	Sb ³⁻
002	H ₂ O	330	H ⁺	760	HSe ⁻
020	Ag ⁺	360	Hg ₂ ²⁺	761	HSeO ₃ ⁻
030	Al ³⁺	361	Hg(OH) ₂ ⁰	762	SeO ₄ ²⁻
060	H ₃ AsO ₃	380	I ⁻	770	H ₄ SiO ₄
061	H ₃ AsO ₄	410	K ⁺	800	Sr ²⁺
090	H ₃ BO ₃	440	Li ⁺	850	Th ⁴⁺
100	Ba ²⁺	460	Mg ²⁺	870	Tl ⁺
130	Br ⁻	470	Mn ²⁺	871	Tl(OH) ₃ ⁰
140	CO ₃ ²⁻	471	Mn ³⁺	890	U ³⁺
141	Fulvate	480	MoO ₂ ²⁻	891	U ⁴⁺
142	Humate	490	NH ₄ ⁺	892	UO ₂ ⁺
143(a)	CN ⁻	491	NO ₂ ⁻	893	UO ₂ ²⁺
144(a)	OCN ⁻	492	NO ₃ ⁻	900	V ²⁺
150	Ca ²⁺	500	Na ⁺	901	V ³⁺
160	Cd ²⁺	540	Ni ²⁺	902	VO ²⁺
180	Cl ⁻	580	PO ₄ ³⁻	903	VO ₂ ⁺
210	Cr ²⁺	600	Pb ²⁺	950	Zn ²⁺
211	Cr(OH) ₂ ⁺	670	Ra ²⁺	990	SOH1
212	CrO ₄ ²⁻	680	Rb ⁺	991	SOH2
220	Cs ⁺	730	HS ⁻	992	XPS10
230	Cu ⁺	731	S	993	XPSIB
231	Cu ²⁺	732	SO ₄ ²⁻	994	XPSID
270	F ⁻	740(a)	Sb(OH) ₃ ⁰	995	SOHB
280	Fe ²⁺	741(a)	Sb(OH) ₆ ⁻		

(a) Introduced in this report.

The components or basis species do not necessarily have the same form as the element they represent; an example of this is arsenic. The H_3AsO_4 component (identification number 061) is used to designate the V oxidation state of arsenic. The only restriction on the specification of components is that a component cannot be a combination of other components. Oxidation/reduction reactions, as written in MINTEQA2, are an exception to this rule.

AQUEOUS COMPLEXES OF COMPONENTS

Aqueous complexes are formed by combining components; they are sometimes called "derived" species. For example, the species CdHCO_3^+ is a species (complex) that is derived from three components, Cd^{2+} , CO_3^{2-} , and H^+ .

The identification number (ID) for complexes are seven-digit numbers with the first three digits representing the ID number of the cationic component and the next three digits representing the anionic component. The last digit is an arbitrary designation to distinguish between complexes that contain different stoichiometries for the same cationic and anionic components and perhaps other minor components as well.

SOLID COMPONENTS

Identification numbers for solids(a) are seven-digit numbers composed of three subcodes: a mineralogical class, the leading cation in the solid, and an arbitrary designation for distinction. The first two digits in the seven-digit ID number designate the mineralogical class of the solid. This mineral classification is described in Dana and Ford (1957) and used in Robie, Hemingway, and Fisher (1979). The mineral-group ID numbers are given in Table A.3. The next three digits in the mineral or solid-phase ID number represent the leading cation in the chemical formula for the mineral or solid. In these three digits for the leading cation, the last digit is arbitrary to distinguish oxidation states. The last two digits in the seven-digit ID number are an arbitrary designation to distinguish between minerals or solids that would otherwise have the same identification number

(a) See Peterson et al. (1987) for a listing of solids in MINTEQA2.

TABLE A.3. MINTEQ Identification Numbers for Mineral Groups

MINTEQ ID Number	Mineral Group	MINTEQ ID Number	Mineral Group
00	elements	70	phosphates
10	sulfides, thiosulfates	72	arsenates
11	cyanides	73	vanadates
12	selenides	74	molybdates, molybdates
14	antimonides	75	uranates
20	oxides and hydroxides, simple metals	76	tungstates
30	multiple oxides	77 ^(a)	cyanogenates
40	bromides	80	orthosilicates
41	chlorides	82	chain silicates
42	fluorides	84	framework silicates
43	iodides	86	sheet silicates
50	carbonates	90	acetates
51	nitrates	91	oxalates
52	borates	92	citrate

(a) Introduced in this report.

(e.g., minerals or solids having the same chemical formula, but distinct structures) or that belong to the same mineralogical class and have the same leading cation, but different minor components.

REFERENCES

Dana, E. S., and W. E. Ford. 1957. A Textbook of Mineralogy. John Wiley and Sons, Inc., New York, New York.

Peterson, S. R., C. J. Hostetler, W. J. Deutsch, and C. E. Cowan. 1987. MINTEQ User's Manual. PNL-6106, Pacific Northwest Laboratory, Richland, Washington.

Robie, R. A., B. S. Hemingway, and J. R. Fisher. 1979. Thermodynamic Properties of Minerals and Related Substances at 298.15 K and 1 Bar Pressure and at Higher Temperatures. Geological Survey Bulletin 1452, reprinted with corrections, U.S. Government Printing Office, Washington, D.C.

Wagman, D. D., W. H. Evans, V. B. Parker, R. H. Schumm, I. Halow, S. M. Bailey, K. L. Churney and R. L. Nuttall. 1982. "The NBS Table of Chemical Thermodynamic Properties - Selected Values for Inorganic and C1 and C2 Organic Substances in SI Units." J. Phys. Chem. Ref. Data: 11, Supplement No. 2.

APPENDIX B

COMPLETE SUMMARY FOR THERMODYNAMIC DATA OF CYANIDE

APPENDIX B

COMPLETE SUMMARY FOR THERMODYNAMIC DATA OF CYANIDE

The data tabulation follows the order of data presentation for compounds in the most complete reference for the thermodynamic data reviewed. This is the National Bureau of Standards publication by Wagman et al. (1982). The order of data tabulation by element in Wagman et al. (1982) is shown in Table B.1, along with the MINTEQ ID for the element. In addition, the page number where the element is first referenced in the thermodynamic tabulation for cyanide, Table B.2, is included.

The thermodynamic data are listed in Table B.2. The column heading "In 82" refers to Wagman et al. (1982). Under this heading, the page number and order of presentation of cyanide on that page in 82WE is listed. The order is listed under the heading 'ID', but the numerical value in the order is increased and multiplied by ten. This expansion of the numerical order facilitates the following:

- listing all data in units of kilocalories because the database for MINTEQ is conventionally assembled in those units
- listing data reported in the units of kilojoules on one line and listing the same data on the following line in units of kilocalories
- using an ID number for a summary line for each compound
- cross-referencing the MINTEQ identification number on the summary line for selected compounds to include in MINTEQ with the citation in Wagman et al. (1982)
- inserting additional data from other sources without disturbing the ID sequence since the last number was initially selected as zero for each ID number. This allows insertion of up to nine lines between initially selected ID numbers.

TABLE B.1. Data Tabulation by NBS Order Number of Elements

NBS Order No.	Element	MINTEQ Number	Data Start on page	NBS Order No.	Element	MINTEQ Number	Data Start on page
1	O	56		49	Tc	83	
2	H	33		50	Re	69	
3	He	34		51	Cr	21	B.29
4	Ne	53		52	Mo	48	
5	Ar	5		53	W	91	
6	Kr	42		54	V	90	
7	Xe	92		55	Nb	51	
8	Rn	71		56	Ta	81	
9	F	27		57	Ti	86	
10	Cl	18		58	Zr	96	
11	Br	13		59	Hf	35	
12	I	38	B.7	60	Sc	75	
13	At	7		61	Y	93	
14	S	73		62	Lu	45	
15	Se	76		63	Yb	94	
16	Te	84		64	Tm	88	
17	Po	63		65	Er	25	
18	N	49	B.4	66	Ho	37	
19	P	58		67	Dy	24	
20	As	6		68	Tb	82	
21	Sb	74		69	Gd	31	
22	Bi	12		70	Eu	26	
23	C	14	B.3	71	Sm	78	
24	Si	77		72	Pm	62	
25	Ge	32		73	Nd	52	
26	Sn	79		74	Pr	64	
27	Pb	60	B.8	75	Ce	17	
28	B	9		76	La	43	B.30
29	Al	3		84	Cm	19	
30	Ga	30		85	Am	4	
31	In	39		86	Pu	66	
32	Tl	87	B.8	87	Np	55	
33	Zn	95	B.9	88	U	89	
34	Cd	16	B.10	89	Pa	59	
35	Hg	36	B.12	90	Th	85	
36	Cu	23	B.16	91	Ac	1	
37	Ag	2	B.17	92	Be	11	
38	Au	8	B.19	93	Mg	46	B.30
39	Ni	54	B.20	94	Ca	15	B.33
40	Co	20	B.21	95	Sr	80	B.38
41	Fe	28	B.22	96	Ba	10	B.41
42	Pd	61	B.28	97	Ra	67	
43	Rh	70		98	Li	44	B.45
44	Ru	72		99	Na	50	B.48
45	Pt	65	B.29	100	K	41	B.58
46	Ir	40		101	Rb	68	B.72
47	Os	57		102	Cs	22	B.78
48	Mn	47	B.29	103	Fr	29	

TABLE B.2. Complete Summary for Thermodynamic Data of Cyanide(a)

MINTeq Number	Location		Form	Compound	Energy Units				Data Sources(e)
	In 82WE	Page ID			(Q) State	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°	
			(b)		(c) (d)	(Q/mol)	(Q/mol)	(Q/mol·K)	
	89	18	CN ⁻		*J ao	172.4	158.8	94.1	82WE 2-89
	89	28	CN ⁻		!C ao	41.20	35.99	22.5	82WE 2-89
	89	38	CN ⁻	std. state, m = 1	*C ao	41.2	36.8	22.5	68WE 122
	89	48	CN ⁻		!C ao	41.2	36.8	27.6	78BS 36 (R1 NBS Series)

(a) Values indicated by 'NA' are not available in the literature reviewed in this study.

(b) S = solid, A = aqueous. There are three codes under the general form for the compound:

A-# and S-# indicate that the compound was selected for the MINTeq data base, i.e.,

A-# for aqueous compounds selected, and S-# for solids selected.

A-1 and S-1 indicate that elements are not in the MINTeq database, or that 'ai' and 'aq' forms of aqueous solutions are not in the MINTeq database.

A-2 and S-2 indicate that ΔG is not available and hence cannot be included in the MINTeq database.

(c) *C = data reported in units of kcal; *J = data reported in units of kJoule; !C = data in units of kcal calculated from the *J data; i.e., !C = *J/4.184. The summary line for each chemical formulation is listed in units of kcal since the database for MINTeq is conventionally assembled in units of kcal.

(d) The reference code lists in order

1) the last two digits of the year when the reference was published,

2) the first letter of the surnames of the first two authors listed for the reference, and

3) the page number in the reference on which the data are listed.

A second source of the data is provided in parentheses, which used the data in the first reference. The number of significant figures in the data listed in this table is taken from the first reference. A semicolon separates additional references for succeeding entries. A semicolon is also used to distinguish multiple references for $\Delta G_f^\circ, 298$, $\Delta H_f^\circ, 298$, and S_{298}° .

(e) Symbols used in the table for physical states follow the convention of Wagman et al. (1982). Symbols used in earlier NBS reports are listed after those in Wagman et al. (1982).

ai, a = aqueous solution, ionized substance standard, m = 1 mol/kg.

ao = aqueous solution, un-ionized substance, standard state, m = 1 mol/kg, or an ion for which here no further ionization is considered.

aq, au = aqueous solution, concentration unspecified - Such solutions may be assumed to be "dilute".

cr = crystalline solid - The symbols above occasionally are modified by number to distinguish two substance in the same state: a numeral is appended to the physical state designation, e.g., cr2, cr3, etc. A more general designation is i2, i3, etc.

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol.K)	Data Sources
Summary data selected for reasons 2 and 3(a)								
89	58	A-8	CN ⁻ std. state, n = 1	*C so	41.2	36.8	22.5	82WE 2-89
143	89	61	A-8	CN ⁻ Selected as basis specie for MINTeq				
89	106		DCN ⁻	*J so	-97.4	-146.8	166.7	82WE 2-89
89	118		OCN ⁻	IC so	-23.3	-34.89	25.58	82WE 2-89
89	128		DCN ⁻	*C sq	-23.3	-34.9	25.5	88WE 122
89	138		OCN ⁻	*C so	-23.3	-34.9	38.6	78BS 36 (R1 NBS Series)
Summary data selected for reasons 2 and 3								
89	148	A-8	DCN ⁻ cyanogen	*C so	-23.3	-34.9	25.5	82WE 2-89
144	89	141	A-8	DCN ⁻ Selected as basis specie for MINTeq				
89	88		N ₃ CN	*J cr	NA	387.4	NA	82WE 2-89
89	78		N ₃ CN	IC cr	NA	92.59	NA	82WE 2-89
89	88		N ₃ CN	*C cr	NA	92.6	NA	88WE 122
Summary data selected for reason 2								
89	98	S-2	N ₃ CN cyanogen azide	*C cr	NA	92.6	NA	82WE 2-89
89	91		NH ₄ Fe(CN) ₆ ³⁻	*C so	143.78	78.35	64.88	86CR

(a) Summary line selected to represent the data listed in the prior lines for this compound.

The reasons used to select the data included in the summary line follow:

1. After change of energy units, the significant figures for data in 82WE are the same as earlier NBS publications.
2. Significant figures for data taken from earlier NBS document with energy units reported in kcal.
3. Data in NBS documentation selected as commonly accepted value.
4. Only data reviewed in this study.
5. Errata revision from earlier National Bureau of Standards publication.
6. More recent documentation than Wagman et al. (1982), or other early documentation.

There are three additional summary lines for each compound which is selected for the MINTeq database.

First line: Chemical reaction selected to represent the formation of the compound.

Second line: Number selected for MINTeq followed by the chemical compound.

Third line: The first number in the compound column represents the number of basis species used. This is followed by several groups of paired entries that represent the contribution from each basis species. In each group, the first entry is the number of basis species required; the second entry is the identification number used to represent the basis species.

TABLE B.2. (contd)

MINTEQA	In 82WE			Units	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°	
Number	Page	ID	Form	Compound	Q	State	(Q/mol)	Data Sources
Summary data selected for reason 4								
	89	92		$\text{NH}_4\text{Fe}(\text{CN})_6^{3-}$	*C	ao	143.78	78.35 64.88 86CR
4981431	89	94	A-8	$\text{NH}_4^+ + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{NH}_4\text{Fe}(\text{CN})_6^{3-}$				
	89	95	A-8	4981431 $\text{NH}_4\text{Fe}(\text{CN})_6^{3-}$				
	89	96		3 1.000 498 1.000 286 6.000 143				
	89	96		$(\text{NH}_4)_2\text{Fe}(\text{CN})_6^{2-}$	*C	ao	123.78	48.88 188.88 86CR
Summary data selected for reason 4								
	89	97	A-8	$(\text{NH}_4)_2\text{Fe}(\text{CN})_6^{2-}$	*C	ao	123.78	48.88 188.88 86CR
4981432	89	98	A-8	$2\text{NH}_4^+ + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow (\text{NH}_4)_2\text{Fe}(\text{CN})_6^{2-}$				
	89	99	A-8	4981432 $(\text{NH}_4)_2\text{Fe}(\text{CN})_6^{2-}$				
	89	101		3 2.000 498 1.000 286 6.000 143				
	89	102		$\text{NH}_5\text{Fe}(\text{CN})_6^{2-}$	*C	ao	139.23	78.95 82.87 86CR
Summary data selected for reason 4								
	89	103		$\text{NH}_5\text{Fe}(\text{CN})_6^{2-}$	*C	ao	139.23	78.95 82.87 86CR
4981433	89	105	A-8	$\text{NH}_4^+ + \text{H}^+ + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{NH}_5\text{Fe}(\text{CN})_6^{2-}$				
	89	106	A-8	4981433 $\text{NH}_5\text{Fe}(\text{CN})_6^{2-}$				
	89	107		4 1.000 498 1.000 338 1.000 286 6.000 143				
	89	149		HCN	*C	ao	28.64	25.67 29.64 78SM 28
	89	150		HCN	*J	ao	119.7	167.1 124.7 82WE 2-89
	89	166		HCN	!C	ao	28.61	25.66 29.66 82WE 2-89
	89	176		HCN un-ionized; std. stat, n = 1	*C	aq	28.6	25.6 29.6 88WE 122
	89	186		HCN std. stat, n = 1	*C	aq	41.2	36.8 22.5 88WE 122
	89	196		HCN undissociated complex	*C	ao	28.6	25.6 29.6 78BS 53 (R1 NBS Series)
	89	191		HCN	*C	ao	28.64	NA NA 87B
Summary data selected for reasons 2 and 3								
	89	200	A-8	HCN un-ionized; std. stat, n = 1	*C	ao	28.6	25.6 29.6 82WE 2-89
3381431	89	201	A-8	$\text{CN}^- + \text{H}^+ \leftrightarrow \text{HCN}$				
	89	202	A-8	3381431 HCN				

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
89 203	2	1.000 143 1.000 330					
89 210	NH ₂ CN		*J cr3	NA	59.0	NA	82WE 2-89
89 220	NH ₂ CN		!C cr3	NA	14.1	NA	82WE 2-89
89 230	NH ₂ CN		*C cr3	NA	14.1	NA	88WE 123
Summary data selected for reason 1							
89 240	S-2 NH ₂ CN	cyanamide	!C cr3	NA	14.1	NA	82WE 2-89
89 250	NH ₂ CN cyanamide in 600 H ₂ O		*J	NA	74.5	NA	82WE 2-89
89 260	NH ₂ CN cyanamide in 600 H ₂ O		!C	NA	17.8	NA	82WE 2-89
89 270	NH ₂ CN cyanamide in 600 H ₂ O		*C aq	NA	17.8	NA	88WE 123
Summary data selected for reason 1							
89 280	A-2 NH ₂ CN cyanamide in 600 H ₂ O		!C	NA	17.8	NA	82WE 2-89
89 290	NH ₄ CN		*J cr	NA	0.42	NA	82WE 2-89
89 300	NH ₄ CN		!C cr	NA	0.10	NA	82WE 2-89
89 310	NH ₄ CN		*C cr	NA	0.10	NA	88WE 123
Summary data selected for reason 1							
89 320	S-2 NH ₄ CN		!C cr	NA	0.10	NA	82WE 2-89
89 330	NH ₄ CN		*J ai	93.0	10.0	207.5	82WE 2-89
89 340	NH ₄ CN		!C ai	22.2	4.30	49.60	82WE 2-89
89 350	NH ₄ CN std. state, n = 1		*C aq	22.2	4.3	49.6	88WE 123
Summary data selected for reason 2							
89 360	A-1 NH ₄ CN std. state, n = 1		*C ai	22.2	4.3	49.6	82WE 2-89
90 10	NH ₄ CN		*J aq	NA	32.2	NA	82WE 2-90
90 20	NH ₄ CN		!C aq	NA	7.70	NA	82WE 2-90
90 30	NH ₄ CN		*C aq	NA	7.70	NA	88WE 123
Summary data selected for reason 1							
90 40	A-2 NH ₄ CN		!C aq	NA	7.70	NA	82WE 2-90
90 50	HOCN		*J ai2	-97.4	-148.0	100.7	82WE 2-90
90 60	HOCN	cyanic acid	!C ai2	-23.3	-34.80	25.50	82WE 2-90
90 70	HOCN	std. state, n = 1, ionized	*C aq	-23.3	-34.9	25.5	88WE 124
Summary data selected for reason 2							
90 80	A-1 HOCN	std. state, n = 1, ionized	*C ai2	-23.3	-34.9	25.5	82WE 2-90
90 90	HOCN		*J ao2	-117.1	-154.30	144.8	82WE 2-90
90 100	HOCN	cyanic acid	!C ao2	-27.99	-36.000	34.61	82WE 2-90

TABLE B.2. (contd)

MINTEQA	In 82WE			Units	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°	Data Sources		
Number	Page	ID	Form	Compound	Q State (Q/mol)	(Q/mol)	(Q/mol·K)			
	98	110		HOCN un-ionized, std. state, m=1	*C aq	-28.8	-36.9	34.6	88WE 124	
	98	111		HOCN	*C ao	-28.86	-36.98	34.72	76SM 28	
Summary data selected for reason 2										
	98	120	A-8	HOCN un-ionized, std. state, m=1	*C ao	-28.8	-36.9	34.6	82WE 2-98	
3381441	98	121	A-8	$\text{OCN}^- + \text{H}^+ \leftrightarrow \text{HOCN}$						
	98	122	A-8	3381441 HOCN						
	98	123		2	1.888 144	1.888 338				
	91	18		NH ₄ OCN	*J cr2	NA	-384.89	NA	82WE 2-91	
	91	26		NH ₄ OCN	!C cr2	NA	-72.751	NA	82WE 2-91	
Summary data selected for reason 4										
	91	38	S-2	NH ₄ OCN	ammonium cyanogen	!C cr2	NA	-72.751	NA	82WE 2-91
	91	48		NH ₄ OCN	*J ai2	-178.9	-278.7	228.1	82WE 2-91	
	91	58		NH ₄ OCN	!C ai2	-42.28	-88.61	52.61	82WE 2-91	
Summary data selected for reason 4										
	91	68	A-1	NH ₄ OCN	ammonium cyanogen	!C ai2	-42.28	-88.61	52.61	82WE 2-91
	91	78		CNCl	*J l	NA	112.89	NA	82WE 2-91	
	91	88		CNCl	!C l	NA	26.798	NA	82WE 2-91	
Summary data selected for reason 4										
	91	98	A-2	CNCl	cyanogen chloride	!C l	NA	26.798	NA	82WE 2-91
	92	18		CNBr	*J cr	NA	148.5	NA	82WE 2-92	
	92	28		CNBr	!C cr	NA	33.58	NA	82WE 2-92	
	92	38		CNBr	*C cr	NA	33.58	NA	88WE 129	
Summary data selected for reason 1										
	92	48	S-2	CNBr	cyanogen bromide	!C cr	NA	33.58	NA	82WE 2-92
	92	58		CNI	*J cr	185.83	166.15	98.2	82WE 2-92	
	92	68		CNI	!C cr	44.223	39.711	23.8	82WE 2-92	
	92	78		CNI	*C cr	44.22	39.71	23.8	88WE 129	
Summary data selected for reason 2										
	92	88	S-8	CNI	cyanogen iodide	*C cr	44.22	39.71	23.8	82WE 2-92
1138881	92	81	S-8	$\text{CN}^- + \text{I}^- \leftrightarrow \text{CNI} + 2\text{e}^-$						

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units g State	$\Delta G_f^\circ, 298$ (g/mol)	$\Delta H_f^\circ, 298$ (g/mol)	S_{298}° (g/mol·K)	Data Sources
92	82	S-8	1138881 CNI					
92	83		3 1.000 143 1.000 388 -1.000 1					
92	96		CNI	*J ai	188.89	177.8	126.1	82WE 2-92
92	106		CNI	!C ai	44.955	42.56	29.96	82WE 2-92
Summary data selected for reason 4								
92	118	A-1	CNI	!C ai	44.955	42.56	29.96	82WE 2-92
92	128		I ₂ CN ⁻	*J ao	136.14	NA	NA	82WE 2-92
92	138		I ₂ CN ⁻	!C ao	32.538	NA	NA	82WE 2-92
92	148		I ₂ CN ⁻ std. state, n = 1	*C aq	32.53	NA	NA	88WE 129
Summary data selected for reason 2								
92	158	A-8	I ₂ CN ⁻ std. state, n = 1	*C ao	32.54	NA	NA	82WE 2-92
3881432	92	161	A-8 CN ⁻ + 2I ⁻ ↔ I ₂ CN ⁻ + 2e ⁻					
92	162	A-8	3881432 I ₂ CN ⁻					
92	163		3 1.000 143 2.000 388 -2.000 1					
188	18		I(CN) ₂ ⁻	*J ao	358.24	NA	NA	82WE 2-188
188	28		I(CN) ₂ ⁻	!C ao	85.621	NA	NA	82WE 2-188
188	38		I(CN) ₂ ⁻ std. state, n = 1	*C aq	85.61	NA	NA	88WE 188
Summary data selected for reason 2								
188	48	A-8	I(CN) ₂ ⁻ std. state, n = 1	*C ao	85.62	NA	NA	82WE 2-188
3881433	188	41	A-8 2CN ⁻ + I ⁻ ↔ I(CN) ₂ ⁻ + 2e ⁻					
188	42	A-8	3881433 I(CN) ₂ ⁻					
188	43		3 2.000 143 1.000 388 -2.000 1					
121	18		Pb(CN) ₂ ·2PbO·H ₂ O	*J cr	NA	-517.6	NA	82WE 2-121
121	28		Pb(CN) ₂ ·2PbO·H ₂ O	!C cr	NA	-123.7	NA	82WE 2-121
Summary data selected for reason 4								
121	38	S-2	Pb(CN) ₂ ·2PbO·H ₂ O	!C cr	NA	-123.7	NA	82WE 2-121
137	18		Tl(CN) ₄ ⁻	*J ao	783.	NA	NA	82WE 2-137

TABLE B.2. (contd)

WINTER Number	In 82WE Page ID	Form	Compound	Units g State	$\Delta G_f^\circ, 298$ (J/mol)	$\Delta H_f^\circ, 298$ (J/mol)	S_{298}° (J/mol·K)	Data Sources
137	28		$\text{Ti}(\text{CN})_4^-$	IC ao	188.	NA	NA	82WE 2-137
Summary data selected for reason 4								
137	38	A-8	$\text{Ti}(\text{CN})_4^-$	IC ao	188.	NA	NA	82WE 2-137
8781431	137	31	A-8	$4\text{CN}^- + \text{Ti}^+ \leftrightarrow \text{Ti}(\text{CN})_4^- + 2e^-$				
137	32	A-8	8781431 $\text{Ti}(\text{CN})_4^-$					
137	33		3 4.888 143 1.888 878 -2.888 1					
143	18		$\text{Zn}(\text{CN})_2$	*J cr	NA	95.8	NA	82WE 2-143
143	28		$\text{Zn}(\text{CN})_2$	IC cr	NA	22.9	NA	82WE 2-143
143	36		$\text{Zn}(\text{CN})_2$	*C cr	NA	22.9	NA	88WE 246
Summary data selected for reason 1								
143	46	A-2	$\text{Zn}(\text{CN})_2$	IC cr	NA	22.9	NA	82WE 2-143
143	41		$\text{Zn}(\text{CN})_2^0$	*C aq	32.1	24.34	32.56	78SM 26
Summary data selected for reason 4								
143	42	A-8	$\text{Zn}(\text{CN})_2^0$	*C aq	32.1	24.34	32.56	78SM 26
9581436	143	43	A-8	$2\text{CN}^- + \text{Zn}^{2+} \leftrightarrow \text{Zn}(\text{CN})_2^0$				
143	44	A-8	2 2.888 143 1.888 958					
143	45		$\text{Zn}(\text{CN})_3^-$	*C ao	66.51	51.14	46.98	78SM 26
Summary data selected for reason 4								
143	48	A-8	$\text{Zn}(\text{CN})_3^-$	*C ao	66.51	51.14	46.98	78SM 26
9581432	143	47	A-8	$3\text{CN}^- + \text{Zn}^{2+} \leftrightarrow \text{Zn}(\text{CN})_3^-$				
143	49	A-8	2 3.888 143 1.888 958					
143	49		$\text{Zn}(\text{CN})_4^{2-}$	*C ao	186.44	79.44	59.99	78SM 26
143	58		$\text{Zn}(\text{CN})_4^{2-}$	*J ao	446.9	342.8	226.	82WE 2-143
143	68		$\text{Zn}(\text{CN})_4^{2-}$	IC ao	186.8	81.81	54.8	82WE 2-143
143	78		$\text{Zn}(\text{CN})_4^{2-}$ std. state, $m = 1$	*C ao	186.8	81.8	54.	88WE 246
143	88		$\text{Zn}(\text{CN})_4^{2-}$	*C aq	186.4	82.8	86.5	78BS 89 (R5 Latimer 1952)
Summary data selected for reason 2								
143	98		$\text{Zn}(\text{CN})_4^{2-}$ std. state, $m = 1$	*C ao	186.8	81.8	54.	82WE 2-143

TABLE B.2. (contd)

WINTERQ Number	In 82WE Page ID Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
9501431	143 92 A-8	$4\text{CN}^- + \text{Zn}^{2+} \leftrightarrow \text{Zn}(\text{CN})_4^{2-}$					
	143 93 A-8	9501431 $\text{Zn}(\text{CN})_4^{2-}$					
	143 94	2 4.000 143 1.000 950					
	143 100	$(\text{Zn}(\text{CN})_2)_3 \cdot \text{ZnO}$	*J cr	NA	-57.7	NA	82WE 2-143
	143 110	$(\text{Zn}(\text{CN})_2)_3 \cdot \text{ZnO}$	!C cr	NA	-13.8	NA	82WE 2-143
	143 120	$(\text{Zn}(\text{CN})_2)_3 \cdot \text{ZnO}$	*C cr	NA	-13.8	NA	68WE 248
Summary data selected for reason 1							
	140 130 S-2	$(\text{Zn}(\text{CN})_2)_3 \cdot \text{ZnO}$	!C cr	NA	-13.8	NA	82WE 2-143
	140 9	CdCN^+	*C ao	15.36	NA	NA	76SM 27
	140 10	CdCN^+	*J ao	54.4	NA	NA	82WE 2-140
	140 20	CdCN^+	!C ao	15.4	NA	NA	82WE 2-140
	140 30	CdCN^+ std. state, $n = 1$	*C aq	15.4	NA	NA	68WE 259
Summary data selected for reason 1							
	140 40 A-8	CdCN^+	!C ao	15.4	NA	NA	82WE 2-140
1001431	140 41 A-8	$\text{CN}^- + \text{Cd}^{2+} \leftrightarrow \text{CdCN}^+$					
	140 42 A-8	1001431 CdCN^+					
	140 43	2 1.000 143 1.000 100					
	140 50	$\text{Cd}(\text{CN})_2$	*J cr	NA	162.3	NA	82WE 2-140
	140 60	$\text{Cd}(\text{CN})_2$	!C cr	NA	38.79	NA	82WE 2-140
	140 70	$\text{Cd}(\text{CN})_2$	*C cr	NA	38.8	NA	68WE 260
Summary data selected for reason 2							
	140 80 S-2	$\text{Cd}(\text{CN})_2$	*C cr	NA	38.8	NA	82WE 2-140
	140 90	$\text{Cd}(\text{CN})_2$	*J ai	267.4	225.5	115.1	82WE 2-140
	140 100	$\text{Cd}(\text{CN})_2$	!C ai	53.91	53.90	27.51	82WE 2-140
	140 110	$\text{Cd}(\text{CN})_2$ std. state, $n = 1$	*C aq	53.9	53.9	27.5	68WE 260
Summary data selected for reason 2							
	140 120 A-1	$\text{Cd}(\text{CN})_2$ std. state, $n = 1$	*C ai	53.9	53.9	27.5	82WE 2-140
	140 120	$\text{Cd}(\text{CN})_2$	*C ao	48.69	48.66	34.78	76SM 27
	140 130	$\text{Cd}(\text{CN})_2$	*J ao	268.0	NA	NA	82WE 2-140
	140 140	$\text{Cd}(\text{CN})_2$	!C ao	49.71	NA	NA	82WE 2-140
	140 150	$\text{Cd}(\text{CN})_2$ undissoc.; std. state, $n=1$	*C aq	49.7	NA	NA	68WE 260

TABLE B.2. (contd)

WINTER Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G^\circ_{f,298}$ (Q/mol)	$\Delta H^\circ_{f,298}$ (Q/mol)	S°_{298} (Q/mol·K)	Data Sources
Summary data selected for reason 2								
148	168	A-8	$\text{Cd}(\text{CN})_2^0$ undissoc.; std. state, $m=1$	C so	49.71	48.88	34.73	82WE 2-148; 76SM 27
1881432	148	161	A-8	$2\text{CN}^- + \text{Cd}^{2+} \leftrightarrow \text{Cd}(\text{CN})_2^0$				
148	162	A-8	1881432 $\text{Cd}(\text{CN})_2^0$					
148	163		2 2.888 143 1.888 168					
148	178		$\text{Cd}(\text{CN})_2$ in 888 H_2O	*J	NA	169.8	NA	82WE 2-148
148	188		$\text{Cd}(\text{CN})_2$ in 888 H_2O	!C	NA	48.39	NA	82WE 2-148
148	198		$\text{Cd}(\text{CN})_2$ in 888 H_2O	*C aq	NA	48.4	NA	88WE 268
Summary data selected for reason 2								
148	208	A-2	$\text{Cd}(\text{CN})_2^0$ in 888 H_2O	*C aq	NA	48.89	NA	82WE 2-148
148	209		$\text{Cd}(\text{CN})_3^-$	*C so	83.71	88.26	49.18	76SM 27
148	218		$\text{Cd}(\text{CN})_3^-$	*J so	354.9	NA	NA	82WE 2-148
148	228		$\text{Cd}(\text{CN})_3^-$	!C so	84.82	NA	NA	82WE 2-148
148	238		$\text{Cd}(\text{CN})_3^-$ std. state, $m = 1$	*C so	84.8	NA	NA	88WE 268
Summary data selected for reason 2								
148	248	A-8	$\text{Cd}(\text{CN})_3^-$ std. state, $m = 1$	*C so	84.82	88.26	49.18	82WE 2-148; 76SM 27
1881433	148	241	A-8	$3\text{CN}^- + \text{Cd}^{2+} \leftrightarrow \text{Cd}(\text{CN})_3^-$				
148	242	A-8	1881433 $\text{Cd}(\text{CN})_3^-$					
148	243		2 3.888 143 1.888 188					
148	249		$\text{Cd}(\text{CN})_4^{2-}$	*C so	121.82	99.16	84.92	76SM 27
148	258		$\text{Cd}(\text{CN})_4^{2-}$	*J so	587.6	428.8	322.	82WE 2-148
148	268		$\text{Cd}(\text{CN})_4^{2-}$	!C so	121.3	182.3	77.7	82WE 2-148
148	278		$\text{Cd}(\text{CN})_4^{2-}$ std. state, $m = 1$	*C so	121.3	182.3	77.	88WE 268
148	288		$\text{Cd}(\text{CN})_4^{2-}$	*C so	121.3	182.3	87.7	78BS 38 (R1 NBS Series)
Summary data selected for reasons 2 and 3								
148	298	A-8	$\text{Cd}(\text{CN})_4^{2-}$ std. state, $m = 1$	*C so	121.3	182.3	77.7	82WE 2-148

TABLE B.2. (contd)

MINTeq	In 82WE				Units	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°	
Number	Page	ID	Form	Compound	Q State	(kJ/mol)	(kJ/mol)	(J/mol.K)	Data Sources
1861434	148	291	A-8	$4\text{CN}^- + \text{Cd}^{2+} \leftrightarrow \text{Cd}(\text{CN})_4^{2-}$					
	148	292	A-8	1861434 $\text{Cd}(\text{CN})_4^{2-}$					
	148	293		2 4.888 143 1.888 186					
	148	300		$(\text{Cd}(\text{CN})_2)_2 \cdot \text{CdO} \cdot 5\text{H}_2\text{O}$	*J cr	NA	-1588.4	NA	82WE 2-148
	148	310		$(\text{Cd}(\text{CN})_2)_2 \cdot \text{CdO} \cdot 5\text{H}_2\text{O}$	!C cr	NA	-358.86	NA	82WE 2-148
	148	320		$(\text{Cd}(\text{CN})_2)_2 \cdot \text{CdO} \cdot 5\text{H}_2\text{O}$	*C cr	NA	-358.6	NA	88WE 200
Summary data selected for reason 2									
	148	330	S-2	$(\text{Cd}(\text{CN})_2)_2 \cdot \text{CdO} \cdot 5\text{H}_2\text{O}$	*C cr	NA	-358.6	NA	82WE 2-148
	153	9		HgCN^+	*C ao	57.38	63.47	13.81	76SM 27
	153	10		HgCN^+	*J ao	233.9	225.6	84.6	82WE 2-153
	153	20		HgCN^+	!C ao	55.90	63.90	20.2	82WE 2-153
	153	30		HgCN^+ std. state, m=1, rev. 89WE10+C aq		55.9	63.9	20.2	81WE 110
	153	40		HgCN^+ ΔG_f° in 89WE10 was 55.9	*C aq	55.9	64.9	16.2	78BS 57 (R1 NBS Series)
Summary data selected for reasons 2, 3 and 5									
	153	50		HgCN^+ std. state, m = 1	*C ao	55.9	63.9	20.2	82WE 2-153
3811431	153	52	A-8	$\text{CN}^- + 2\text{H}^+ + \text{Hg}(\text{OH})_2^\circ \leftrightarrow \text{HgCN}^+ + 2\text{H}_2\text{O}$					
	153	53	A-8	3811431 HgCN^+					
	153	54		4 1.888 143 1.888 381 2.888 330 -2.888 802					
	153	60		$\text{Hg}(\text{CN})_2$	*C	-85.51	NA	NA	76SM 22
	153	61		$\text{Hg}(\text{CN})_2$	*J cr	NA	263.6	NA	82WE 2-153
	153	70		$\text{Hg}(\text{CN})_2$	!C cr	NA	63.86	NA	82WE 2-153
	153	80		$\text{Hg}(\text{CN})_2$	*C cr	NA	63.8	NA	89WE 10
Summary data selected for reason 2									
	153	90	S-2	$\text{Hg}(\text{CN})_2$	*C cr	NA	63.8	NA	82WE 2-153
	153	99		$\text{Hg}(\text{CN})_2$	*C ao	77.89	68.87	29.90	76SM 27
	153	100		$\text{Hg}(\text{CN})_2$	*J ao	312.2	278.2	165.3	82WE 2-153
	153	110		$\text{Hg}(\text{CN})_2$	!C ao	74.82	68.49	39.61	82WE 2-153
	153	120		$\text{Hg}(\text{CN})_2$ S_{298}° in 89WE 10 was 37.3	*C ao	74.8	68.5	39.5	81WE 110
	153	130		$\text{Hg}(\text{CN})_2$ undissociated complex	*C aq	74.8	65.8	37.3	78BS 56 (R1 NBS Series)
Summary data selected for reasons 2, 3 and 5									
	153	140	A-8	$\text{Hg}(\text{CN})_2$ undissoc.; std. state, m=1	*C ao	74.82	68.49	39.61	82WE 2-153

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
3811432	153 141	A-8	$2\text{CN}^- + 2\text{H}^+ + \text{Hg}(\text{OH})_2^0 \leftrightarrow \text{Hg}(\text{CN})_2^0 + 2\text{H}_2\text{O}$					
	153 142	A-8	3811432 $\text{Hg}(\text{CN})_2$					
	153 143		4 2.000 143 1.000 381 2.000 330 -2.000 002					
	153 149		$\text{Hg}(\text{CN})_3^-$	*C ao	118.03	95.26	47.24	76SM 27
	153 150		$\text{Hg}(\text{CN})_3^-$	*J ao	483.2	397.1	225.1	82WE 2-153
	153 160		$\text{Hg}(\text{CN})_3^-$	!C ao	110.7	94.91	53.00	82WE 2-153
	153 170		$\text{Hg}(\text{CN})_3^-$ S_{298}° was 51.4 in 80WE 10	*C ao	110.7	94.9	53.0	81WE 110
	153 180		$\text{Hg}(\text{CN})_3^-$	*C aq	110.7	94.9	56.4	78BS 55 (R1 NBS Series)
Summary data selected for reasons 2, 3 and 5								
	153 190		$\text{Hg}(\text{CN})_3^-$ std. state, $n = 1$	*C ao	110.7	94.9	53.0	82WE 2-153
3801433	153 192	A-8	$3\text{CN}^- + 2\text{H}^+ + \text{Hg}(\text{OH})_2^0 \leftrightarrow \text{Hg}(\text{CN})_3^- + 2\text{H}_2\text{O}$					
	153 193	A-8	3811433 $\text{Hg}(\text{CN})_3^-$					
	153 194		4 3.000 143 1.000 381 2.000 330 -2.000 002					
	153 194		$\text{Hg}(\text{CN})_4^{2-}$	*C ao	151.01	124.97	59.40	76SM 27
	153 200		$\text{Hg}(\text{CN})_4^{2-}$	*J ao	618.5	526.3	305.	82WE 2-153
	153 210		$\text{Hg}(\text{CN})_4^{2-}$	!C ao	147.8	125.8	72.9	82WE 2-153
	153 220		$\text{Hg}(\text{CN})_4^{2-}$ S_{298}° was 71. in 80WE 10	*C aq	147.8	125.8	73.	81WE 110
	153 230		$\text{Hg}(\text{CN})_4^{2-}$	*C aq	147.8	125.3	81.0	78BS 55 (R1 NBS Series)
Summary data selected for reasons 2, 3 and 5								
	153 240		$\text{Hg}(\text{CN})_4^{2-}$ std. state, $n = 1$	*C ao	147.8	125.8	72.9	82WE 2-153
3811434	153 242	A-8	$4\text{CN}^- + 2\text{H}^+ + \text{Hg}(\text{OH})_2^0 \leftrightarrow \text{Hg}(\text{CN})_4^{2-} + 2\text{H}_2\text{O}$					
	153 243	A-8	3811434 $\text{Hg}(\text{CN})_4^{2-}$					
	153 244		4 4.000 143 1.000 381 2.000 330 -2.000 002					
	153 250		$\text{Hg}(\text{CN})_2 \cdot \text{HgO}$	*J cr	NA	163.0	NA	82WE 2-153

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
153 268		Hg(CN) ₂ ·HgO	!C cr	NA	39.18	NA	82WE 2-153
153 278		Hg(CN) ₂ ·HgO	*C cr	NA	39.18	NA	89WE 18
Summary data selected for reason 1							
153 288	S-2	Hg(CN) ₂ ·HgO	!C cr	NA	39.18	NA	82WE 2-153
153 298		(Hg(CN) ₂) ₃ ·HgO	*J cr	NA	683.8	NA	82WE 2-153
153 308		(Hg(CN) ₂) ₃ ·HgO	!C cr	NA	153.8	NA	82WE 2-153
153 318		(Hg(CN) ₂) ₃ ·HgO	*C cr	NA	158.8	NA	89WE 18
Summary data selected for reason 1							
153 318	S-2	(Hg(CN) ₂) ₃ ·HgO	!C cr	NA	158.8	NA	82WE 2-153
153 318		Hg(CN) ₂ Cl ⁻	*J ao	182.5	NA	NA	82WE 2-153
153 338		Hg(CN) ₂ Cl ⁻	!C ao	43.82	NA	NA	82WE 2-153
153 348		Hg(CN) ₂ Cl ⁻ std. state, n = 1	*C aq	43.8	NA	NA	89WE 18
Summary data selected for reason 2							
153 358	A-8	Hg(CN) ₂ Cl ⁻ std. state, n = 1	*C ao	43.8	NA	NA	82WE 2-153
3811435	153 351	A-8 2CN ⁻ + Cl ⁻ + Hg(OH) ₂ ⁰ + 2H ⁺ ↔ Hg(CN) ₂ Cl ⁻ + 2H ₂ O					
153 352	A-8	3811435 Hg(CN) ₂ Cl ⁻					
153 353		5 2.888 143 1.888 188 1.888 351 2.888 338 -2.888 2					
153 378		Hg(CN) ₃ Cl ²⁻	*J ao	335.	NA	NA	82WE 2-153
153 371		Hg(CN) ₃ Cl ²⁻	!C ao	88.1	NA	NA	82WE 2-153
153 388		Hg(CN) ₃ Cl ²⁻ std. state, n = 1	*C aq	88.	NA	NA	89WE 18
Summary data selected for reason 2							
153 398	A-8	Hg(CN) ₃ Cl ²⁻ std. state, n = 1	*C ao	88.1	NA	NA	82WE 2-153
3811436	153 401	A-8 3CN ⁻ + Cl ⁻ + Hg(OH) ₂ ⁰ + 2H ⁺ ↔ Hg(CN) ₃ Cl ²⁻ + 2H ₂ O					
153 402	A-8	3811436 Hg(CN) ₃ Cl ²⁻					
153 403		6 3.888 143 1.888 188 1.888 351 2.888 338 -2.888 2					
153 418		Hg(CN) ₃ Br ²⁻	*J ao	358.	NA	NA	82WE 2-153
153 411		Hg(CN) ₃ Br ²⁻	!C ao	85.1	NA	NA	82WE 2-153
153 428		Hg(CN) ₃ Br ²⁻ std. state, n = 1	*C aq	85.	NA	NA	89WE 11
Summary data selected for reason 2							
153 438	A-8	Hg(CN) ₃ Br ²⁻ std. state, n = 1	*C ao	85.1	NA	NA	82WE 2-153

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
3811437	153 441	A-8	$3\text{CN}^- + \text{Br}^- + \text{Hg}(\text{OH})_2^\circ + 2\text{H}^+ \leftrightarrow \text{Hg}(\text{CN})_3\text{Br}^{2-} + 2\text{H}_2\text{O}$					
	153 442	A-8	3811437 $\text{Hg}(\text{CN})_3\text{Br}^{2-}$					
	153 443		4 3.866 143 1.866 136 1.866 351 2.866 336 -2.86 882					
	153 456		$\text{Hg}(\text{CN})_2 \cdot \text{NH}_4\text{Cl} \cdot 7.5\text{H}_2\text{O}$	*C cr	NA	-84.1	NA	82WE 10
Summary data selected for reason 4								
	153 451	S-2	$\text{Hg}(\text{CN})_2 \cdot \text{NH}_4\text{Cl} \cdot 7.5\text{H}_2\text{O}$	*C cr	NA	-84.1	NA	82WE 10
	153 466		$\text{Hg}(\text{CN})_2 \cdot \text{NH}_4\text{Br} \cdot \text{H}_2\text{O}$	*C cr	NA	-73.8	NA	82WE 11
Summary data selected for reason 4								
	153 476	S-2	$\text{Hg}(\text{CN})_2 \cdot \text{NH}_4\text{Br} \cdot \text{H}_2\text{O}$	*C cr	NA	-73.8	NA	82WE 11
	153 486		$\text{Hg}(\text{CN})_2 \cdot \text{NH}_4\text{I} \cdot 8.25\text{H}_2\text{O}$	*J cr	NA	-48.6	NA	82WE 2-153
	153 496		$\text{Hg}(\text{CN})_2 \cdot \text{NH}_4\text{I} \cdot 8.25\text{H}_2\text{O}$	!C cr	NA	-9.7	NA	82WE 2-153
	153 506		$\text{Hg}(\text{CN})_2 \cdot \text{NH}_4\text{I} \cdot 8.25\text{H}_2\text{O}$	*C cr	NA	-9.7	NA	82WE 11
Summary data selected for reason 2								
	153 516	S-2	$\text{Hg}(\text{CN})_2 \cdot \text{NH}_4\text{I} \cdot 8.25\text{H}_2\text{O}$	*C cr	NA	-9.7	NA	82WE 2-153
	153 526		$\text{Hg}(\text{CNS})_3(\text{CN})_3^{2-}$	*J ao	553.2	NA	NA	82WE 2-153
	153 536		$\text{Hg}(\text{CNS})_3(\text{CN})_3^{2-}$	!C ao	132.2	NA	NA	82WE 2-153
Summary data selected for reason 4								
	153 546	A-1	$\text{Hg}(\text{CNS})_3(\text{CN})_3^{2-}$	!C ao	132.2	NA	NA	82WE 2-153
	153 556		$(\text{Hg}(\text{CN})_2)_2 \cdot \text{ZnCl}_2 \cdot 7\text{H}_2\text{O}$	*J cr	NA	-1991.2	NA	82WE 2-153
	153 566		$(\text{Hg}(\text{CN})_2)_2 \cdot \text{ZnCl}_2 \cdot 7\text{H}_2\text{O}$	!C cr	NA	-475.91	NA	82WE 2-153
	153 576		$(\text{Hg}(\text{CN})_2)_2 \cdot \text{ZnCl}_2 \cdot 7\text{H}_2\text{O}$	*C cr	NA	-475.9	NA	82WE 12
Summary data selected for reason 2								
	153 586	S-2	$(\text{Hg}(\text{CN})_2)_2 \cdot \text{ZnCl}_2 \cdot 7\text{H}_2\text{O}$	*C cr	NA	-475.9	NA	82WE 2-153
	153 596		$(\text{Hg}(\text{CN})_2)_2 \cdot \text{ZnBr}_2 \cdot 8\text{H}_2\text{O}$	*J cr	NA	-2228.9	NA	82WE 2-153
	153 606		$(\text{Hg}(\text{CN})_2)_2 \cdot \text{ZnBr}_2 \cdot 8\text{H}_2\text{O}$	!C cr	NA	-538.81	NA	82WE 2-153
	153 616		$(\text{Hg}(\text{CN})_2)_2 \cdot \text{ZnBr}_2 \cdot 8\text{H}_2\text{O}$	*C cr	NA	-538.8	NA	82WE 12
Summary data selected for reason 2								
	153 626	S-2	$(\text{Hg}(\text{CN})_2)_2 \cdot \text{ZnBr}_2 \cdot 8\text{H}_2\text{O}$	*C cr	NA	-538.81	NA	82WE 2-153
	153 636		$\text{Hg}(\text{CN})_2 \cdot \text{CdCl}_2 \cdot 2\text{H}_2\text{O}$	*J cr	NA	-739.7	NA	82WE 2-153
	153 646		$\text{Hg}(\text{CN})_2 \cdot \text{CdCl}_2 \cdot 2\text{H}_2\text{O}$	!C cr	NA	-176.8	NA	82WE 2-153
	153 656		$\text{Hg}(\text{CN})_2 \cdot \text{CdCl}_2 \cdot 2\text{H}_2\text{O}$	*C cr	NA	-176.8	NA	82WE 12

TABLE B.2. (contd)

MINTEQA	In 82WE				Units	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°	
Number	Page	ID	Form	Compound	Q State	(Q/mol)	(Q/mol)	(Q/mol·K)	Data Sources
Summary data selected for reason 1									
153	656	S-2		Hg(CN) ₂ ·CdCl ₂ ·2H ₂ O	!C cr	NA	-176.8	NA	82WE 2-153
153	676			Hg(CN) ₂ ·CdBr ₂ ·3H ₂ O	*J cr	NA	-955.6	NA	82WE 2-153
153	666			Hg(CN) ₂ ·CdBr ₂ ·3H ₂ O	!C cr	NA	-228.4	NA	82WE 2-153
153	696			Hg(CN) ₂ ·CdBr ₂ ·3H ₂ O	*C cr	NA	-228.4	NA	69WE 12
Summary data selected for reason 1									
153	766	S-2		Hg(CN) ₂ ·CdBr ₂ ·3H ₂ O	!C cr	NA	-228.4	NA	82WE 2-153
153	716			(Hg(CN) ₂) ₂ ·CdI ₂ ·8H ₂ O	*J cr	NA	-2838.8	NA	82WE 2-153
153	726			(Hg(CN) ₂) ₂ ·CdI ₂ ·8H ₂ O	!C cr	NA	-487.89	NA	82WE 2-153
153	736			(Hg(CN) ₂) ₂ ·CdI ₂ ·8H ₂ O	*C cr	NA	-487.1	NA	69WE 12
Summary data selected for reason 1									
153	746	S-2		(Hg(CN) ₂) ₂ ·CdI ₂ ·8H ₂ O	*C cr	NA	-487.89	NA	82WE 2-158
158	16			CuCN	*J cr	111.3	96.2	84.5	82WE 2-158
158	26			CuCN	!C cr	26.66	23.6	26.2	82WE 2-158
158	36			CuCN	*C cr	26.66	23.6	26.2	69WE 26
Summary data selected for reason 1									
158	46	S-6		CuCN	*C cr	26.66	23.6	26.2	82WE 2-158
1123661	158	41	S-6	CN ⁻ + Cu ⁺ ↔ CuCN					
158	42	S-6		1123661 CuCN					
158	48		2	1.666 143 1.666 236					
158	49			Cu(CN) ₂ ⁻	*C ao	72.22	66.1	31.55	76SM 26
158	56			Cu(CN) ₂ ⁻	*J ao	257.8	NA	NA	82WE 2-158
158	66			Cu(CN) ₂ ⁻	!C ao	61.62	NA	NA	82WE 2-158
158	76			Cu(CN) ₂ ⁻ std. state, n = 1	*C aq	61.6	NA	NA	69WE 26
Summary data selected for reason 2									
158	66	A-6		Cu(CN) ₂ ⁻ std. state, n = 1	*C ao	61.62	66.1	31.55	82WE 2-158; 76SM 26
2361432	158	81	A-6	2CN ⁻ + Cu ⁺ ↔ Cu(CN) ₂ ⁻					
158	82	A-6		2361432 Cu(CN) ₂ ⁻					

TABLE B.2. (contd)

MINTEQA Number	In 82WE Page ID	Form	Compound	Units g State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
158	83	2	2.000 143	1.000 230				
158	84		$\text{Cu}(\text{CN})_3^{2-}$	*C aq	100.14	85.0	41.24	76SM 26
158	90		$\text{Cu}(\text{CN})_3^{2-}$	*J ao	483.8	NA	NA	82WE 2-158
158	100		$\text{Cu}(\text{CN})_3^{2-}$	!C ao	90.51	NA	NA	82WE 2-158
158	110		$\text{Cu}(\text{CN})_3^{2-}$ std. state, $m = 1$	*C aq	90.5	NA	NA	89WE 25
Summary data selected for reason 2								
158	120	A-#	$\text{Cu}(\text{CN})_3^{2-}$ std. state, $m = 1$	*C ao	90.51	85.0	41.24	82WE 2-158; 76SM 26
2301433	158	121	A-# $3\text{CN}^- + \text{Cu}^+ \leftrightarrow \text{Cu}(\text{CN})_3^{2-}$					
158	122	A-#	2301433 $\text{Cu}(\text{CN})_3^{2-}$					
158	123	2	3.000 143	1.000 230				
158	124		$\text{Cu}(\text{CN})_4^{3-}$	*C aq	145.29	109.8	33.05	76SM 26
158	130		$\text{Cu}(\text{CN})_4^{3-}$	*J ao	506.8	NA	NA	82WE 2-158
158	140		$\text{Cu}(\text{CN})_4^{3-}$	!C ao	135.4	NA	NA	82WE 2-158
158	150		$\text{Cu}(\text{CN})_4^{3-}$ std. state, $m = 1$	*C aq	135.4	NA	NA	89WE 25
Summary data selected for reason 1								
158	160	A-#	$\text{Cu}(\text{CN})_4^{3-}$	!C ao	135.4	109.8	33.05	82WE 2-158; 76SM 26
2301431	158	161	A-# $4\text{CN}^- + \text{Cu}^+ \leftrightarrow \text{Cu}(\text{CN})_4^{3-}$					
158	162	A-#	2301431 $\text{Cu}(\text{CN})_4^{3-}$					
158	163	2	4.000 143	1.000 230				
163	18		AgCN	*J cr	156.9	146.0	107.19	82WE 2-163
163	20		AgCN	!C cr	37.50	34.89	25.619	82WE 2-163
163	30		AgCN	*C cr	37.5	34.9	25.62	89WE 37
Summary data selected for reason 2								
163	40	S-#	AgCN	*C cr	37.50	34.89	25.619	82WE 2-163
1102002	163	41	S-# $\text{CN}^- + \text{Ag}^+ \leftrightarrow \text{AgCN}$					
163	42	S-#	1102002 AgCN					

TABLE B.2. (contd)

MINTED	In 82WE				Units	ΔG_f° , 298	ΔH_f° , 298	S_{298}°	
Number	Page	ID	Form	Compound	Q State	(Q/mol)	(Q/mol)	(Q/mol·K)	Data Sources
183	43	2		1.000 143	1.000 020				
183	50		AgCN		*J ai	249.4	256.1	166.9	82WE 2-183
183	60		AgCN		!C ai	59.61	61.21	99.89	82WE 2-183
183	70		AgCN	std. state, n = 1	*C aq	59.6	61.2	99.9	69WE 37
Summary data selected for reason 2									
183	80	A-1	AgCN	std. state, n = 1	*C ai	59.61	61.21	99.89	69WE 37 (82WE 2-183)
183	90		$\text{Ag}(\text{CN})_2^-$		*C aq	72.89	64.38	45.87	76SM 26
183	91		$\text{Ag}(\text{CN})_2^-$		*J ao	305.5	276.3	192.	82WE 2-183
183	100		$\text{Ag}(\text{CN})_2^-$		!C ao	73.02	64.66	45.9	82WE 2-183
183	110		$\text{Ag}(\text{CN})_2^-$	std. state, n = 1	*C aq	73.0	64.6	46.	69WE 37
183	120		$\text{Ag}(\text{CN})_2^-$	(Crias - Cobble Type 3)	*C aq	73.0	64.6	51.0	78BS 28 (R1 NBS Series)
183	130		$\text{Ag}(\text{CN})_2^-$	(Crias - Cobble Type 2)	*C aq	68.3	58.6	46.0	78BS 31 (R1 NBS Series)
Summary data selected for reasons 2 and 3									
183	140	A-0	$\text{Ag}(\text{CN})_2^-$	std. state, n = 1	*C ao	73.02	64.66	45.9	82WE 2-183
0201432	183	141	A-0	$2\text{CN}^- + \text{Ag}^+ \leftrightarrow \text{Ag}(\text{CN})_2^-$					
183	142	A-0	0201432	$\text{Ag}(\text{CN})_2^-$					
183	143	2		2.000 143	1.000 020				
183	145		$\text{Ag}(\text{CN})_3^{2-}$		*C aq	112.83	99.78	70.58	76SM 26
Summary data selected for reason 2									
183	146		$\text{Ag}(\text{CN})_3^{2-}$		*C aq	112.83	99.78	70.58	76SM 26
0201433	183	147		$3\text{CN}^- + \text{Ag}^+ \leftrightarrow \text{Ag}(\text{CN})_3^{2-}$					
183	148	2		3.000 143	1.000 020				
183	150		AgCN ₂		*J cr	NA	235.1	NA	82WE 2-183
183	160		AgCN ₂		!C cr	NA	56.19	NA	82WE 2-183
183	170		AgCN ₂		*C cr	NA	56.2	NA	69WE 37
Summary data selected for reason 2									
183	180	S-2	AgCN ₂	silver cyanamide	*C cr		56.19	NA	82WE 2-183

TABLE B.2. (contd)

WINTER	In 82WE				Units	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°	
Number	Page	ID	Form	Compound	Q State	(Q/mol)	(Q/mol)	(Q/mol·K)	Data Sources
183	198			AgOCN	*C	-4.18	NA	NA	76SM 28
183	191			AgOCN	*J cr2	-58.1	-95.4	121.	82WE 2-183
183	208			AgOCN	!C cr2	-13.9	-22.8	28.9	82WE 2-183
Summary data selected for reason 4									
183	218			AgOCN silver cyanogen	!C cr2	-13.9	-22.8	28.9	82WE 2-183
7714481	183	212	S-#	$\text{OCN}^- + \text{Ag}^+ \leftrightarrow \text{AgOCN crystal}$					
183	213	S-#	7714481	AgOCN					
183	214		2	1.888 144	1.888 828				
183	215			$\text{Ag}(\text{OCN})_2^-$	*C aq	-35.8	NA	NA	76SM 28
Summary data selected for reason 4									
183	218			$\text{Ag}(\text{OCN})_2^-$	*C aq	-35.8	NA	NA	76SM 28
8281448	183	217	A-#	$2\text{OCN}^- + \text{Ag}^+ \leftrightarrow \text{Ag}(\text{OCN})_2^-$					
183	218		2	2.888 144	1.888 828				
183	228			AgCN·NH ₃	*J cr	NA	42.	NA	82WE 2-183
183	238			AgCN·NH ₃	!C cr	NA	18.	NA	82WE 2-183
183	248			AgCN·NH ₃	*C cr	NA	18.	NA	82WE 37
Summary data selected for reason 1									
183	258	S-2		AgCN·NH ₃	!C cr	NA	18.	NA	82WE 2-183
183	259			$\text{Ag}(\text{CN})\text{OH}^-$	*C ao	4.82	NA	NA	76SM 28
183	268			$\text{Ag}(\text{CN})\text{OH}^-$	*J ao	15.5	NA	NA	82WE 2-183
183	278			$\text{Ag}(\text{CN})\text{OH}^-$	!C ao	3.78	NA	NA	82WE 2-183
Summary data selected for reason 4									
183	288	A-#		$\text{Ag}(\text{CN})\text{OH}^-$	!C ao	3.78	NA	NA	82WE 2-183
8281431	183	281	A-#	$\text{CN}^- + \text{Ag}^+ + \text{H}_2\text{O} \leftrightarrow \text{Ag}(\text{CN})\text{OH}^- + \text{H}^+$					
183	282	A-#	8281431	$\text{Ag}(\text{CN})\text{OH}^-$					
183	283		4	1.888 143	1.888 828	1.888 2	-1.888 338		
184	18			$\text{Au}(\text{CN})_2^-$	*J ao	285.8	242.3	172.	82WE 2-184
184	28			$\text{Au}(\text{CN})_2^-$	!C ao	88.31	57.91	41.1	82WE 2-184
184	38			$\text{Au}(\text{CN})_2^-$ std. state, m = 1	*C aq	88.3	57.9	41.	82WE 41

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
Summary data selected for reason 2								
184	48	A-1	$\text{Au}(\text{CN})_2^-$	std. state, m = 1	*C ao	3.3	57.9	41.1 82WE 2-184
189	18		$\text{Ni}(\text{CN})_2$	precipitated	*J cr	NA	127.8	NA 82WE 2-189
189	28		$\text{Ni}(\text{CN})_2$	precipitated	!C cr	NA	38.58	NA 82WE 2-189
189	38		$\text{Ni}(\text{CN})_2$	precipitated	*C cr	NA	38.58???	NA 89WE 51
Summary data selected for reason 2								
189	48		$\text{Ni}(\text{CN})_2$	precipitated	*C cr	NA	38.58	NA 82WE 2-189
189	58		$\text{Ni}(\text{CN})_2$		*J ai	299.2	247.3	59.4 82WE 2-189
189	68		$\text{Ni}(\text{CN})_2$		!C ai	71.51	59.11	14.2 82WE 2-189
189	78		$\text{Ni}(\text{CN})_2$	std. state, m = 1	*C ai	71.5	59.1	14.2 89WE 51
Summary data selected for reason 2								
189	88	A-1	$\text{Ni}(\text{CN})_2$	std. state, m = 1	*C ai	71.51	59.11	14.2 82WE 2-189
189	88		$\text{Ni}(\text{CN})_4^{2-}$		*C ao	111.75	NA	52.58 87B
189	89		$\text{Ni}(\text{CN})_4^{2-}$		*C aq	112.88	87.9	52.58 78SM 28
189	98		$\text{Ni}(\text{CN})_4^{2-}$		*J ao	472.1	387.8	218. 82WE 2-189
189	108		$\text{Ni}(\text{CN})_4^{2-}$		!C ao	112.8	87.91	52.1 82WE 2-189
189	118		$\text{Ni}(\text{CN})_4^{2-}$	std. state, m = 1	*C ao	112.8	87.9	52. 89WE 51
189	128		$\text{Ni}(\text{CN})_4^{2-}$		*C ao	112.8	87.9	52.8 78BS 72 (R1 NBS Series)
Summary data selected for reasons 2 and 3								
189	138	A-8	$\text{Ni}(\text{CN})_4^{2-}$	std. state, m = 1	*C ao	112.8	87.9	52. 82WE 2-189
5481431	189	131	A-8 $4\text{CN}^- + \text{Ni}^{2+} \leftrightarrow \text{Ni}(\text{CN})_4^{2-}$					
189	132	A-8	5481431 $\text{Ni}(\text{CN})_4^{2-}$					
189	133		2 4.888 143 1.888 548					
189	148		$\text{Ni}(\text{CN})_4^-$		*C ao	183.765	NA	NA 78SM 28
Summary data selected for reason 4								
189	141		$\text{Ni}(\text{CN})_4^-$		*C ao	183.765	NA	NA 78SM 28
5481432	189	142	$\text{Ni}^{2+} + \text{H}^+ + 4\text{CN}^- \leftrightarrow \text{Ni}(\text{CN})_4^-$					

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
	169 143	5481432	NiFe(CN)_4^-					
	169 144	3	1.000 548	1.000 330	4.000 143			
	169 150	$\text{NiH}_2(\text{CN})_4^0$		*C ao	97.84	NA	NA	78SM 26
Summary data selected for reason 4								
	169 151	$\text{NiH}_2(\text{CN})_4^0$		*C ao	97.84	NA	NA	78SM 26
5481433	169 152	$\text{Ni}^{2+} + 2\text{H}^+ + 4\text{CN}^- \leftrightarrow \text{NiH}_2(\text{CN})_4^0$						
	169 153	5481433	$\text{NiH}_2(\text{CN})_4^0$					
		3	1.000 548	2.000 330	4.000 143			
	169 160	$\text{NiH}_3(\text{CN})_4^+$		*C ao	93.94	NA	NA	78SM 26
Summary data selected for reason 4								
	169 161	$\text{NiH}_3(\text{CN})_4^+$		*C ao	93.94	NA	NA	78SM 26
5481434	169 162	$\text{Ni}^{2+} + 3\text{H}^+ + 4\text{CN}^- \leftrightarrow \text{NiH}_3(\text{CN})_4^+$						
	169 163	5481434	$\text{NiH}_3(\text{CN})_4^+$					
	169 164	3	1.000 548	3.000 330	4.000 143			
	169 170	Ni(CN)_2^0		*C ao	51.60	NA	NA	78SM 26
Summary data selected for reason 4								
	169 171	Ni(CN)_2^0		*C ao	51.60	NA	NA	78SM 26
5481435	169 172	$\text{Ni}^{2+} + 2\text{CN}^- \leftrightarrow \text{Ni(CN)}_2^0$						
	169 173	5481435	Ni(CN)_2^0					
	169 174	2	1.000 548	2.000 143				
	169 186	Ni(CN)_3^-		*C ao	81.82	NA	NA	78SM 26
5481436	169 181	$\text{Ni}^{2+} + 3\text{CN}^- \leftrightarrow \text{Ni(CN)}_3^-$						
	169 182	5481436	Ni(CN)_3^-					
	169 183	2	1.000 548	3.000 143				
	175 18	Co(CN)_6^{3-}		*J ao	NA	NA	232.6	82WE 2-175
	175 20	Co(CN)_6^{3-}		!C ao	NA	NA	55.59	82WE 2-175
	175 30	Co(CN)_6^{3-}	std. state, m = 1	*C sq	NA	NA	55.6	80WE 69

TABLE B.2. (contd)

WINTER Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S°_{298} (Q/mol·K)	Data Sources
Summary data selected for reason 2								
175	48	A-2	$\text{Co}(\text{CN})_6^{3-}$	std. state, n = 1	*C ao	NA	NA	55.59 82WE 2-175
181	8		$\text{Fe}(\text{CN})_6^{3-}$		*C ao	185.22	NA	NA 87B
181	9		$\text{Fe}(\text{CN})_6^{3-}$		*C aq	186.63	134.3	23.85 76SM 26
181	10		$\text{Fe}(\text{CN})_6^{3-}$		*J ao	729.4	581.9	276.3 82WE 2-181
181	20		$\text{Fe}(\text{CN})_6^{3-}$		!C ao	174.3	134.3	84.68 82WE 2-181
181	30		$\text{Fe}(\text{CN})_6^{3-}$	std. state, n = 1	*C aq	174.3	134.3	84.6 89WE 85
181	40		$\text{Fe}(\text{CN})_6^{3-}$		*C aq	174.3	134.3	79.6 78BS 46 (R1 NBS Series)
181	41		$\text{Fe}(\text{CN})_6^{3-}$		*C aq	174.3	134.3	84.6 82A
Summary data selected for reasons 2 and 3								
181	50	A-8	$\text{Fe}(\text{CN})_6^{3-}$	std. state, n = 1	*C ao	174.3	134.3	84.68 82WE 2-181
2811431	181	51	A-8 $6\text{CN}^- + \text{Fe}^{3+} \leftrightarrow \text{Fe}(\text{CN})_6^{3-}$					
181	52	A-8	2811431 $\text{Fe}(\text{CN})_6^{3-}$					
181	53		2 0.000 143 1.000 281					
181	55		$\text{Fe}_2(\text{CN})_6^0$		*C ao	167.26	NA	NA 76SM 26
Summary data selected for reason								
181	56		$\text{Fe}_2(\text{CN})_6^0$		*C ao	167.26	NA	NA 76SM 26
2811432	181	57	$2\text{Fe}^{3+} + 6\text{CN}^- \leftrightarrow \text{Fe}_2(\text{CN})_6^0$					
181	58		2811432 $\text{Fe}_2(\text{CN})_6^0$					
181	59		2 2.000 281 0.000 143					
181	59.1		$\text{Fe}(\text{CN})_6^{4-}$		*C ao	178.82	NA	NA 87B
181	59.2		$\text{Fe}(\text{CN})_6^{4-}$		*C ao	180.86	168.9	42.69 76SM 26
181	66		$\text{Fe}(\text{CN})_6^{4-}$		*J ao	895.86	455.6	95.8 82WE 2-181
181	70		$\text{Fe}(\text{CN})_6^{4-}$		!C ao	166.13	168.9	22.7 82WE 2-181
181	80		$\text{Fe}(\text{CN})_6^{4-}$	std. state, n = 1	*C aq	166.89	168.9	22.7 89WE 85

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (J/mol)	$\Delta H_f^\circ, 298$ (J/mol)	S_{298}° (J/mol·K)	Data Sources
181	98		$\text{Fe}(\text{CN})_6^{4-}$	*C aq	166.1	108.9	42.7	78BS 46 (R1 NBS Series)
181	91		$\text{Fe}(\text{CN})_6^{4-}$	*C aq	166.1	110.6	48.1	88CR
Summary data selected for reason 6								
181	100	A-8	$\text{Fe}(\text{CN})_6^{4-}$ std. state, $n = 1$	*C ao	166.13	108.9	22.7	82WE 2-181
2881431	181	101	A-8 $6\text{CN}^- + \text{Fe}^{2+} \leftrightarrow \text{Fe}(\text{CN})_6^{4-}$					
181	102	A-8	2881431 $\text{Fe}(\text{CN})_6^{4-}$					
181	103		2 8.866 143 1.888 288					
181	110		$\text{Fe}_4(\text{Fe}(\text{CN})_6)_3$	*J cr	NA	1184.	NA	82WE 2-181
181	120		$\text{Fe}_4(\text{Fe}(\text{CN})_6)_3$	!C cr	NA	283.0	NA	82WE 2-181
181	130		$\text{Fe}_4(\text{Fe}(\text{CN})_6)_3$	*C cr	NA	283.	NA	89WE 86
Summary data selected for reason 2								
181	148	S-2	$\text{Fe}_4(\text{Fe}(\text{CN})_6)_3$	*C cr	NA	283.0	NA	82WE 2-181
181	150		$\text{FeCo}(\text{CN})_5^{3-}$	*J ao	NA	192.9	NA	82WE 2-181
181	160		$\text{FeCo}(\text{CN})_5^{3-}$	!C ao	NA	46.10	NA	82WE 2-181
181	170		$\text{FeCo}(\text{CN})_5^{3-}$ std. state, $n = 1$	*C aq	NA	46.1	NA	89WE 86
Summary data selected for reason 2								
181	180	A-2	$\text{FeCo}(\text{CN})_5^{3-}$ std. state, $n = 1$	*C ao	NA	46.10	NA	82WE 2-181
181	190		$\text{Fe}_2\text{Co}(\text{CN})_5$	*J cr	NA	414.	NA	82WE 2-181
181	200		$\text{Fe}_2\text{Co}(\text{CN})_5$	!C cr	NA	99.0	NA	82WE 2-181
181	210		$\text{Fe}_2\text{Co}(\text{CN})_5$	*C cr	NA	99.	NA	89WE 86
Summary data selected for reason 2								
181	220	S-2	$\text{Fe}_2\text{Co}(\text{CN})_5$	*C cr	NA	99.0	NA	82WE 2-181
181	220		$\text{HFe}(\text{CN})_5^{3-}$	*C ao	168.26	108.4	66.11	76SM 21
181	230		$\text{HFe}(\text{CN})_5^{3-}$	*J ao	671.28	455.6	176.	82WE 2-181
181	240		$\text{HFe}(\text{CN})_5^{3-}$	!C ao	168.44	108.9	42.1	82WE 2-181
181	250		$\text{HFe}(\text{CN})_5^{3-}$ std. state, $n = 16$	*C ao	168.4	108.9	42.	89WE 86

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
181	268		$\text{HFe}(\text{CN})_6^{3-}$	*C ao	168.4	169.6	57.6	78BS 54 (R1 NBS Series)
181	268		$\text{HFe}(\text{CN})_6^{3-}$	*C ao	168.14	116.54	48.86	86CR
181	268		$\text{HFe}(\text{CN})_6^{3-}$	*C ao	154.41	NA	NA	87B
Summary data selected for reason 6								
181	270		$\text{HFe}(\text{CN})_6^{3-}$	*C ao	168.14	116.54	48.86	86CR
2881432	181	271	A-8 $6\text{CN}^- + \text{Fe}^{2+} + \text{H}^+ \leftrightarrow \text{HFe}(\text{CN})_6^{3-}$					
181	272	A-8	2881432 $\text{HFe}(\text{CN})_6^{3-}$					
181	273		3 6.888 143 1.888 288 1.888 338					
181	279		$\text{H}_2\text{Fe}(\text{CN})_6^{2-}$	*C ao	158.59	169.54	63.32	78SM 21
181	288		$\text{H}_2\text{Fe}(\text{CN})_6^{2-}$	*J ao	658.66	455.6	218.	82WE 2-181
181	298		$\text{H}_2\text{Fe}(\text{CN})_6^{2-}$	!C ao	157.41	168.9	52.1	82WE 2-181
181	308		$\text{H}_2\text{Fe}(\text{CN})_6^{2-}$ std. state, n = 1	*C aq	157.37	168.9	52.	69WE 86
181	318		$\text{H}_2\text{Fe}(\text{CN})_6^{2-}$	*C aq	157.41	168.9	52.1	78BS 54 (R1 NBS Series)
181	311		$\text{H}_2\text{Fe}(\text{CN})_6^{2-}$	*C aq	158.8	111.6	62.85	86CR
181	312		$\text{H}_2\text{Fe}(\text{CN})_6^{2-}$	*C ao	157.14	NA	NA	87B
Summary data selected for reason 6								
181	328	A-8	$\text{H}_2\text{Fe}(\text{CN})_6^{2-}$ std. state, n = 1	*C ao	158.8	111.6	62.85	86CR
2881433	181	321	A-8 $6\text{CN}^- + 2\text{H}^+ + \text{Fe}^{2+} \leftrightarrow \text{H}_2\text{Fe}(\text{CN})_6^{2-}$					
181	322	A-8	2881433 $\text{H}_2\text{Fe}(\text{CN})_6^{2-}$					
181	323		3 6.888 143 2.888 338 1.888 288					
181	338		$\text{H}_3\text{Fe}(\text{CN})_6$	*J aq	NA	588.6	NA	82WE 2-181
181	348		$\text{H}_3\text{Fe}(\text{CN})_6$	!C aq	NA	135.9	NA	82WE 2-181
181	358		$\text{H}_3\text{Fe}(\text{CN})_6$	*C aq	NA	135.9	NA	69WE 86
Summary data selected for reason 1								
181	368	A-2	$\text{H}_3\text{Fe}(\text{CN})_6$	!C aq	NA	135.9	NA	82WE 2-181

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (kJ/mol)	$\Delta H_f^\circ, 298$ (kJ/mol)	S_{298}° (J/mol·K)	Data Sources
181 378		$H_3Fe(CN)_6^-$	*J ao	NA	456.6	NA	82WE 2-181
181 388		$H_3Fe(CN)_6^-$	!C ao	NA	188.9	NA	82WE 2-181
181 488		$H_3Fe(CN)_6^-$ std. state, $m = 1$	*C aq	NA	188.9	NA	69WE 86
Summary data selected for reason 1							
181 418	A-2	$H_3Fe(CN)_6^-$	!C ao	NA	188.9	NA	82WE 2-181
181 428		$H_4Fe(CN)_6$	*J cr	NA	482.8	NA	82WE 2-181
181 438		$H_4Fe(CN)_6$	!C cr	NA	118.6	NA	82WE 2-181
181 448		$H_4Fe(CN)_6$	*C cr	NA	118.6	NA	69WE 86
Summary data selected for reason 1							
181 458	S-2	$H_4Fe(CN)_6$	!C cr	NA	118.8	NA	82WE 2-181
181 468		$H_4Fe(CN)_6$	*J aq	NA	481.1	NA	82WE 2-181
181 478		$H_4Fe(CN)_6$	!C aq	NA	118.2	NA	82WE 2-181
181 488		$H_4Fe(CN)_6$	*C aq	NA	118.2	NA	69WE 86
Summary data selected for reason 1							
181 498	A-2	$H_4Fe(CN)_6$	!C aq	NA	118.2	NA	82WE 2-181
181 508		$(NH_4)_4Fe(CN)_6$	*J aq	NA	-81.9	NA	82WE 2-181
181 518		$(NH_4)_4Fe(CN)_6$	!C aq	NA	-14.8	NA	82WE 2-181
181 528		$(NH_4)_4Fe(CN)_6$	*C aq	NA	-14.8	NA	69WE 86
Summary data selected for reason 1							
181 538	A-2	$(NH_4)_4Fe(CN)_6$	!C aq	NA	-14.8	NA	82WE 2-181
181 548		$(NH_4)_4Fe(CN)_6 \cdot 6H_2O$	*J cr	NA	-1882.9	NA	82WE 2-181
181 558		$(NH_4)_4Fe(CN)_6 \cdot 6H_2O$	!C cr	NA	-438.98	NA	82WE 2-181
181 568		$(NH_4)_4Fe(CN)_6 \cdot 6H_2O$	*C cr	NA	-438.9	NA	69WE 86
Summary data selected for reason 2							
181 578	S-2	$(NH_4)_4Fe(CN)_6 \cdot 6H_2O$	*C cr	NA	-438.98	NA	82WE 2-181
181 588		$HFeCo(CN)_5^{2-}$	*J ao	NA	192.5	NA	82WE 2-181
181 598		$HFeCo(CN)_5^{2-}$	!C ao	NA	46.81	NA	82WE 2-181
181 608		$HFeCo(CN)_5^{2-}$ std. state, $m = 1$	*C aq	NA	46.8	NA	69WE 86
Summary data selected for reason 2							
181 618	A-2	$HFeCo(CN)_5^{2-}$ std. state, $m = 1$	*C ao	NA	46.81	NA	82WE 2-181

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
181	628		$H_2FeCo(CN)_5^-$	*J ao	NA	193.7	NA	82WE 2-181
181	638		$H_2FeCo(CN)_5^-$	!C ao	NA	46.38	NA	82WE 2-181
181	648		$H_2FeCo(CN)_5^-$ std. state, n = 1	*C aq	NA	48.3	NA	89WE 87
Summary data selected for reason 2								
181	658	A-2	$H_2FeCo(CN)_5^-$ std. state, n = 1	*C ao	NA	48.38	NA	82WE 2-181
181	668		$H_2FeCo(CN)_5^-$	*J aq	NA	197.	NA	82WE 2-181
181	678		$H_2FeCo(CN)_5^-$	!C aq	NA	47.1	NA	82WE 2-181
181	688		$H_2FeCo(CN)_5^-$	*C aq	NA	47.	NA	89WE 87
Summary data selected for reason 2								
181	698	A-2	$H_3FeCo(CN)_5$	*C aq	NA	47.1	NA	82WE 2-181
181	708		$H_3FeCo(CN)_5 \cdot H_2O$	*J cr	NA	-87.	NA	82WE 2-181
181	718		$H_3FeCo(CN)_5 \cdot H_2O$	!C cr	NA	-16.	NA	82WE 2-181
181	728		$H_3FeCo(CN)_5 \cdot H_2O$	*C cr	NA	-16.	NA	89WE 87
Summary data selected for reason 1								
181	738	S-2	$H_3FeCo(CN)_5 \cdot H_2O$	!C cr	NA	-16.	NA	82WE 2-181
181	748		$Pb_2Fe(CN)_8 \cdot 3H_2O$	*J cr	-168.8	NA	NA	82WE 2-181
181	758		$Pb_2Fe(CN)_8 \cdot 3H_2O$	!C cr	-48.15	NA	NA	82WE 2-181
181	768		$Pb_2Fe(CN)_8 \cdot 3H_2O$	*C cr	-48.2	NA	NA	89WE 87
Summary data selected for reason 2								
181	778	S-8	$Pb_2Fe(CN)_8 \cdot 3H_2O$	*C cr	-48.15	NA	NA	82WE 2-181
1168881	181	771	S-8 $6CN^- + 2Pb^{2+} + Fe^{2+} + 3H_2O \leftrightarrow Pb_2Fe(CN)_8 \cdot 3H_2O$					
181	772	S-8	1168881 $Pb_2Fe(CN)_8 \cdot 3H_2O$					
181	773		4 8.888 143 2.888 888 1.888 288 3.888 2					
181	798		$TiFe(CN)_6^{3-}$	*J ao	644.9	464.8	292.9	82WE 2-181
181	791		$TiFe(CN)_6^{3-}$	!C ao	154.1	111.1	78.88	82WE 2-181
181	808		$TiFe(CN)_6^{3-}$ std. state, n = 1	*C aq	154.1	111.1	78.8	89WE 88
Summary data selected for reason 2								

TABLE B.2. (contd)

WINTER Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (kJ/mol)	$\Delta H_f^\circ, 298$ (kJ/mol)	S_{298}° (J/mol·K)	Data Sources
	181 810	A-8	$\text{TiFe}(\text{CN})_6^{3-}$ std. state, $n = 1$	*C so	154.1	111.1	78.8	82WE 2-181
8701432	181 811	A-8	$6\text{CN}^- + \text{Ti}^+ + \text{Fe}^{2+} \leftrightarrow \text{TiFe}(\text{CN})_6^{3-}$					
	181 812	A-8	8701432 $\text{TiFe}(\text{CN})_6^{3-}$					
	181 813		3 8.888 143 1.888 870 1.888 280					
	181 830		$\text{Ti}_4\text{Fe}(\text{CN})_8 \cdot 2\text{H}_2\text{O}$	*J cr	26.8	NA	NA	82WE 2-181
	181 831		$\text{Ti}_4\text{Fe}(\text{CN})_8 \cdot 2\text{H}_2\text{O}$	!C cr	6.36	NA	NA	82WE 2-181
	181 848		$\text{Ti}_4\text{Fe}(\text{CN})_8 \cdot 2\text{H}_2\text{O}$	*C cr	6.3	NA	NA	89WE 88
Summary data selected for reason 2								
	181 850	S-8	$\text{Ti}_4\text{Fe}(\text{CN})_8 \cdot 2\text{H}_2\text{O}$	*C cr	6.36	NA	NA	82WE 2-181
1187001	181 851	S-8	$6\text{CN}^- + 4\text{Ti}^+ + \text{Fe}^{2+} + 2\text{H}_2\text{O} \leftrightarrow \text{Ti}_4\text{Fe}(\text{CN})_8 \cdot 2\text{H}_2\text{O}$					
	181 852	S-8	1187001 $\text{Ti}_4\text{Fe}(\text{CN})_8 \cdot 2\text{H}_2\text{O}$					
	181 853		4 8.888 143 4.888 870 1.888 280 2.888 2					
	181 870		$\text{Zn}_2\text{Fe}(\text{CN})_8 \cdot 2\text{H}_2\text{O}$	*J cr	-163.8	NA	NA	82WE 2-181
	181 871		$\text{Zn}_2\text{Fe}(\text{CN})_8 \cdot 2\text{H}_2\text{O}$	!C cr	-38.96	NA	NA	82WE 2-181
	181 880		$\text{Zn}_2\text{Fe}(\text{CN})_8 \cdot 2\text{H}_2\text{O}$	*C cr	-39.8	NA	NA	89WE 88
Summary data selected for reason 2								
	181 890	S-8	$\text{Zn}_2\text{Fe}(\text{CN})_8 \cdot 2\text{H}_2\text{O}$	*C cr	-38.96	NA	NA	82WE 2-181
1195001	181 891	S-8	$6\text{CN}^- + 2\text{Zn}^{2+} + \text{Fe}^{2+} + 2\text{H}_2\text{O} \leftrightarrow \text{Zn}_2\text{Fe}(\text{CN})_8 \cdot 2\text{H}_2\text{O}$					
	181 892	S-8	1195001 $\text{Zn}_2\text{Fe}(\text{CN})_8 \cdot 2\text{H}_2\text{O}$					
	181 893		4 8.888 143 2.888 950 1.888 280 2.888 2					
	181 910		$\text{Cd}_2\text{Fe}(\text{CN})_8 \cdot 7\text{H}_2\text{O}$	*J cr	-1219.8	NA	NA	82WE 2-181
	181 911		$\text{Cd}_2\text{Fe}(\text{CN})_8 \cdot 7\text{H}_2\text{O}$	!C cr	-291.49	NA	NA	82WE 2-181
	181 920		$\text{Cd}_2\text{Fe}(\text{CN})_8 \cdot 7\text{H}_2\text{O}$	*C cr	-291.6	NA	NA	89WE 88
Summary data selected for reason 2								
	181 930	S-8	$\text{Cd}_2\text{Fe}(\text{CN})_8 \cdot 7\text{H}_2\text{O}$	*C cr	-291.49	NA	NA	82WE 2-181
1116001	181 931	S-8	$6\text{CN}^- + 2\text{Cd}^{2+} + \text{Fe}^{2+} + 7\text{H}_2\text{O} \leftrightarrow \text{Cd}_2\text{Fe}(\text{CN})_8 \cdot 7\text{H}_2\text{O}$					
	181 932	S-8	1116001 $\text{Cd}_2\text{Fe}(\text{CN})_8 \cdot 7\text{H}_2\text{O}$					
	181 933		4 8.888 143 2.888 160 1.888 280 7.888 2					

TABLE B.2. (contd)

MINTEQ Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
181 950			$\text{Cu}_2\text{Fe}(\text{CN})_6$	*J cr	736.6	NA	NA	82WE 2-181
181 951			$\text{Cu}_2\text{Fe}(\text{CN})_6$	!C cr	176.0	NA	NA	82WE 2-181
181 960			$\text{Cu}_2\text{Fe}(\text{CN})_6$	*C cr	176.0	NA	NA	89WE 89
Summary data selected for reason 1								
181 970	S-0		$\text{Cu}_2\text{Fe}(\text{CN})_6$	!C cr	176.0	NA	NA	82WE 2-181
1123102	181 981	S-0	$6\text{CN}^- + 2\text{Cu}^{2+} + \text{Fe}^{2+} \leftrightarrow \text{Cu}_2\text{Fe}(\text{CN})_6$					
	181 982	S-0	1123102 $\text{Cu}_2\text{Fe}(\text{CN})_6$					
181 983			3 6.000 143 2.000 231 1.000 280					
181 990			$\text{Ag}_4\text{Fe}(\text{CN})_6 \cdot \text{H}_2\text{O}$	*J cr	514.8	NA	NA	82WE 2-181
181 992			$\text{Ag}_4\text{Fe}(\text{CN})_6 \cdot \text{H}_2\text{O}$	!C cr	123.0	NA	NA	82WE 2-181
181 1000			$\text{Ag}_4\text{Fe}(\text{CN})_6 \cdot \text{H}_2\text{O}$	*C cr	123.0	NA	NA	89WE 89
Summary data selected for reason 1								
181 1010	S-0		$\text{Ag}_4\text{Fe}(\text{CN})_6 \cdot \text{H}_2\text{O}$	!C cr	123.0	NA	NA	82WE 2-181
1102001	181 1011	S-0	$6\text{CN}^- + 4\text{Ag}^+ + \text{Fe}^{2+} + \text{H}_2\text{O} \leftrightarrow \text{Ag}_4\text{Fe}(\text{CN})_6 \cdot \text{H}_2\text{O}$					
	181 1012	S-0	1102001 $\text{Ag}_4\text{Fe}(\text{CN})_6 \cdot \text{H}_2\text{O}$					
181 1013			4 6.000 143 4.000 020 1.000 280 1.000 2					
183 10			$\text{Pd}(\text{CN})_4^{2-}$	*J ao	289.	NA	NA	82WE 2-183
183 20			$\text{Pd}(\text{CN})_4^{2-}$	!C ao	69.1	NA	NA	82WE 2-183
183 30			$\text{Pd}(\text{CN})_4^{2-}$ std. state, $n = 1$	*C aq	69.	NA	NA	89WE 92
Summary data selected for reason 2								
183 40			$\text{Pd}(\text{CN})_4^{2-}$ std. state, $n = 1$	*C ao	69.1	NA	NA	82WE 2-183
183 50			$\text{Pd}(\text{CN})_2$	*J cr	NA	205.4	NA	82WE 2-183
183 60			$\text{Pd}(\text{CN})_2$	!C cr	NA	49.09	NA	82WE 2-183
183 70			$\text{Pd}(\text{CN})_2$ Note revision from 89WE 92	*C cr	NA	49.1	NA	81WE 121
Summary data selected for reasons 2 and 5								
183 80	S-2		$\text{Pd}(\text{CN})_2$	*C cr	NA	49.09	NA	82WE 2-183
183 90			$\text{Pd}(\text{CN})_4^{2-}$	*J ao	620.	NA	NA	82WE 2-183
183 100			$\text{Pd}(\text{CN})_4^{2-}$	!C ao	150.	NA	NA	82WE 2-183
183 110			$\text{Pd}(\text{CN})_4^{2-}$ std. state, $n = 1$	*C aq	150.	NA	NA	89WE 92

TABLE B.2. (contd)

WINTER	In 82WE				Units	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°	
Number	Page	ID	Form	Compound	Q State	(Q/mol)	(Q/mol)	(Q/mol·K)	Data Sources
Summary data selected for reason 1									
183	128			$\text{Pd}(\text{CN})_4^{2-}$	IC ao	156.	NA	NA	82WE 2-183
187	18			$(\text{Pt}(\text{CN})_4)^{2-}$	*J ao	718.5	NA	NA	82WE 2-187
187	28			$(\text{Pt}(\text{CN})_4)^{2-}$	IC ao	169.8	NA	NA	82WE 2-187
Summary data selected for reason 4									
187	38	A-1		$(\text{Pt}(\text{CN})_4)^{2-}$	IC ao	169.8	NA	NA	82WE 2-187
193	18			$\text{Mn}(\text{CN})_6^{4-}$	*J aq	NA	556.	NA	82WE 2-193
193	28			$\text{Mn}(\text{CN})_6^{4-}$	IC aq	NA	133.	NA	82WE 2-193
193	38			$\text{Mn}(\text{CN})_6^{4-}$	*C aq	NA	133.	NA	89WE 114
Summary data selected for reason 1									
193	48	A-2		$\text{Mn}(\text{CN})_6^{4-}$	IC aq	NA	133.	NA	82WE 2-193
194	18			$\text{Mn}_2\text{Fe}(\text{CN})_8$	*J cr	162.4	NA	NA	82WE 2-194
194	28			$\text{Mn}_2\text{Fe}(\text{CN})_8$	IC cr	38.82	NA	NA	82WE 2-194
194	38			$\text{Mn}_2\text{Fe}(\text{CN})_8$	*C cr	38.8	NA	NA	89WE 115
Summary data selected for reason 2									
194	48	S-8		$\text{Mn}_2\text{Fe}(\text{CN})_8$	*C cr	38.82	NA	NA	82WE 2-194
1147814	194	41	S-8	$8\text{CN}^- + 2\text{Mn}^{2+} + \text{Fe}^{2+} \leftrightarrow \text{Mn}_2\text{Fe}(\text{CN})_8$					
194	42	S-8	1147814	$\text{Mn}_2\text{Fe}(\text{CN})_8$					
194	43		3	8.888 143	2.888 475	1.888 288			
199	18			CrCN	*J cr	124.7	NA	NA	82WE 2-199
199	28			CrCN	IC cr	29.88	NA	NA	82WE 2-199
Summary data selected for reason 4. Note that CrN on page 2-199 should be CrCN. Personal communication from Vivian B. Parker, NBS, October 29, 1987.									
199	38	S-8		CrCN	IC cr	29.88	NA	NA	82WE 2-199
1121881	199	31	S-8	$\text{CN}^- + \text{Cr}^{2+} + e^- \leftrightarrow \text{CrCN}$					
199	32	S-8	1121881	CrCN					
199	33		3	1.888 143	1.888 218	1.888 1			
199	48			Cr ₂ CN	*J cr	127.6	NA	NA	82WE 2-199

TABLE B.2. (contd)

WINTER	In 82WE				Units	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°		
Number	Page	ID	Form	Compound	Q	State	(Q/mol)	(Q/mol)	(Q/mol-K)	Data Sources
	199	58		Cr ₂ CN	!C	cr	38.58	NA	NA	82WE 2-199
Summary data selected for reason 4. Note that Cr ₂ N on page 2-199 should be Cr ₂ CN. Personal communication from Vivian B. Parker, NBS, October 29, 1987.										
	199	58	S-8	Cr ₂ CN	!C	cr	38.58	NA	NA	82WE 2-199
1121002	199	61	S-8	CN ⁻ + 2Cr ²⁺ + 3e ⁻ ↔ Cr ₂ CN						
	199	62	S-8	1121002 Cr ₂ CN						
	199	63		3	1.000	143	2.000	218	3.000	1
	245	18		La ₂ (CN) ₂ 3	*J	cr	NA	-833.	NA	82WE 2-245
	245	28		La ₂ (CN) ₂ 3	!C	cr	NA	-199.		82WE 2-245
Summary data selected for reason 4										
	245	38	S-2	La ₂ (CN) ₂ 3 cyanamide	!C	cr	NA	-199.		82WE 2-245
	265	18		MgCN ₂	*J	cr	NA	-252.8	NA	82WE 2-265
	265	28		MgCN ₂	!C	cr	NA	-68.38	NA	82WE 2-265
	265	38		MgCN ₂	*C	cr	NA	-68.3	NA	71PW 24
Summary data selected for reason 2										
	265	48	S-2	MgCN ₂ cyanamide	*C	cr	NA	-68.38	NA	82WE 2-265
	265	58		Mg(CN) ₂	*J	aq	NA	-164.	NA	82WE 2-265
	265	68		Mg(CN) ₂	!C	aq	NA	-39.2	NA	82WE 2-265
	265	78		Mg(CN) ₂	*C	aq	NA	-39.2	NA	71PW 24
Summary data selected for reason 1										
	265	88	A-2	Mg(CN) ₂	!C	aq	NA	-39.2	NA	82WE 2-265
	265	98		MgHg(CN) ₄	*J	aq	NA	61.2	NA	82WE 2-265
	265	108		MgHg(CN) ₄	!C	aq	NA	19.4	NA	82WE 2-265
	265	118		MgHg(CN) ₄	*C	aq	NA	19.4	NA	71PW 26
Summary data selected for reason 1										
	265	128	A-2	MgHg(CN) ₄	!C	aq	NA	19.4	NA	82WE 2-265
	265	138		Mg(Hg(CN) ₃) ₂	*J	aq	NA	341.4	NA	82WE 2-265
	265	148		Mg(Hg(CN) ₃) ₂	!C	aq	NA	61.68	NA	82WE 2-265
	265	158		Mg(Hg(CN) ₃) ₂	*C	aq	NA	61.6	NA	71PW 26

TABLE B.2. (contd)

MINTER Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
Summary data selected for reason 2								
265	168	A-2	Mg(Hg(CN)3)2	*C aq	NA	81.68	NA	82WE 2-265
265	178		(Hg(CN)2)2·MgCl2	*J aq	NA	-238.9	NA	82WE 2-265
265	188		(Hg(CN)2)2·MgCl2	!C aq	NA	-57.18	NA	82WE 2-265
Summary data selected for reason 4								
265	198	A-2	(Hg(CN)2)2·MgCl2	!C aq	NA	-57.18	NA	82WE 2-265
265	208		(Hg(CN)2)2·MgCl2·8H2O	*J cr	NA	-1993.7	NA	82WE 2-265
265	218		(Hg(CN)2)2·MgCl2·8H2O	!C cr	NA	-476.51	NA	82WE 2-265
Summary data selected for reason 4								
265	228	S-2	(Hg(CN)2)2·MgCl2·8H2O	!C cr	NA	-476.51	NA	82WE 2-265
265	238		(Hg(CN)2)2·MgBr2	*J aq	NA	-158.6	NA	82WE 2-265
265	248		(Hg(CN)2)2·MgBr2	!C aq	NA	-35.99	NA	82WE 2-265
Summary data selected for reason 4								
265	258	A-2	(Hg(CN)2)2·MgBr2	!C aq	NA	-35.99	NA	82WE 2-265
265	268		(Hg(CN)2)2·MgBr2·8H2O	*J cr	NA	-2581.6	NA	82WE 2-265
265	278		(Hg(CN)2)2·MgBr2·8H2O	!C cr	NA	-597.98	NA	82WE 2-265
Summary data selected for reason 4								
265	288	S-2	(Hg(CN)2)2·MgBr2·8H2O	!C cr	NA	-597.98	NA	82WE 2-265
265	298		(Hg(CN)2)2·MgI2	*J aq	NA	-35.1	NA	82WE 2-265
265	308		(Hg(CN)2)2·MgI2	!C aq	NA	-8.39	NA	82WE 2-265
Summary data selected for reason 4								
265	318	A-2	(Hg(CN)2)2·MgI2	!C aq	NA	-8.39	NA	82WE 2-265
265	328		(Hg(CN)2)2·MgI2·8H2O	*J cr	NA	-2482.5	NA	82WE 2-265
265	338		(Hg(CN)2)2·MgI2·8H2O	!C cr	NA	-574.21	NA	82WE 2-265
Summary data selected for reason 4								
265	348	S-2	(Hg(CN)2)2·MgI2·8H2O	!C cr	NA	-574.21	NA	82WE 2-265
265	349		MgFe(CN)6 ⁻	*C ao	61.79	NA	NA	78SM 22
265	358		MgFe(CN)6 ⁻	*J ao	258.7	NA	NA	82WE 2-265
265	368		MgFe(CN)6 ⁻	!C ao	61.83	NA	NA	82WE 2-265
265	378		MgFe(CN)6 ⁻ Revision of WE 27	*C ao	61.8	NA	NA	81WE 128

TABLE B.2. (contd)

WINTER Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
265	376		$\text{MgFe}(\text{CN})_6^-$	*C ao	61.89	23.51	46.66	82A
Summary data selected for reasons 2 and 5								
265	386	A-8	$\text{MgFe}(\text{CN})_6^-$	!C ao	61.83	23.51	46.69	82WE 2-265; 82A
4681431	265	381	A-8	$8\text{CN}^- + \text{Mg}^{2+} + \text{Fe}^{3+} \leftrightarrow \text{MgFe}(\text{CN})_6^-$				
265	382	A-8	4681431 $\text{MgFe}(\text{CN})_6^-$					
265	383		3 8.666 143 1.666 466 1.666 281					
265	399		$\text{MgFe}(\text{CN})_6^{2-}$	*C ao	52.25	NA	NA	76SM 21
265	406		$\text{MgFe}(\text{CN})_6^{2-}$	*J ao	218.5	NA	NA	82WE 2-265
265	416		$\text{MgFe}(\text{CN})_6^{2-}$	!C ao	52.22	NA	NA	82WE 2-265
265	426		$\text{MgFe}(\text{CN})_6^{2-}$ Revision of WE 27	*C aq	52.2	NA	NA	81WE 126
Summary data selected for reasons 2 and 5								
265	436	A-8	$\text{MgFe}(\text{CN})_6^{2-}$	!C ao	52.22	NA	NA	82WE 2-265
4681432	265	431	A-8	$8\text{CN}^- + \text{Mg}^{2+} + \text{Fe}^{2+} \leftrightarrow \text{MgFe}(\text{CN})_6^{2-}$				
265	432	A-8	4681432 $\text{MgFe}(\text{CN})_6^{2-}$					
265	433		3 8.666 143 1.666 466 1.666 286					
265	456		$\text{Mg}_2\text{Fe}(\text{CN})_6$ from $\text{Fe}(\text{CN})_6^{4-}$	*J ai	-214.5	-478.2	-181.2	82WE 2-265
265	466		$\text{Mg}_2\text{Fe}(\text{CN})_6$ from $\text{Fe}(\text{CN})_6^{4-}$	!C ai	-51.27	-114.3	-43.31	82WE 2-265
265	476		$\text{Mg}_2\text{Fe}(\text{CN})_6$ std. state, $n = 1$	*C aq	-51.3	-114.3	-43.3	71PW 27
Summary data selected for reason 2								
265	486	A-1	$\text{Mg}_2\text{Fe}(\text{CN})_6$ std. state, $n = 1$	*C ai	-51.27	-114.3	-43.31	82WE 2-265
265	496		$\text{Mg}_2\text{Fe}(\text{CN})_6$ in 1500 H ₂ O	*J	NA	-487.44	NA	82WE 2-265
265	506		$\text{Mg}_2\text{Fe}(\text{CN})_6$ in 1500 H ₂ O	!C	NA	-111.72	NA	82WE 2-265
265	516		$\text{Mg}_2\text{Fe}(\text{CN})_6$ in 1500 H ₂ O	*Caq	NA	-111.72	NA	71PW 27

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
Summary data selected for reason 1								
266	528	A-2	$Mg_2Fe(CN)_6$ in 1500 H ₂ O	!C	NA	-111.72	NA	82WE 2-266
266	18		$Mg_2Fe(CN)_6$ in ∞ H ₂ O	*Jaq	NA	-478.2	NA	82WE 2-266
266	28		$Mg_2Fe(CN)_6$ in ∞ H ₂ O	!C	NA	-114.3	NA	82WE 2-266
266	38		$Mg_2Fe(CN)_6$ in ∞ H ₂ O	*C	NA	-114.3	NA	71PW 27
Summary data selected for reason 1								
266	48	A-2	$Mg_2Fe(CN)_6$ in ∞ H ₂ O	!C	NA	-114.3	NA	82WE 2-266
272	18		CaCN ₂	*J cr	NA	-358.6	NA	82WE 2-272
272	28		CaCN ₂	!C cr	NA	-83.88	NA	82WE 2-272
272	38		CaCN ₂	*C cr	NA	-83.8	NA	71PW 47
Summary data selected for reason 2								
272	48	S-2	CaCN ₂ cyanamide	*C cr	NA	-83.88	NA	82WE 2-272
272	58		Ca(CN) ₂	*J cr	NA	-184.5	NA	82WE 2-272
272	68		Ca(CN) ₂	!C cr	NA	-44.18	NA	82WE 2-272
272	78		Ca(CN) ₂	*C cr	NA	-44.1	NA	71PW 47
Summary data selected for reason 2								
272	88	S-2	Ca(CN) ₂	*C cr	NA	-44.18	NA	82WE 2-272
272	98		Ca(CN) ₂	*J aq	NA	-238.1	NA	82WE 2-272
272	108		Ca(CN) ₂	!C aq	NA	-56.91	NA	82WE 2-272
272	118		Ca(CN) ₂	*C aq	NA	-56.9	NA	71PW 47
Summary data selected for reason 2								
272	128	A-2	Ca(CN) ₂	*C aq	NA	-56.91	NA	82WE 2-272
273	18		(CaO) ₃ ·Ca(CN) ₂ ·15H ₂ O	*J cr	NA	-6728.	NA	82WE 2-273
273	28		(CaO) ₃ ·Ca(CN) ₂ ·15H ₂ O	!C cr	NA	-1888.	NA	82WE 2-273
273	38		(CaO) ₃ ·Ca(CN) ₂ ·15H ₂ O	*C cr	NA	-1888.	NA	71PW 47
Summary data selected for reason 1								
273	48	S-2	(CaO) ₃ ·Ca(CN) ₂ ·15H ₂ O	!C cr	NA	-1888.	NA	82WE 2-273
274	18		CaHg(CN) ₄ in 788 H ₂ O	*J	NA	-8.4	NA	82WE 2-274
274	28		CaHg(CN) ₄ in 788 H ₂ O	!C	NA	-2.8		82WE 2-274
Summary data selected for reason 4								
274	38	A-2	CaHg(CN) ₄ in 788 H ₂ O	!C	NA	-2.8		82WE 2-274
274	48		CaHg ₂ (CN) ₈ in 1688 H ₂ O	*J	NA	275.3	NA	82WE 2-274
274	58		CaHg ₂ (CN) ₈ in 1688 H ₂ O	!C	NA	85.88	NA	82WE 2-274

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
Summary data selected for reason 4								
274	66	A-2	$\text{CaHg}_2(\text{CN})_6$	in 1000 H ₂ O	!C	NA	65.86	82WE 2-274
274	76		$\text{CaCl}_2 \cdot 2\text{Hg}(\text{CN})_2$	in 1000 H ₂ O	*J	NA	-311.7	82WE 2-274
274	86		$\text{CaCl}_2 \cdot 2\text{Hg}(\text{CN})_2$	in 1000 H ₂ O	!C	NA	-74.56	82WE 2-274
Summary data selected for reason 4								
274	96	A-2	$\text{CaCl}_2 \cdot 2\text{Hg}(\text{CN})_2$	in 1000 H ₂ O	!C	NA	-74.56	82WE 2-274
274	106		$\text{CaCl}_2 \cdot 2\text{Hg}(\text{CN})_2 \cdot 6\text{H}_2\text{O}$		*J cr	NA	-2683.6	82WE 2-274
274	116		$\text{CaCl}_2 \cdot 2\text{Hg}(\text{CN})_2 \cdot 6\text{H}_2\text{O}$		!C cr	NA	-497.99	82WE 2-274
Summary data selected for reason 4								
274	126	S-2	$\text{CaCl}_2 \cdot 2\text{Hg}(\text{CN})_2 \cdot 6\text{H}_2\text{O}$		!C cr	NA	-497.99	82WE 2-274
274	136		$\text{CaBr}_2 \cdot 2\text{Hg}(\text{CN})_2$	in 1000 H ₂ O	*J	NA	-224.3	82WE 2-274
274	146		$\text{CaBr}_2 \cdot 2\text{Hg}(\text{CN})_2$	in 1000 H ₂ O	!C	NA	-53.61	82WE 2-274
Summary data selected for reason 4								
274	156	A-2	$\text{CaBr}_2 \cdot 2\text{Hg}(\text{CN})_2$	in 1000 H ₂ O	!C	NA	-53.61	82WE 2-274
274	166		$\text{CaBr}_2 \cdot 2\text{Hg}(\text{CN})_2 \cdot 7\text{H}_2\text{O}$		*J cr	NA	-2364.1	82WE 2-274
274	176		$\text{CaBr}_2 \cdot 2\text{Hg}(\text{CN})_2 \cdot 7\text{H}_2\text{O}$		!C cr	NA	-556.69	82WE 2-274
Summary data selected for reason 4								
274	186	S-2	$\text{CaBr}_2 \cdot 2\text{Hg}(\text{CN})_2 \cdot 7\text{H}_2\text{O}$		!C cr	NA	-556.69	82WE 2-274
274	196		$\text{CaI}_2 \cdot 2\text{Hg}(\text{CN})_2$	in 1000 H ₂ O	*J	NA	-169.2	82WE 2-274
274	206		$\text{CaI}_2 \cdot 2\text{Hg}(\text{CN})_2$	in 1000 H ₂ O	!C	NA	-26.16	82WE 2-274
Summary data selected for reason 4								
274	216	A-2	$\text{CaI}_2 \cdot 2\text{Hg}(\text{CN})_2$	in 1000 H ₂ O	!C	NA	-26.16	82WE 2-274
274	226		$\text{CaI}_2 \cdot 2\text{Hg}(\text{CN})_2 \cdot 7\text{H}_2\text{O}$		*J cr	NA	-2199.9	82WE 2-274
274	236		$\text{CaI}_2 \cdot 2\text{Hg}(\text{CN})_2 \cdot 7\text{H}_2\text{O}$		!C cr	NA	-525.79	82WE 2-274
Summary data selected for reason 4								
274	246	S-2	$\text{CaI}_2 \cdot 2\text{Hg}(\text{CN})_2 \cdot 7\text{H}_2\text{O}$		!C cr	NA	-525.79	82WE 2-274
274	256		$\text{CaAg}(\text{CN})_3$	in 1200 H ₂ O	*J	NA	-122.6	82WE 2-274
274	266		$\text{CaAg}(\text{CN})_3$	in 1200 H ₂ O	!C	NA	-29.36	82WE 2-274
Summary data selected for reason 4								
274	276	A-2	$\text{CaAg}(\text{CN})_3$	in 1200 H ₂ O	!C	NA	-29.36	82WE 2-274
274	286		$\text{CaAg}_2(\text{CN})_4$	in 550 H ₂ O	*J	NA	-3.8	82WE 2-274

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol.K)	Data Sources
274	298		$\text{CaAg}_2(\text{CN})_4$ in 550 H ₂ O	!C	NA	-8.91	NA	82WE 2-274
Summary data selected for reason 4								
274	306	A-2	$\text{CaAg}_2(\text{CN})_4$ in 550 H ₂ O	!C	NA	-8.91	NA	82WE 2-274
274	309		$\text{CaFe}(\text{CN})_6^-$	*C ao	38.14	6.18	72.82	76SM 22
274	310		$\text{CaFe}(\text{CN})_6^-$	*J ao	159.5	NA	NA	82WE 2-274
274	320		$\text{CaFe}(\text{CN})_6^-$	!C ao	38.12	NA	NA	82WE 2-274
274	321		$\text{CaFe}(\text{CN})_6^-$	!C ao	38.24	5.16	66.53	82A
Summary data selected for reason 4								
274	330		$\text{CaFe}(\text{CN})_6^-$	!C ao	38.12	5.16	66.53	82WE 2-274; 82A
1501431	274	332	A-8 $8\text{CN}^- + \text{Ca}^{2+} + \text{Fe}^{3+} \leftrightarrow \text{CaFe}(\text{CN})_6^-$					
274	333	A-8	1501431 $\text{CaFe}(\text{CN})_6^-$					
274	334		3 8.000 143 1.000 150 1.000 281					
274	349		$\text{CaFe}(\text{CN})_6^{2-}$	*C ao	28.65	-18.74	46.44	76SM 21
274	350		$\text{CaFe}(\text{CN})_6^{2-}$	*J ao	119.8	NA	NA	82WE 2-274
274	351		$\text{CaFe}(\text{CN})_6^{2-}$	!C ao	28.63	NA	NA	82WE 2-274
274	352		$\text{CaFe}(\text{CN})_6^{2-}$	!C ao	28.26	-18.14	37.65	86CR
Summary data selected for reason 6								
274	360	A-8	$\text{CaFe}(\text{CN})_6^{2-}$	!C ao	28.26	-18.14	37.65	86CR
1501432	274	361	A-8 $8\text{CN}^- + \text{Ca}^{2+} + \text{Fe}^{2+} \leftrightarrow \text{CaFe}(\text{CN})_6^{2-}$					
274	362	A-8	1501432 $\text{CaFe}(\text{CN})_6^{2-}$					
274	363		3 8.000 143 1.000 150 1.000 280					
274	368		$\text{Ca}_2\text{Fe}(\text{CN})_6$ from $\text{Fe}(\text{CN})_6^{4-}$	*J ai	-412.87	-838.1	-11.8	82WE 2-274
274	381		$\text{Ca}_2\text{Fe}(\text{CN})_6$ from $\text{Fe}(\text{CN})_6^{4-}$	!C ai	-98.487	-158.8	-2.78	82WE 2-274

TABLE B.2. (contd)

MINTEQA	In 82WE				Units	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°	
Number	Page	ID	Form	Compound	Q State	(Q/mol)	(Q/mol)	(Q/mol·K)	Data Sources
Summary data selected for reason 4									
274	398	A-1		$\text{Ca}_2\text{Fe}(\text{CN})_6$ from $\text{Fe}(\text{CN})_6^{4-}$	!C ai	-98.487	-158.6	-2.78	82WE 2-274
274	408			$\text{Ca}_2\text{Fe}(\text{CN})_6$	*J ao	-441.7	NA	NA	82WE 2-274
274	410			$\text{Ca}_2\text{Fe}(\text{CN})_6$	!C ao	-185.6	NA	NA	82WE 2-274
274	411			$\text{Ca}_2\text{Fe}(\text{CN})_6$	!C ao	-185.82	-149.48	28.91	86CR
274	412			$\text{Ca}_2\text{Fe}(\text{CN})_6$	*C ao	-182.13	NA	NA	76SM 21
Summary data selected for reason 6									
274	426			$\text{Ca}_2\text{Fe}(\text{CN})_6$	!C ao	-185.82	-149.48	28.91	86CR
1581433	274	421	A-8	$6\text{CN}^- + 2\text{Ca}^{2+} + \text{Fe}^{2+} \leftrightarrow \text{Ca}_2\text{Fe}(\text{CN})_6$					
	274	422	A-8	1581433 $\text{Ca}_2\text{Fe}(\text{CN})_6$					
274	423		3	6.888 143 2.888 158 1.888 288					
274	448			$\text{Ca}_2\text{Fe}(\text{CN})_6$ in 1588 H_2O	*J	NA	-824.55	NA	82WE 2-274
274	441			$\text{Ca}_2\text{Fe}(\text{CN})_6$ in 1588 H_2O	!C	NA	-149.27	NA	82WE 2-274
Summary data selected for reason 4									
274	458	A-2		$\text{Ca}_2\text{Fe}(\text{CN})_6$ in 1588 H_2O	!C	NA	-149.27	NA	82WE 2-274
274	468			$\text{Ca}_2\text{Fe}(\text{CN})_6$ in 2888 H_2O	*J	NA	-824.34	NA	82WE 2-274
274	478			$\text{Ca}_2\text{Fe}(\text{CN})_6$ in 2888 H_2O	!C	NA	-149.22	NA	82WE 2-274
Summary data selected for reason 4									
274	488	A-2		$\text{Ca}_2\text{Fe}(\text{CN})_6$ in 2888 H_2O	!C	NA	-149.22	NA	82WE 2-274
274	498			$\text{Ca}_2\text{Fe}(\text{CN})_6$ in 5888 H_2O	*J	NA	-824.59	NA	82WE 2-274
274	508			$\text{Ca}_2\text{Fe}(\text{CN})_6$ in 5888 H_2O	!C	NA	-149.28	NA	82WE 2-274
Summary data selected for reason 4									
274	518	A-2		$\text{Ca}_2\text{Fe}(\text{CN})_6$ in 5888 H_2O	!C	NA	-149.28	NA	82WE 2-274
274	528			$\text{Ca}_2\text{Fe}(\text{CN})_6$ in 58,888 H_2O	*J	NA	-826.6	NA	82WE 2-274
274	538			$\text{Ca}_2\text{Fe}(\text{CN})_6$ in 58,888 H_2O	!C	NA	-149.8	NA	82WE 2-274
Summary data selected for reason 4									
274	548	A-2		$\text{Ca}_2\text{Fe}(\text{CN})_6$ in 58,888 H_2O	!C	NA	-149.8	NA	82WE 2-274
274	558			$\text{Ca}_2\text{Fe}(\text{CN})_6$ in 188,888 H_2O	*J	NA	-827.81	NA	82WE 2-274
274	568			$\text{Ca}_2\text{Fe}(\text{CN})_6$ in 188,888 H_2O	!C	NA	-149.88	NA	82WE 2-274

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
Summary data selected for reason 4								
274	578	A-2	$\text{Ca}_2\text{Fe}(\text{CN})_8$	in 186,888 H_2O	IC	NA	-149.88	NA 82WE 2-274
274	588		$\text{Ca}_2\text{Fe}(\text{CN})_8$	in $\infty \text{H}_2\text{O}$	*J	NA	-838.1	NA 82WE 2-274
274	598		$\text{Ca}_2\text{Fe}(\text{CN})_8$	in $\infty \text{H}_2\text{O}$	IC	NA	-158.6	NA 82WE 2-274
Summary data selected for reason 4								
274	608	A-2	$\text{Ca}_2\text{Fe}(\text{CN})_8$	in $\infty \text{H}_2\text{O}$	IC	NA	-158.6	NA 82WE 2-274
274	818		$\text{Ca}_2\text{Fe}(\text{CN})_8 \cdot 11\text{H}_2\text{O}$		*J cr	NA	-3781.1	NA 82WE 2-274
274	828		$\text{Ca}_2\text{Fe}(\text{CN})_8 \cdot 11\text{H}_2\text{O}$		IC cr	NA	-983.78	NA 82WE 2-274
274	838		$\text{Ca}_2\text{Fe}(\text{CN})_8 \cdot 11\text{H}_2\text{O}$		*C cr	NA	-983.7	NA 71PW 54
Summary data selected for reason 2								
274	848	S-2	$\text{Ca}_2\text{Fe}(\text{CN})_8 \cdot 11\text{H}_2\text{O}$		*C cr	NA	-983.78	NA 82WE 2-274
274	858		$\text{Ca}_3(\text{Fe}(\text{CN})_6)_2$	from $\text{Fe}(\text{CN})_6^{3-}$	*J ai	-281.9	-584.6	381.2 82WE 2-274
274	868		$\text{Ca}_3(\text{Fe}(\text{CN})_6)_2$	from $\text{Fe}(\text{CN})_6^{3-}$	IC ai	-48.28	-128.6	91.11 82WE 2-274
274	878		$\text{Ca}_3(\text{Fe}(\text{CN})_6)_2$	std. state, $m = 1$	*C aq	-48.3	-128.6	91.1 71PW 54
Summary data selected for reason 2								
274	888	A-1	$\text{Ca}_3(\text{Fe}(\text{CN})_6)_2$	std. state, $m = 1$	*C ai	-48.28	-128.6	91.11 82WE 2-274
275	18		$\text{Ca}_3(\text{Fe}(\text{CN})_6)_2$	in $\infty \text{H}_2\text{O}$	*J	NA	-584.6	NA 82WE 2-275
275	28		$\text{Ca}_3(\text{Fe}(\text{CN})_6)_2$	in $\infty \text{H}_2\text{O}$	IC	NA	-128.6	NA 82WE 2-275
275	38		$\text{Ca}_3(\text{Fe}(\text{CN})_6)_2$	in $\infty \text{H}_2\text{O}$	*C	NA	-128.6	NA 71PW 54
Summary data selected for reason 1								
275	48	A-2	$\text{Ca}_3(\text{Fe}(\text{CN})_6)_2$	in $\infty \text{H}_2\text{O}$	IC	NA	-128.6	NA 82WE 2-275
275	58		$\text{CaH}_2\text{Fe}(\text{CN})_8$		*J aq	NA	-84.5	NA 82WE 2-275
275	68		$\text{CaH}_2\text{Fe}(\text{CN})_8$		IC aq	NA	-28.2	NA 82WE 2-275
Summary data selected for reason 4								
275	78	A-2	$\text{CaH}_2\text{Fe}(\text{CN})_8$		IC aq	NA	-28.2	NA 82WE 2-275
275	71		$\text{CaHFe}(\text{CN})_8^{2-}$		*C ao	24.14	-17.84	55.16 86CR
Summary data selected for reason 4								
275	72		$\text{CaHFe}(\text{CN})_8^{2-}$		*C ao	24.14	-17.84	55.16 86CR
1581434	275	74	A-8	$\text{Ca}^{2+} + \text{H}^+ + \text{Fe}^{2+} + 6\text{CN}^- + e^- \leftrightarrow \text{CaHFe}(\text{CN})_8^{2-}$				
275	75	A-8	1581434	$\text{CaHFe}(\text{CN})_8^{2-}$				

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
275	76	5	1.000 156	1.000 336	1.000 280	6.000 143	1.000 001
280	10	Sr(CN) ₂	*J aq	NA	-238.5	NA	82WE 2-280
280	20	Sr(CN) ₂	!C aq	NA	-57.00	NA	82WE 2-280
280	30	Sr(CN) ₂	*C aq	NA	-57.0	NA	71PW 71
Summary data selected for reason 2							
280	40	A-2 Sr(CN) ₂	*C aq	NA	-57.00	NA	82WE 2-280
280	50	Sr(CN) ₂ ·4H ₂ O	*J cr	NA	-1396.2	NA	82WE 2-280
280	60	Sr(CN) ₂ ·4H ₂ O	!C cr	NA	-333.70	NA	82WE 2-280
280	70	Sr(CN) ₂ ·4H ₂ O	*C cr	NA	-333.7	NA	71PW 71
Summary data selected for reason 2							
280	80	S-2 Sr(CN) ₂ ·4H ₂ O	*C cr	NA	-333.70	NA	82WE 2-280
280	90	SrHg(CN) ₄	*J aq	NA	-16.8	NA	82WE 2-280
280	100	SrHg(CN) ₄	!C aq	NA	-3.90	NA	82WE 2-280
280	110	SrHg(CN) ₄	*C aq	NA	-3.9	NA	71PW 73
Summary data selected for reason 2							
280	120	A-2 SrHg(CN) ₄	*C aq	NA	-3.90	NA	82WE 2-280
280	130	Sr(Hg(CN) ₃) ₂	*J aq	NA	258.6	NA	82WE 2-280
280	140	Sr(Hg(CN) ₃) ₂	!C aq	NA	61.81	NA	82WE 2-280
280	150	Sr(Hg(CN) ₃) ₂	*C aq	NA	61.8	NA	71PW 73
Summary data selected for reason 2							
280	160	A-2 Sr(Hg(CN) ₃) ₂	*C aq	NA	61.8	NA	82WE 2-280
280	170	SrCl ₂ ·2Hg(CN) ₂	*J aq	NA	-323.4	NA	82WE 2-280
280	180	SrCl ₂ ·2Hg(CN) ₂	!C aq	NA	-77.20	NA	82WE 2-280
Summary data selected for reason 4							
280	190	A-2 SrCl ₂ ·2Hg(CN) ₂	!C aq	NA	-77.20	NA	82WE 2-280
280	200	SrCl ₂ ·2Hg(CN) ₂ ·6H ₂ O	*J cr	NA	-2107.5	NA	82WE 2-280
280	210	SrCl ₂ ·2Hg(CN) ₂ ·6H ₂ O	!C cr	NA	-503.70	NA	82WE 2-280
Summary data selected for reason 4							
280	220	S-2 SrCl ₂ ·2Hg(CN) ₂ ·6H ₂ O	!C cr	NA	-503.70	NA	82WE 2-280
280	230	SrBr ₂ ·2Hg(CN) ₂	*J aq	NA	-236.0	NA	82WE 2-280
280	240	SrBr ₂ ·2Hg(CN) ₂	!C aq	NA	-56.41	NA	82WE 2-280

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta H_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
Summary data selected for reason 4								
266	256	A-2	SrBr ₂ ·2Hg(CN) ₂	!C aq	NA	-56.41	NA	82WE 2-266
266	266		SrBr ₂ ·2Hg(CN) ₂ ·6H ₂ O	*J cr	NA	-2632.2	NA	82WE 2-266
266	276		SrBr ₂ ·2Hg(CN) ₂ ·6H ₂ O	!C cr	NA	-485.71	NA	82WE 2-266
Summary data selected for reason 4								
266	286	S-2	SrBr ₂ ·2Hg(CN) ₂ ·6H ₂ O	!C cr	NA	-485.71	NA	82WE 2-266
266	296		SrI ₂ ·2Hg(CN) ₂	*J aq	NA	-121.8	NA	82WE 2-266
266	306		SrI ₂ ·2Hg(CN) ₂	!C aq	NA	-29.11	NA	82WE 2-266
Summary data selected for reason 4								
266	316	A-2	SrI ₂ ·2Hg(CN) ₂	!C aq	NA	-29.11	NA	82WE 2-266
266	326		SrI ₂ ·2Hg(CN) ₂ ·7H ₂ O	*J cr	NA	-2269.2	NA	82WE 2-266
266	336		SrI ₂ ·2Hg(CN) ₂ ·7H ₂ O	!C cr	NA	-528.61	NA	82WE 2-266
Summary data selected for reason 4								
266	346	S-2	SrI ₂ ·2Hg(CN) ₂ ·7H ₂ O	!C cr	NA	-528.61	NA	82WE 2-266
266	356		SrAg(CN) ₃	*J aq	NA	-164.4	NA	82WE 2-266
266	366		SrAg(CN) ₃	!C aq	NA	-39.29	NA	82WE 2-266
266	376		SrAg(CN) ₃	*C aq	NA	-39.3	NA	71PW 74
Summary data selected for reason 2								
266	386	A-2	SrAg(CN) ₃	*C aq	NA	-39.29	NA	82WE 2-266
266	396		Sr(Ag(CN) ₂) ₂	*J aq	NA	-1.7	NA	82WE 2-266
266	406		Sr(Ag(CN) ₂) ₂	!C aq	NA	-6.41	NA	82WE 2-266
266	416		Sr(Ag(CN) ₂) ₂	*C aq	NA	-6.4	NA	71PW 74
Summary data selected for reason 2								
266	426	A-2	Sr(Ag(CN) ₂) ₂	*C aq	NA	-6.41	NA	82WE 2-266
266	436		SrNi(CN) ₄	*J aq	NA	-164.4	NA	82WE 2-266
266	446		SrNi(CN) ₄	!C aq	NA	-39.29	NA	82WE 2-266
266	456		SrNi(CN) ₄	*C aq	NA	-39.3	NA	71PW 74
Summary data selected for reason 2								
266	466	A-2	SrNi(CN) ₄	*C aq	NA	-39.29	NA	82WE 2-266
281	16		SrFe(CN) ₆ ⁻	*J ao	153.7	NA	NA	82WE 2-281
281	26		SrFe(CN) ₆ ⁻	!C ao	36.74	NA	NA	82WE 2-281
281	36		SrFe(CN) ₆ ⁻	*C aq	36.7	NA	NA	71PW 75

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
281	31	$\text{SrFe}(\text{CN})_6^-$	*C aq	37.8	4.12	78.4	82A
281	32	$\text{SrFe}(\text{CN})_6^-$	*C so	38.93	NA	NA	76SM 22
Summary data selected for reasons 2 and 4							
281	48	$\text{SrFe}(\text{CN})_6^-$	*C so	38.74	4.12	78.4	82WE 2-281 (82A)
8881431	281	42 A-8 $\text{Sr}^{2+} + \text{Fe}^{3+} + 6\text{CN}^- \leftrightarrow \text{SrFe}(\text{CN})_6^-$					
281	43	A-8 8881431 $\text{SrFe}(\text{CN})_6^-$					
281	44	3 1.888 888 1.888 281 8.888 143					
281	58	$\text{Sr}_2\text{Fe}(\text{CN})_8$ from $\text{Fe}(\text{CN})_6^{4-}$	*J ai	-423.87	-636.8	29.7	82WE 2-281
281	61	$\text{Sr}_2\text{Fe}(\text{CN})_8$ from $\text{Fe}(\text{CN})_6^{4-}$	!C ai	-181.31	-152.8	7.18	82WE 2-281
281	78	$\text{Sr}_2\text{Fe}(\text{CN})_8$ std. state, $n = 1$	*C aq	-181.33	-152.8	7.1	71PW 76
Summary data selected for reason 2							
281	88	A-1 $\text{Sr}_2\text{Fe}(\text{CN})_8$ std. state, $n = 1$	*C ai	-181.31	-152.8	7.18	82WE 2-281
281	98	$\text{Sr}_2\text{Fe}(\text{CN})_8$ in 1,888,888 H_2O	*J	NA	-634.84	NA	82WE 2-281
281	188	$\text{Sr}_2\text{Fe}(\text{CN})_8$ in 1,888,888 H_2O	!C	NA	-151.73	NA	82WE 2-281
281	118	$\text{Sr}_2\text{Fe}(\text{CN})_8$ in 1,888,888 H_2O	*C	NA	-151.73	NA	71PW 76
Summary data selected for reason 1							
281	128	A-2 $\text{Sr}_2\text{Fe}(\text{CN})_8$ in 1,888,888 H_2O	!C	NA	-151.73	NA	82WE 2-281
281	138	$\text{Sr}_2\text{Fe}(\text{CN})_8$ in $\infty \text{H}_2\text{O}$	*J	NA	-636.8	NA	82WE 2-281
281	148	$\text{Sr}_2\text{Fe}(\text{CN})_8$ in $\infty \text{H}_2\text{O}$	!C	NA	-152.8	NA	82WE 2-281
281	158	$\text{Sr}_2\text{Fe}(\text{CN})_8$ in $\infty \text{H}_2\text{O}$	*C	NA	-152.8	NA	71PW 76
Summary data selected for reason 1							
281	188	A-2 $\text{Sr}_2\text{Fe}(\text{CN})_8$ in $\infty \text{H}_2\text{O}$	!C	NA	-152.8	NA	82WE 2-281
281	178	$\text{Sr}_3(\text{Fe}(\text{CN})_6)_2$ in 188,888 H_2O	*J	NA	-518.95	NA	82WE 2-281
281	188	$\text{Sr}_3(\text{Fe}(\text{CN})_6)_2$ in 188,888 H_2O	!C	NA	-122.12	NA	82WE 2-281
281	198	$\text{Sr}_3(\text{Fe}(\text{CN})_6)_2$ in 188,888 H_2O	*C	NA	-122.55	NA	71PW 76
Summary data selected for reason 2							
281	208	A-2 $\text{Sr}_3(\text{Fe}(\text{CN})_6)_2$ in 188,888 H_2O	*C	NA	-122.12	NA	82WE 2-281
281	218	$\text{Sr}_3(\text{Fe}(\text{CN})_6)_2$ in $\infty \text{H}_2\text{O}$	*J	NA	-513.8	NA	82WE 2-281
281	228	$\text{Sr}_3(\text{Fe}(\text{CN})_6)_2$ in $\infty \text{H}_2\text{O}$	!C	NA	-122.8	NA	82WE 2-281
281	238	$\text{Sr}_3(\text{Fe}(\text{CN})_6)_2$ in $\infty \text{H}_2\text{O}$	*C	NA	-122.8	NA	71PW 76

TABLE B.2. (contd)

WINTER	In 82WE				Units	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°			
Number	Page	ID	Form	Compound	Q	State	(Q/mol)	(Q/mol)	(Q/mol·K)	Date	Sources
Summary data selected for reason 1											
281	248	A-2		$\text{Sr}_3(\text{Fe}(\text{CN})_6)_2$ in $\infty \text{H}_2\text{O}$	!C	NA	-122.8	NA		82WE	2-281
281	258			$\text{Sr}_3(\text{FeCo}(\text{CN})_6)_2$	*J	cr	NA	-1882.4	NA	82WE	2-281
281	268			$\text{Sr}_3(\text{FeCo}(\text{CN})_6)_2$	!C	cr	NA	-258.78	NA	82WE	2-281
281	278			$\text{Sr}_3(\text{FeCo}(\text{CN})_6)_2$	*C	cr	NA	-258.7	NA	71PW	78
Summary data selected for reason 2											
281	288	S-2		$\text{Sr}_3(\text{FeCo}(\text{CN})_6)_2$	*C	cr	NA	-258.78	NA	82WE	2-281
281	298			$\text{Sr}_3(\text{FeCo}(\text{CN})_6)_2$	*J	aq	NA	-1255.5	NA	82WE	2-281
281	308			$\text{Sr}_3(\text{FeCo}(\text{CN})_6)_2$	!C	aq	NA	-388.31	NA	82WE	2-281
281	318			$\text{Sr}_3(\text{FeCo}(\text{CN})_6)_2$	*C	aq	NA	-388.3	NA	71PW	78
Summary data selected for reason 2											
281	328	A-2		$\text{Sr}_3(\text{FeCo}(\text{CN})_6)_2$	*C	aq	NA	-388.31	NA	82WE	2-281
281	338			$\text{Sr}_3(\text{FeCo}(\text{CN})_6)_2 \cdot 4\text{H}_2\text{O}$	*J	cr	NA	-2259.4	NA	82WE	2-281
281	348			$\text{Sr}_3(\text{FeCo}(\text{CN})_6)_2 \cdot 4\text{H}_2\text{O}$	!C	cr	NA	-548.81	NA	82WE	2-281
281	358			$\text{Sr}_3(\text{FeCo}(\text{CN})_6)_2 \cdot 4\text{H}_2\text{O}$	*C	cr	NA	-548.8	NA	71PW	78
Summary data selected for reason 2											
281	368	S-2		$\text{Sr}_3(\text{FeCo}(\text{CN})_6)_2 \cdot 4\text{H}_2\text{O}$	*C	cr	NA	-548.81	NA	82WE	2-281
286	18			$\text{Ba}(\text{CN})_2$	*J	cr	NA	-218.4	NA	82WE	2-288
286	28			$\text{Ba}(\text{CN})_2$	!C	cr	NA	-52.28	NA	82WE	2-288
286	38			$\text{Ba}(\text{CN})_2$	*C	cr	NA	-52.2	NA	71PW	95
Summary data selected for reason 2											
286	48	S-2		$\text{Ba}(\text{CN})_2$	*C	cr	NA	-52.28	NA	82WE	2-288
286	58			$\text{Ba}(\text{CN})_2$	*J	ai	NA	-238.1	NA	82WE	2-288
286	68			$\text{Ba}(\text{CN})_2$	!C	ai	NA	-55.88	NA	82WE	2-288
286	78			$\text{Ba}(\text{CN})_2$	*C	aq	NA	-55.8	NA	71PW	95
Summary data selected for reason 2											
286	88	A-2		$\text{Ba}(\text{CN})_2$	*C	ai	NA	-55.88	NA	82WE	2-288
286	98			$\text{Ba}(\text{CN})_2 \cdot \text{H}_2\text{O}$	*J	cr	NA	-528.5	NA	82WE	2-288
286	108			$\text{Ba}(\text{CN})_2 \cdot \text{H}_2\text{O}$	!C	cr	NA	-124.4	NA	82WE	2-288
286	118			$\text{Ba}(\text{CN})_2 \cdot \text{H}_2\text{O}$	*C	cr	NA	-124.4	NA	71PW	95
Summary data selected for reason 1											
286	128	S-2		$\text{Ba}(\text{CN})_2 \cdot \text{H}_2\text{O}$	!C	cr	NA	-124.4	NA	82WE	2-288

TABLE B.2. (contd)

MINTEQA Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta H_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
286	138		Ba(CN) ₂ ·2H ₂ O	*J cr	NA	-817.8	NA	82WE 2-286
286	148		Ba(CN) ₂ ·2H ₂ O	!C cr	NA	-195.4	NA	82WE 2-286
286	158		Ba(CN) ₂ ·2H ₂ O	*C cr	NA	-195.4	NA	71PW 95
Summary data selected for reason 1								
286	168	S-2	Ba(CN) ₂ ·2H ₂ O	!C cr	NA	-195.4	NA	82WE 2-286
287	18		BaHg(CN) ₄	*J aq	NA	-3.8	NA	82WE 2-287
287	28		BaHg(CN) ₄	!C aq	NA	-8.91	NA	82WE 2-287
287	38		BaHg(CN) ₄	*C aq	NA	-8.9	NA	71PW 98
Summary data selected for reason 2								
287	48	A-2	BaHg(CN) ₄	*C aq	NA	-8.91	NA	82WE 2-287
287	58		Ba(Hg(CN) ₃) ₂	*J aq	NA	286.9	NA	82WE 2-287
287	68		Ba(Hg(CN) ₃) ₂	!C aq	NA	63.79	NA	82WE 2-287
287	78		Ba(Hg(CN) ₃) ₂	*C aq	NA	63.8	NA	71PW 98
Summary data selected for reason 2								
287	88	A-2	Ba(Hg(CN) ₃) ₂	*C aq	NA	63.79	NA	82WE 2-287
287	98		BaCl ₂ ·2Hg(CN) ₂	*J aq	NA	-315.1	NA	82WE 2-287
287	108		BaCl ₂ ·2Hg(CN) ₂	!C aq	NA	-75.31	NA	82WE 2-287
287	118		BaCl ₂ ·2Hg(CN) ₂	*C aq	NA	-75.3	NA	71PW 98
Summary data selected for reason 2								
287	128	A-2	BaCl ₂ ·2Hg(CN) ₂	*C aq	NA	-75.31	NA	82WE 2-287
287	138		BaCl ₂ ·2Hg(CN) ₂ ·5H ₂ O	*J cr	NA	-1819.6	NA	82WE 2-287
287	148		BaCl ₂ ·2Hg(CN) ₂ ·5H ₂ O	!C cr	NA	-434.89	NA	82WE 2-287
287	158		BaCl ₂ ·2Hg(CN) ₂ ·5H ₂ O	*C cr	NA	-434.9	NA	71PW 98
Summary data selected for reason 2								
287	168	S-2	BaCl ₂ ·2Hg(CN) ₂ ·5H ₂ O	*C cr	NA	-434.89	NA	82WE 2-287
287	178		BaBr ₂ ·2Hg(CN) ₂	*J aq	NA	-227.8	NA	82WE 2-287
287	188		BaBr ₂ ·2Hg(CN) ₂	!C aq	NA	-54.48	NA	82WE 2-287
287	198		BaBr ₂ ·2Hg(CN) ₂	*C aq	NA	-54.4	NA	71PW 98
Summary data selected for reason 2								
287	208	A-2	BaBr ₂ ·2Hg(CN) ₂	*C aq	NA	-54.48	NA	82WE 2-287
287	218		BaBr ₂ ·2Hg(CN) ₂ ·7H ₂ O	*J cr	NA	-2318.8	NA	82WE 2-287
287	228		BaBr ₂ ·2Hg(CN) ₂ ·7H ₂ O	!C cr	NA	-554.21	NA	82WE 2-287
287	238		BaBr ₂ ·2Hg(CN) ₂ ·7H ₂ O	*C cr	NA	-554.2	NA	71PW 98

TABLE B.2. (contd)

MINTeq	In 82WE				Units	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°	
Number	Page	ID	Form	Compound	Q State	(Q/mol)	(Q/mol)	(Q/mol·K)	Data Sources
Summary data selected for reason 2									
287	248	S-2		BaBr ₂ ·2Hg(CN) ₂ ·7H ₂ O	*C cr	NA	-554.21	NA	82WE 2-287
287	258			(Hg(CN) ₂) ₂ ·BaI ₂	*J aq	NA	-113.8	NA	82WE 2-287
287	268			(Hg(CN) ₂) ₂ ·BaI ₂	!C aq	NA	-27.81	NA	82WE 2-287
287	278			(Hg(CN) ₂) ₂ ·BaI ₂	*C aq	NA	-27.8	NA	71PW 99
Summary data selected for reason 2									
287	288	A-2		(Hg(CN) ₂) ₂ ·BaI ₂	*C aq	NA	-27.81	NA	82WE 2-287
287	298			(Hg(CN) ₂) ₂ ·BaI ₂ ·6H ₂ O	*J cr	NA	-1924.6	NA	82WE 2-287
287	308			(Hg(CN) ₂) ₂ ·BaI ₂ ·6H ₂ O	!C cr	NA	-459.99	NA	82WE 2-287
287	318			(Hg(CN) ₂) ₂ ·BaI ₂ ·6H ₂ O	*C cr	NA	-459.8	NA	71PW 99
Summary data selected for reason 2									
287	328	S-2		(Hg(CN) ₂) ₂ ·BaI ₂ ·6H ₂ O	*C cr	NA	-459.89	NA	82WE 2-287
287	338			BaAg(CN) ₃	*J aq	NA	-119.7	NA	82WE 2-287
287	348			BaAg(CN) ₃	!C aq	NA	-28.81	NA	82WE 2-287
287	358			BaAg(CN) ₃	*C aq	NA	-28.8	NA	71PW 99
Summary data selected for reason 2									
287	368	A-2		BaAg(CN) ₃	*C aq	NA	-28.81	NA	82WE 2-287
287	378			Ba(Ag(CN) ₂) ₂	*J aq	NA	7.9	NA	82WE 2-287
287	388			Ba(Ag(CN) ₂) ₂	!C aq	NA	1.9	NA	82WE 2-287
287	398			Ba(Ag(CN) ₂) ₂	*C aq	NA	1.9	NA	71PW 99
Summary data selected for reason 1									
287	408	A-2		Ba(Ag(CN) ₂) ₂	!C aq	NA	1.9	NA	82WE 2-287
287	418			Ba(Ni(CN) ₄)	*J aq	NA	-142.7	NA	82WE 2-287
287	428			Ba(Ni(CN) ₄)	!C aq	NA	-34.11	NA	82WE 2-287
287	438			Ba(Ni(CN) ₄)	*C aq	NA	-34.1	NA	71PW 99
Summary data selected for reason 2									
287	448	A-2		Ba(Ni(CN) ₄)	*C aq	NA	-34.11	NA	82WE 2-287
287	458			Ba ₂ Fe(CN) ₆	*J aq	NA	-609.8	NA	82WE 2-287
287	468			Ba ₂ Fe(CN) ₆	!C aq	NA	-145.7	NA	82WE 2-287
287	478			Ba ₂ Fe(CN) ₆	*C aq	NA	-145.7	NA	71PW 99

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol-K)	Data Sources
Summary data selected for reason 1								
287	480	A-2	$\text{Ba}_2\text{Fe}(\text{CN})_8$	IC aq	NA	-145.7	NA	82WE 2-287
287	481		$\text{BaFe}(\text{CN})_6^-$	*C ao	36.35	NA	NA	76SM 22
287	481		$\text{BaFe}(\text{CN})_6^-$	*C ao	36.45	6.22	81.15	82A
Summary data selected for reason								
287	482	A-5	$\text{BaFe}(\text{CN})_6^-$	*C ao	36.45	6.22	81.15	82A
1001431	287	483	A-5 $\text{Ba}^{+2} + \text{Fe}^{+3} + 6\text{CN}^- \leftrightarrow \text{BaFe}(\text{CN})_6^-$					
287	484	A-5	1001431 $\text{BaFe}(\text{CN})_6^-$					
287	485		3 1.000 100 1.000 281 6.000 143					
287	486		$\text{BaFe}(\text{CN})_6^-$	*Caq	26.93	NA	NA	76SM 21
Summary data selected for reason 4								
287	487		$\text{BaFe}(\text{CN})_6^-$	*C	26.93	NA	NA	76SM 21
1001438	287	488	$\text{Ba}^+ + \text{Fe}^{3+} + 6\text{CN}^- \leftrightarrow \text{BaFe}(\text{CN})_6^-$					
287	489		3 1.000 100 1.000 281 6.000 143					
287	490		$\text{Ba}_2\text{Fe}(\text{CN})_8 \cdot 6\text{H}_2\text{O}$	*J cr	NA	-2372.3	NA	82WE 2-287
287	500		$\text{Ba}_2\text{Fe}(\text{CN})_8 \cdot 6\text{H}_2\text{O}$	IC cr	NA	-566.99	NA	82WE 2-287
287	510		$\text{Ba}_2\text{Fe}(\text{CN})_8 \cdot 6\text{H}_2\text{O}$	*C cr	NA	-567.0	NA	71PW 99
Summary data selected for reason 2								
287	520	S-2	$\text{Ba}_2\text{Fe}(\text{CN})_8 \cdot 6\text{H}_2\text{O}$	*C cr	NA	-567.0	NA	71PW 99
287	530		$\text{Ba}_3(\text{Fe}(\text{CN})_6)_2$ from $\text{Fe}(\text{CN})_6^{3-}$	*J ai	-223.6	-489.1	569.4	82WE 2-287
287	540		$\text{Ba}_3(\text{Fe}(\text{CN})_6)_2$ from $\text{Fe}(\text{CN})_6^{3-}$	IC ai	-53.44	-116.9	136.1	82WE 2-287
287	550		$\text{Ba}_3(\text{Fe}(\text{CN})_6)_2$ std. state., n = 1	*C aq	-53.5	-116.9	136.1	71PW 99
Summary data selected for reason 2								
287	560	A-1	$\text{Ba}_3(\text{Fe}(\text{CN})_6)_2$ std. state., n = 1	*C ai	-53.44	-116.9	136.1	82WE 2-287
287	570		$\text{Ba}_3(\text{Fe}(\text{CN})_6)_2$ in 100,000 H_2O	*J	NA	-486.1	NA	82WE 2-287
287	580		$\text{Ba}_3(\text{Fe}(\text{CN})_6)_2$ in 100,000 H_2O	IC	NA	-116.2	NA	82WE 2-287
287	590		$\text{Ba}_3(\text{Fe}(\text{CN})_6)_2$ in 100,000 H_2O	*C	NA	-116.18	NA	71PW 100

TABLE B.2. (contd)

WINTER	In 82WE				Units	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°	
Number	Page	ID	Form	Compound	Q State	(Q/mol)	(Q/mol)	(Q/mol-K)	Data Sources
Summary data selected for reason 2									
287	808	A-2		$\text{Ba}_3(\text{Fe}(\text{CN})_6)_2$ in 188,888 H_2O	*C	NA	-116.2	NA	82WE 2-287
287	818			$\text{Ba}_3(\text{Fe}(\text{CN})_6)_2$ in $\infty \text{H}_2\text{O}$	*J	NA	-489.1	NA	82WE 2-287
287	828			$\text{Ba}_3(\text{Fe}(\text{CN})_6)_2$ in $\infty \text{H}_2\text{O}$	!C	NA	-116.9	NA	82WE 2-287
287	838			$\text{Ba}_3(\text{Fe}(\text{CN})_6)_2$ in $\infty \text{H}_2\text{O}$	*C	NA	-116.9	NA	71PW 186
Summary data selected for reason 1									
287	848	A-2		$\text{Ba}_3(\text{Fe}(\text{CN})_6)_2$ in $\infty \text{H}_2\text{O}$	!C	NA	-116.9	NA	82WE 2-287
287	858			$\text{Ba}_3(\text{FeCo}(\text{CN})_5)_2$	*J cr	NA	-1142.7	NA	82WE 2-287
287	868			$\text{Ba}_3(\text{FeCo}(\text{CN})_5)_2$	!C cr	NA	-273.11	NA	82WE 2-287
287	878			$\text{Ba}_3(\text{FeCo}(\text{CN})_5)_2$	*C cr	NA	-273.1	NA	71PW 186
Summary data selected for reason 2									
287	888	S-2		$\text{Ba}_3(\text{FeCo}(\text{CN})_5)_2$	*C cr	NA	-273.11	NA	82WE 2-287
287	898			$\text{Ba}_3(\text{FeCo}(\text{CN})_5)_2$	*J aq	NA	-1219.2	NA	82WE 2-287
287	708			$\text{Ba}_3(\text{FeCo}(\text{CN})_5)_2$	!C aq	NA	-291.48	NA	82WE 2-287
287	718			$\text{Ba}_3(\text{FeCo}(\text{CN})_5)_2$	*C aq	NA	-291.4	NA	71PW 186
Summary data selected for reason 2									
287	728	A-2		$\text{Ba}_3(\text{FeCo}(\text{CN})_5)_2$	*C aq	NA	-291.48	NA	82WE 2-287
287	738			$\text{Ba}_3(\text{FeCo}(\text{CN})_5)_2 \cdot 11\text{H}_2\text{O}$	*J cr	NA	-4391.5	NA	82WE 2-287
287	748			$\text{Ba}_3(\text{FeCo}(\text{CN})_5)_2 \cdot 11\text{H}_2\text{O}$	!C cr	NA	-1849.8	NA	82WE 2-287
287	758			$\text{Ba}_3(\text{FeCo}(\text{CN})_5)_2 \cdot 11\text{H}_2\text{O}$	*C cr	NA	-1849.8	NA	71PW 186
Summary data selected for reason 1									
287	768	S-2		$\text{Ba}_3(\text{FeCo}(\text{CN})_5)_2 \cdot 11\text{H}_2\text{O}$	!C cr	NA	-1849.8	NA	82WE 2-287
287	778			$\text{BaH}_2\text{Fe}(\text{CN})_6$	*J aq	NA	-78.2	NA	82WE 2-287
287	788			$\text{BaH}_2\text{Fe}(\text{CN})_6$	!C aq	NA	-18.7	NA	82WE 2-287
287	798			$\text{BaH}_2\text{Fe}(\text{CN})_6$	*C aq	NA	-18.7	NA	71PW 18687
Summary data selected for reason 1									
287	808	A-2		$\text{BaH}_2\text{Fe}(\text{CN})_6$	!C aq	NA	-18.7	NA	82WE 2-287
298	18			LiCN in 118 H_2O	*J	NA	-125.1	NA	82WE 2-298
298	28			LiCN in 118 H_2O	!C	NA	-29.9	NA	82WE 2-298
298	38			LiCN in 118 H_2O	*C	NA	-29.9	NA	81WE 19

TABLE B.2. (contd)

WINTER	In 82WE				Units	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°	
Number	Page	ID	Form	Compound	Q State	(Q/mol)	(Q/mol)	(Q/mol·K)	Data Sources
Summary data selected for reason 1									
296	48	A-2	LiCN	in 118 H ₂ O	!C	NA	-29.9	NA	82WE 2-296
296	58		LiCN	in 228 H ₂ O	*J	NA	-126.6	NA	82WE 2-296
296	68		LiCN	in 228 H ₂ O	!C	NA	-38.88	NA	82WE 2-296
296	78		LiCN	in 228 H ₂ O	*C	NA	-38.8	NA	81WE 19
Summary data selected for reason 2									
296	88	A-2	LiCN	in 228 H ₂ O	*C	NA	-38.8	NA	82WE 2-296
297	18		LiCN·0.5Hg(CN) ₂	in 338 H ₂ O	*J	NA	-12.6	NA	82WE 2-297
297	28		LiCN·0.5Hg(CN) ₂	in 338 H ₂ O	!C	NA	-3.81	NA	82WE 2-297
297	38		LiCN·0.5Hg(CN) ₂	in 338 H ₂ O	*C	NA	-3.8	NA	81WE 21
Summary data selected for reason 2									
297	48	A-2	LiCN·0.5Hg(CN) ₂	in 338 H ₂ O	*C	NA	-3.81	NA	82WE 2-297
297	58		LiCN·Hg(CN) ₂	in 558 H ₂ O	*J	NA	128.4	NA	82WE 2-297
297	68		LiCN·Hg(CN) ₂	in 558 H ₂ O	!C	NA	29.49	NA	82WE 2-297
297	78		LiCN·Hg(CN) ₂	in 558 H ₂ O	*C	NA	29.5	NA	81WE 21
Summary data selected for reason 2									
297	88	A-2	LiCN·Hg(CN) ₂	in 558 H ₂ O	*C	NA	29.49	NA	82WE 2-297
297	98		LiCl·0.5Hg(CN) ₂	in 338 H ₂ O	*J	NA	-386.3	NA	82WE 2-297
297	108		LiCl·0.5Hg(CN) ₂	in 338 H ₂ O	!C	NA	-73.21	NA	82WE 2-297
297	118		LiCl·0.5Hg(CN) ₂	in 338 H ₂ O	*C	NA	-73.2	NA	81WE 21
Summary data selected for reason 2									
297	128	A-2	LiCl·0.5Hg(CN) ₂	in 338 H ₂ O	*C	NA	-73.21	NA	82WE 2-297
297	138		LiCl·Hg(CN) ₂	in 558 H ₂ O	*J	NA	-187.4	NA	82WE 2-297
297	148		LiCl·Hg(CN) ₂	in 558 H ₂ O	!C	NA	-48.81	NA	82WE 2-297
297	158		LiCl·Hg(CN) ₂	in 558 H ₂ O	*C	NA	-48.8	NA	81WE 21
Summary data selected for reason 2									
297	168	A-2	LiCl·Hg(CN) ₂	in 558 H ₂ O	*C	NA	-48.81	NA	82WE 2-297
297	178		LiBr·0.5Hg(CN) ₂	in 388 H ₂ O	*J	NA	-262.3	NA	82WE 2-297
297	188		LiBr·0.5Hg(CN) ₂	in 388 H ₂ O	!C	NA	-82.69	NA	82WE 2-297
297	198		LiBr·0.5Hg(CN) ₂	in 388 H ₂ O	*C	NA	-82.7	NA	81WE 21

TABLE B.2. (contd)

MINTeq	In 82WE			Compound	Units	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°	Data Sources
Number	Page	ID	Form		Q	State	(Q/mol)	(Q/mol)	
Summary data selected for reason 2									
297	205	A-2	LiBr·0.5Hg(CN) ₂	in 300 H ₂ O	*C	NA	-82.69	NA	82WE 2-297
297	210		LiBr·Hg(CN) ₂	in 550 H ₂ O	*J	NA	-128.4	NA	82WE 2-297
297	220		LiBr·Hg(CN) ₂	in 550 H ₂ O	!C	NA	-29.49	NA	82WE 2-297
297	230		LiBr·Hg(CN) ₂	in 550 H ₂ O	*C	NA	-29.5	NA	81WE 21
Summary data selected for reason 2									
297	240	A-2	LiBr·Hg(CN) ₂	in 550 H ₂ O	*C	NA	-29.49	NA	82WE 2-297
298	10		LiBr·Hg(CN) ₂ ·3.5H ₂ O		*J cr	NA	-1161.1	NA	82WE 2-298
298	20		LiBr·Hg(CN) ₂ ·3.5H ₂ O		!C cr	NA	-277.51	NA	82WE 2-298
298	30		LiBr·Hg(CN) ₂ ·3.5H ₂ O		*C cr	NA	-277.5	NA	81WE 21
Summary data selected for reason 2									
298	40	S-2	LiBr·Hg(CN) ₂ ·3.5H ₂ O		*C cr	NA	-277.51	NA	82WE 2-298
298	50		LiI·0.5Hg(CN) ₂	in 330 H ₂ O	*J	NA	-201.7	NA	82WE 2-298
298	60		LiI·0.5Hg(CN) ₂	in 330 H ₂ O	!C	NA	-48.21	NA	82WE 2-298
298	70		LiI·0.5Hg(CN) ₂	in 330 H ₂ O	*C	NA	-48.2	NA	81WE 21
Summary data selected for reason 2									
298	80	A-2	LiI·0.5Hg(CN) ₂	in 330 H ₂ O	*C	NA	-48.21	NA	82WE 2-298
298	90		LiI·Hg(CN) ₂	in 550 H ₂ O	*J	NA	-86.5	NA	82WE 2-298
298	100		LiI·Hg(CN) ₂	in 550 H ₂ O	!C	NA	-15.9	NA	82WE 2-298
298	110		LiI·Hg(CN) ₂	in 550 H ₂ O	*C	NA	-15.9	NA	81WE 21
Summary data selected for reason 1									
298	120	A-2	LiI·Hg(CN) ₂	in 550 H ₂ O	!C	NA	-15.9	NA	82WE 2-298
298	130		LiI·Hg(CN) ₂ ·3.5H ₂ O		*J cr	NA	-1160.8	NA	82WE 2-298
298	140		LiI·Hg(CN) ₂ ·3.5H ₂ O		!C cr	NA	-265.01	NA	82WE 2-298
298	150		LiI·Hg(CN) ₂ ·3.5H ₂ O		*C cr	NA	-265.0	NA	81WE 21
Summary data selected for reason 2									
298	160	S-2	LiI·Hg(CN) ₂ ·3.5H ₂ O		*C cr	NA	-265.01	NA	82WE 2-298
298	170		LiFe(CN) ₆ ³⁻		*J ao	391.0	NA	NA	82WE 2-298
298	180		LiFe(CN) ₆ ³⁻		!C ao	93.64	NA	NA	82WE 2-298
298	190		LiFe(CN) ₆ ³⁻		*C ao	93.6	NA	NA	81WE 21
298	191		LiFe(CN) ₆ ³⁻		*C ao	93.19	47.99	54.12	86CR

TABLE B.2. (contd)

MINTeq	In 82WE				Units	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°	
Number	Page	ID	Form	Compound	Q State	(Q/mol)	(Q/mol)	(Q/mol.K)	Data Sources
Summary data selected for reason 6									
	298	280	A-8	$\text{LiFe}(\text{CN})_6^{3-}$	*C ao	93.19	47.99	54.12	86CR
4481431	298	281	A-8	$6\text{CN}^- + \text{Li}^+ + \text{Fe}^{2+} \leftrightarrow \text{LiFe}(\text{CN})_6^{3-}$					
	298	282	A-8	4481431 $\text{LiFe}(\text{CN})_6^{3-}$					
	298	283		3 6.888 143 1.888 448 1.888 288					
	298	284		$\text{Li}_2\text{Fe}(\text{CN})_6^{2-}$	*C ao	21.93	-21.92	58.12	86CR
Summary data selected for reason 4									
	298	284	A-8	$\text{Li}_2\text{Fe}(\text{CN})_6^{2-}$	*C ao	21.93	-21.92	58.12	86CR
4481432	298	285	A-8	$2\text{Li}^+ + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{Li}_2\text{Fe}(\text{CN})_6^{2-}$					
	298	286	A-8	4481432 $\text{Li}_2\text{Fe}(\text{CN})_6^{2-}$					
	298	287		3 2.888 448 1.888 288 6.888 143					
	298	288		$\text{LiHFe}(\text{CN})_6^{2-}$	*C ao	88.37	47.14	87.88	86CR
Summary data selected for reason 4									
	298	289	A-8	$\text{LiHFe}(\text{CN})_6^{2-}$	*C ao	88.37	47.14	87.88	86CR
4481433	298	210	A-8	$\text{Li}^+ + \text{H}^+ + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{LiHFe}(\text{CN})_6^{2-}$					
	298	211	A-8	4481433 $\text{LiHFe}(\text{CN})_6^{2-}$					
	298	212		4 1.888 448 1.888 338 1.888 288 6.888 143					
	318	18	NaCN	cr I, cubic	*J cr	-76.43	-87.49	116.88	82WE 2-316
	318	28	NaCN	cr I, cubic	!C cr	-18.27	-28.91	27.829	82WE 2-316
	318	38	NaCN	cr I, cubic	*C cr	-18.27	-28.91	27.83	81WE 42
	318	48	NaCN	cr I, cubic	*C cr	NA	-28.99	NA	76WE 33
Summary data selected for reason 2									
	318	58	S-8	NaCN	cr I, cubic	*C cr	-18.27	-28.91	27.83 82WE 2-316
1158881	318	51	S-8	$\text{CN}^- + \text{Na}^+ \leftrightarrow \text{NaCN}$					
	318	52	S-8	1158881 NaCN					
	318	53		2 1.888 143 1.888 588					

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
316	66	NaCN	cr II, orthorhombic	*J cr2	NA	-90.75	NA	82WE 2-316
316	70	NaCN	cr II, orthorhombic	!C cr2	NA	-21.69	NA	82WE 2-316
316	86	NaCN	cr II, orthorhombic	*C cr2	NA	-21.69	NA	81WE 42
316	96	NaCN	cr II, orthorhombic	*C cr2	NA	-21.69	NA	76WE 36
Summary data selected for reason 1								
316	106	S-2 NaCN	cr II, orthorhombic	!C cr2	NA	-21.69	NA	82WE 2-316
316	116	NaCN		*J ai	-89.5	-89.5	153.1	82WE 2-316
316	126	NaCN		!C ai	-21.4	-21.4	36.59	82WE 2-316
316	136	NaCN		*C a	-21.4	-21.4	36.6	81WE 42
316	146	NaCN		*C a	-21.4	-21.4	36.6	76WE 33
316	156	NaCN	undissociated complex	*C aq	-14.7	-19.1	21.8	76BS 70; 52L
Summary data selected for reasons 2 and 3								
316	166	A-1 NaCN		*C ai	-21.4	-21.4	36.59	82WE 2-316
316	176	NaCN	in 266 H ₂ O	*J	NA	-87.9	NA	82WE 2-316
316	186	NaCN	in 266 H ₂ O	!C	NA	-21.6	NA	82WE 2-316
316	196	NaCN	in 266 H ₂ O	*C	NA	-21.6	NA	81WE 42
316	206	NaCN	in 266 H ₂ O	*C	NA	-21.6	NA	76WE 33
Summary data selected for reason 1								
316	216	A-2 NaCN	in 266 H ₂ O	!C	NA	-21.6	NA	82WE 2-316
316	226	NaCN·1/2H ₂ O		*J cr	NA	-235.77	NA	82WE 2-316
316	236	NaCN·1/2H ₂ O		!C cr	NA	-56.35	NA	82WE 2-316
316	246	NaCN·1/2H ₂ O		*C cr	NA	-56.35	NA	81WE 42
316	256	NaCN·1/2H ₂ O		*C cr	NA	-56.35	NA	76WE 33
Summary data selected for reason 1								
316	266	S-2 NaCN·1/2H ₂ O		!C cr	NA	-56.35	NA	82WE 2-316
316	276	NaCN·2H ₂ O		*J cr	NA	-679.77	NA	82WE 2-316
316	286	NaCN·2H ₂ O		!C cr	NA	-162.47	NA	82WE 2-316
316	296	NaCN·2H ₂ O		*C cr	NA	-162.47	NA	81WE 42
316	306	NaCN·2H ₂ O		*C cr	NA	-162.47	NA	76WE 33
Summary data selected for reason 1								
316	316	S-2 NaCN·2H ₂ O		!C cr	NA	-162.47	NA	82WE 2-316
317	16	NaCNI ₂		*J ai	-125.75	NA	NA	82WE 2-317
317	26	NaCNI ₂		!C ai	-36.855	NA	NA	82WE 2-317
317	36	NaCNI ₂		*C a	-36.86	NA	NA	81WE 42

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol.K)	Data Sources
Summary data selected for reason 2								
317	48	A-1	NaCNH ₂	*C ai	-38.86	NA	NA	82WE 2-317
317	56		Na(CN) ₂ I	*J ai	NA	98.32	NA	82WE 2-317
317	66		Na(CN) ₂ I	IC ai	NA	23.82	NA	82WE 2-317
317	76		Na(CN) ₂ I	*C a	NA	23.82	NA	81WE 42
Summary data selected for reason 1								
317	86	A-2	Na(CN) ₂ I	IC ai	NA	23.82	NA	82WE 2-317
326	16		NaTi(CN) ₄ from Ti(CN) ₄ ³⁻	*J ai	439.	NA	NA	82WE 2-326
326	26		NaTi(CN) ₄ from Ti(CN) ₄ ³⁻	IC ai	185.	NA	NA	82WE 2-326
Summary data selected for reason 4								
326	36	A-1	NaTi(CN) ₄ from Ti(CN) ₄ ³⁻	IC ai	185.	NA	NA	82WE 2-326
326	46		Na ₂ Zn(CN) ₄	*J ai	-76.9	-138.1	343.	82WE 2-326
326	56		Na ₂ Zn(CN) ₄	IC ai	-18.4	-33.81	82.8	82WE 2-326
326	66		Na ₂ Zn(CN) ₄	*C ai	-18.4	-33.8	82.	81WE 46
Summary data selected for reason 2								
326	76	A-1	Na ₂ Zn(CN) ₄	*C ai	-18.4	-33.81	82.	82WE 2-326
326	86		NaCd(CN) ₃	*J ai	92.9	NA	NA	82WE 2-326
326	96		NaCd(CN) ₃	IC ai	22.2	NA	NA	82WE 2-326
326	106		NaCd(CN) ₃	*C a	22.2	NA	NA	81WE 46
Summary data selected for reason 1								
326	116	A-1	NaCd(CN) ₃	IC ai	22.2	NA	NA	82WE 2-326
326	126		Na ₂ Cd(CN) ₄	*J ai	-16.3	-52.3	439.	82WE 2-326
326	136		Na ₂ Cd(CN) ₄	IC ai	-3.98	-12.5	185.	82WE 2-326
326	146		Na ₂ Cd(CN) ₄	*C a	-3.9	-12.5	185.	81WE 46
Summary data selected for reason 1								
326	156	A-1	Na ₂ Cd(CN) ₄	IC ai	-3.98	-12.5	185.	82WE 2-326
321	16		NaHg(CN) ₃	*J ai	281.3	156.9	284.1	82WE 2-321
321	26		NaHg(CN) ₃	IC ai	48.11	37.58	67.9	82WE 2-321
321	36		NaHg(CN) ₃	*C ai	48.1	37.5	67.9	81WE 46
Summary data selected for reason 2								
321	46	A-1	NaHg(CN) ₃	*C ai	48.1	37.58	67.9	82WE 2-321

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
321	55	Na ₂ Hg(CN) ₄	*J ai	94.6	46.8	423.	82WE 2-321
321	65	Na ₂ Hg(CN) ₄	!C ai	22.6	11.8	161.	82WE 2-321
321	75	Na ₂ Hg(CN) ₄	*C a	22.6	11.8	161.1	81WE 46
Summary data selected for reason 2							
321	85	A-1 Na ₂ Hg(CN) ₄	*C ai	22.6	11.8	161	82WE 2-321
321	95	NaHg(CN) ₂ Cl	in 558 H ₂ O *J	NA	-131.8	NA	82WE 2-321
321	105	NaHg(CN) ₂ Cl	in 558 H ₂ O !C	NA	-31.31	NA	82WE 2-321
321	115	NaHg(CN) ₂ Cl	in 558 H ₂ O *C	NA	-31.3	NA	81WE 46
Summary data selected for reason 2							
321	125	A-2 NaHg(CN) ₂ Cl	in 558 H ₂ O *C	NA	-31.31	NA	82WE 2-321
321	135	NaHg(CN) ₂ Cl ₂ ·1.25H ₂ O	*J cr	NA	-526.5	NA	82WE 2-321
321	145	NaHg(CN) ₂ Cl ₂ ·1.25H ₂ O	!C cr	NA	-124.4	NA	82WE 2-321
321	155	NaHg(CN) ₂ Cl ₂ ·1.25H ₂ O	*C cr	NA	-124.4	NA	81WE 46
Summary data selected for reason 1							
321	165	S-2 NaHg(CN) ₂ Cl ₂ ·1.25H ₂ O	!C cr	NA	-124.4	NA	82WE 2-321
321	175	Na ₂ Hg(CN) ₂ Cl ₂	in 558 H ₂ O *J	NA	-536.8	NA	82WE 2-321
321	185	Na ₂ Hg(CN) ₂ Cl ₂	in 558 H ₂ O !C	NA	-128.3	NA	82WE 2-321
321	195	Na ₂ Hg(CN) ₂ Cl ₂	in 558 H ₂ O *C	NA	-128.3	NA	81WE 46
Summary data selected for reason 1							
321	205	A-2 Na ₂ Hg(CN) ₂ Cl ₂	in 558 H ₂ O !C	NA	-128.3	NA	82WE 2-321
321	215	NaHg(CN) ₂ Br	in 558 H ₂ O *J	NA	-87.9	NA	82WE 2-321
321	225	NaHg(CN) ₂ Br	in 558 H ₂ O !C	NA	-21.8	NA	82WE 2-321
321	235	NaHg(CN) ₂ Br	in 558 H ₂ O *C	NA	-21.8	NA	81WE 46
Summary data selected for reason 1							
321	245	A-2 NaHg(CN) ₂ Br	in 558 H ₂ O !C	NA	-21.8	NA	82WE 2-321
321	255	NaHg(CN) ₂ Br·2H ₂ O	*J cr	NA	-786.4	NA	82WE 2-321
321	265	NaHg(CN) ₂ Br·2H ₂ O	!C cr	NA	-169.3	NA	82WE 2-321
321	275	NaHg(CN) ₂ Br·2H ₂ O	*C cr	NA	-169.3	NA	81WE 46
Summary data selected for reason 1							
321	285	S-2 NaHg(CN) ₂ Br·2H ₂ O	!C cr	NA	-169.3	NA	82WE 2-321
321	295	Na ₂ Hg(CN) ₂ Br ₂	in 558 H ₂ O *J	NA	-453.1	NA	82WE 2-321
321	315	Na ₂ Hg(CN) ₂ Br ₂	in 558 H ₂ O !C	NA	-188.3	NA	82WE 2-321
321	325	Na ₂ Hg(CN) ₂ Br ₂	in 558 H ₂ O *C	NA	-188.3	NA	81WE 47

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
Summary data selected for reason 1							
321	338 A-2	$\text{Na}_2\text{Hg}(\text{CN})_2\text{Br}_2$	in 558 H ₂ O !C	NA	-108.3	NA	82WE 2-321
321	348	$\text{NaHg}(\text{CN})_2\text{I}$	in 558 H ₂ O *J	NA	-28.24	NA	82WE 2-321
321	358	$\text{NaHg}(\text{CN})_2\text{I}$	in 558 H ₂ O !C	NA	-8.758	NA	82WE 2-321
321	368	$\text{NaHg}(\text{CN})_2\text{I}$	in 558 H ₂ O *C	NA	-8.75	NA	81WE 47
Summary data selected for reason 2							
321	378 A-2	$\text{NaHg}(\text{CN})_2\text{I}$	in 558 H ₂ O *C	NA	-8.758	NA	82WE 2-321
321	388	$\text{NaHg}(\text{CN})_2\text{I} \cdot 2\text{H}_2\text{O}$	*J cr	NA	648.4	NA	82WE 2-321
321	398	$\text{NaHg}(\text{CN})_2\text{I} \cdot 2\text{H}_2\text{O}$	!C cr	NA	154.5	NA	82WE 2-321
321	408	$\text{NaHg}(\text{CN})_2\text{I} \cdot 2\text{H}_2\text{O}$	*C cr	NA	154.5	NA	81WE 47
Summary data selected for reason 1							
321	418 S-2	$\text{NaHg}(\text{CN})_2\text{I} \cdot 2\text{H}_2\text{O}$	!C cr	NA	154.5	NA	82WE 2-321
321	428	$\text{Na}_2\text{Hg}(\text{CN})_2\text{I}_2$	in 558 H ₂ O *J	NA	-328.4	NA	82WE 2-321
321	438	$\text{Na}_2\text{Hg}(\text{CN})_2\text{I}_2$	in 558 H ₂ O !C	NA	-78.49	NA	82WE 2-321
321	448	$\text{Na}_2\text{Hg}(\text{CN})_2\text{I}_2$	in 558 H ₂ O *C	NA	-78.5	NA	81WE 47
Summary data selected for reason 2							
321	458 A-2	$\text{Na}_2\text{Hg}(\text{CN})_2\text{I}_2$	in 558 H ₂ O *C	NA	-78.49	NA	82WE 2-321
321	468	$\text{NaCu}(\text{CN})_2$	*J ai	-4.2	NA	NA	82WE 2-321
321	478	$\text{NaCu}(\text{CN})_2$	!C ai	-1.8	NA	NA	82WE 2-321
321	488	$\text{NaCu}(\text{CN})_2$	*C ai	-1.8	NA	NA	81WE 47
Summary data selected for reason 1							
321	498 A-1	$\text{NaCu}(\text{CN})_2$	!C ai	-1.8	NA	NA	82WE 2-321
321	508	$\text{Na}_2\text{Cu}(\text{CN})_3$	*J ai	-128.6	NA	NA	82WE 2-321
321	518	$\text{Na}_2\text{Cu}(\text{CN})_3$	!C ai	-28.68	NA	NA	82WE 2-321
321	528	$\text{Na}_2\text{Cu}(\text{CN})_3$	*C ai	-28.7	NA	NA	81WE 47
Summary data selected for reason 2							
321	538 A-1	$\text{Na}_2\text{Cu}(\text{CN})_3$	*C ai	-28.68	NA	NA	82WE 2-321
321	548	$\text{Na}_3\text{Cu}(\text{CN})_4$	*J ai	-219.2	NA	NA	82WE 2-321
321	558	$\text{Na}_3\text{Cu}(\text{CN})_4$	!C ai	-52.39	NA	NA	82WE 2-321
321	568	$\text{Na}_3\text{Cu}(\text{CN})_4$	*C ai	-52.4	NA	NA	81WE 47
Summary data selected for reason 2							
321	578 A-1	$\text{Na}_3\text{Cu}(\text{CN})_4$	*C ai	-52.39	NA	NA	82WE 2-321

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
321	500		NaAg(CN) ₂	*J ai	43.6	36.12	251.	82WE 2-821
321	500		NaAg(CN) ₂	!C ai	10.4	7.199	60.0	82WE 2-321
321	600		NaAg(CN) ₂	*C ai	10.4	7.20	60.	81WE 47
321	610		NaAg(CN) ₂	*C ai	10.4	7.2	60.	76WE 37
Summary data selected for reason 2								
321	620	A-1	NaAg(CN) ₂	*C ai	10.4	7.19	60.	82WE 2-321
321	630		Na ₂ Ag(CN) ₃	*J ai	NA	-63.3	NA	82WE 2-321
321	640		Na ₂ Ag(CN) ₃	!C ai	NA	-15.13	NA	82WE 2-321
321	650		Na ₂ Ag(CN) ₃	*C ai	NA	-15.13	NA	81WE 47
Summary data selected for reason 1								
321	660	A-2	Na ₂ Ag(CN) ₃	!C ai	NA	-15.13	NA	82WE 2-321
322	10		NaAu(CN) ₂	*J ai	23.9	2.1	230.	82WE 2-322
322	20		NaAu(CN) ₂	!C ai	5.71	0.50	55.0	82WE 2-322
322	30		NaAu(CN) ₂	*C ai	5.7	0.5	55.	81WE 47
322	40		NaAu(CN) ₂	*C ai	5.7	0.5	55.	76WE 30
Summary data selected for reason 2								
322	50	A-1	NaAu(CN) ₂	*C ai	5.7	0.5	55.0	82WE 2-322
322	60		Na ₂ Ni(CN) ₄	*J ai	-51.8	-112.5	335.	82WE 2-322
322	70		Na ₂ Ni(CN) ₄	!C ai	-12.4	-26.89	80.1	82WE 2-322
322	80		Na ₂ Ni(CN) ₄	*C ai	-12.4	-26.9	80.	81WE 47
Summary data selected for reason 2								
322	90	A-1	Na ₂ Ni(CN) ₄	*C ai	-12.4	-26.89	80.1	82WE 2-322
322	100		Na ₃ Co(CN) ₆	*J ai	NA	NA	409.0	82WE 2-322
322	110		Na ₃ Co(CN) ₆	!C ai	NA	NA	97.90	82WE 2-322
322	120		Na ₃ Co(CN) ₆	*C ai	NA	NA	97.9	81WE 47
322	130		Na ₃ Co(CN) ₆	*C ai	NA	NA	97.9	76WE 30
Summary data selected for reason 2								
322	140	A-2	Na ₃ Co(CN) ₆	*C ai	NA	NA	97.9	82WE 2-322
322	150		Na ₃ Fe(CN) ₆	*J ai	-56.4	-158.6	447.3	82WE 2-322
322	160		Na ₃ Fe(CN) ₆	!C ai	-13.5	-37.91	100.9	82WE 2-322
322	170		Na ₃ Fe(CN) ₆	*C a	-13.5	-37.9	100.9	81WE 48
322	180		Na ₃ Fe(CN) ₆	*C a	-13.5	-37.9	100.9	76WE 30
Summary data selected for reason 2								
322	190	A-1	Na ₃ Fe(CN) ₆	*C ai	-13.5	-37.91	100.9	82WE 2-322

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
322 200		$\text{Na}_3\text{Fe}(\text{CN})_6$ in 100,000 H_2O	*J	NA	-157.90	NA	82WE 2-322
322 210		$\text{Na}_3\text{Fe}(\text{CN})_6$ in 100,000 H_2O	!C	NA	-37.730	NA	82WE 2-322
322 220		$\text{Na}_3\text{Fe}(\text{CN})_6$ in 100,000 H_2O	*C	NA	-37.74	NA	81WE 48
322 230		$\text{Na}_3\text{Fe}(\text{CN})_6$ in 100,000 H_2O	*C	NA	-37.74	NA	78WE 38
Summary data selected for reason 2							
322 240	A-2	$\text{Na}_3\text{Fe}(\text{CN})_6$ in 100,000 H_2O	*C	NA	-37.74	NA	82WE 2-322
322 241		$\text{NaFe}(\text{CN})_6^{3-}$	*C ao	100.29	52.37	60.48	86CR
Summary data selected for reason 4							
322 242	A-8	$\text{NaFe}(\text{CN})_6^{3-}$	*C ao	100.29	52.37	60.48	86CR
5001431	322 243	A-8 $\text{Na}^+ + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{NaFe}(\text{CN})_6^{3-}$					
322 244	A-8	5001431 $\text{NaFe}(\text{CN})_6^{3-}$					
322 245		3 1.000 500 1.000 200 6.000 143					
322 246		$\text{Na}_2\text{Fe}(\text{CN})_6^{2-}$	*C ao	36.67	-5.16	67.56	86CR
Summary data selected for reason 4							
322 247	A-8	$\text{Na}_2\text{Fe}(\text{CN})_6^{2-}$	*C ao	36.67	-5.16	67.56	86CR
5001432	322 248	A-8 $2\text{Na}^+ + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{Na}_2\text{Fe}(\text{CN})_6^{2-}$					
322 249	A-8	5001432 $\text{Na}_2\text{Fe}(\text{CN})_6^{2-}$					
322 250		3 2.000 500 1.000 200 6.000 143					
322 251		$\text{NaHFe}(\text{CN})_6^{2-}$	*C ao	95.59	51.87	63.89	86CR
Summary data selected for reason 4							
322 252	A-8	$\text{NaHFe}(\text{CN})_6^{2-}$	*C ao	95.59	51.87	63.89	86CR
5001433	322 253	A-8 $\text{Na}^+ + \text{H}^+ + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{NaHFe}(\text{CN})_6^{2-}$					
322 254	A-8	5001433 $\text{NaHFe}(\text{CN})_6^{2-}$					
322 255		4 1.000 500 1.000 330 1.000 200 6.000 143					
322 256		$\text{Na}_3\text{Fe}(\text{CN})_6$	*J ai	-352.63	-505.0	331.	82WE 2-322
322 260		$\text{Na}_3\text{Fe}(\text{CN})_6$	!C ai	-84.257	-120.7	79.1	82WE 2-322

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta H_f^{\circ}, 298$ (Q/mol)	$\Delta H_f^{\circ}, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
322	270		$\text{Na}_3\text{Fe}(\text{CN})_6$	*C a	-84.28	-128.7	79.1	81WE 48
322	280		$\text{Na}_3\text{Fe}(\text{CN})_6$	*C a	-84.28	-128.7	79.1	76WE 38
Summary data selected for reason 2								
322	290	A-1	$\text{Na}_3\text{Fe}(\text{CN})_6$	*C ai	-84.28	-128.7	79.1	82WE 2-322
322	300		$\text{Na}_3\text{FeCo}(\text{CN})_6$	*J cr	NA	-581.7	NA	82WE 2-322
322	310		$\text{Na}_3\text{FeCo}(\text{CN})_6$	!C cr	NA	-119.9	NA	82WE 2-322
322	320		$\text{Na}_3\text{FeCo}(\text{CN})_6$	*C cr	NA	-119.9	NA	81WE 48
322	330		$\text{Na}_3\text{FeCo}(\text{CN})_6$	*C cr	NA	-119.9	NA	76WE 38
Summary data selected for reason 1								
322	340	S-2	$\text{Na}_3\text{FeCo}(\text{CN})_6$	!C cr	NA	-119.9	NA	82WE 2-322
322	350		$\text{Na}_3\text{FeCo}(\text{CN})_6$	*J aq	NA	-525.9	NA	82WE 2-322
322	360		$\text{Na}_3\text{FeCo}(\text{CN})_6$	!C aq	NA	-125.7	NA	82WE 2-322
322	370		$\text{Na}_3\text{FeCo}(\text{CN})_6$	*C au	NA	-125.7	NA	81WE 48
322	380		$\text{Na}_3\text{FeCo}(\text{CN})_6$	*C au	NA	-125.7	NA	76WE 38
Summary data selected for reason 1								
322	390	A-2	$\text{Na}_3\text{FeCo}(\text{CN})_6$	!C aq	NA	-125.7	NA	82WE 2-322
322	400		$\text{NaFeCo}(\text{CN})_5 \cdot 7\text{H}_2\text{O}$	*J cr	NA	-2557.3	NA	82WE 2-322
322	410		$\text{NaFeCo}(\text{CN})_5 \cdot 7\text{H}_2\text{O}$	!C cr	NA	-811.21	NA	82WE 2-322
322	420		$\text{NaFeCo}(\text{CN})_5 \cdot 7\text{H}_2\text{O}$	*C cr	NA	-811.2	NA	81WE 48
322	430		$\text{NaFeCo}(\text{CN})_5 \cdot 7\text{H}_2\text{O}$	*C cr	NA	-811.2	NA	76WE 38
Summary data selected for reason 2								
322	440	S-2	$\text{NaFeCo}(\text{CN})_5 \cdot 7\text{H}_2\text{O}$	*C cr	NA	-811.21	NA	82WE 2-322
322	450		$\text{NaH}_3\text{Fe}(\text{CN})_6$ from $\text{H}_3\text{Fe}(\text{CN})_6^-$	*J ai	NA	215.5	NA	82WE 2-322
322	460		$\text{NaH}_3\text{Fe}(\text{CN})_6$ from $\text{H}_3\text{Fe}(\text{CN})_6^-$	!C ai	NA	51.51	NA	82WE 2-322
322	470		$\text{NaH}_3\text{Fe}(\text{CN})_6$ from $\text{H}_3\text{Fe}(\text{CN})_6^-$	*C ai	NA	51.5	NA	81WE 48
322	480		$\text{NaH}_3\text{Fe}(\text{CN})_6$ from $\text{H}_3\text{Fe}(\text{CN})_6^-$	*C ai	NA	51.5	NA	76WE 38
Summary data selected for reason 2								
322	490	A-2	$\text{NaH}_3\text{Fe}(\text{CN})_6$ from $\text{H}_3\text{Fe}(\text{CN})_6^-$	*C ai	NA	51.51	NA	82WE 2-322
322	500		$\text{Na}_2\text{H}_2\text{Fe}(\text{CN})_6$ from $\text{H}_2\text{Fe}(\text{CN})_6^{2-}$	*J ai	134.77	-24.7	335.	82WE 2-322
322	510		$\text{Na}_2\text{H}_2\text{Fe}(\text{CN})_6$ from $\text{H}_2\text{Fe}(\text{CN})_6^{2-}$	!C ai	32.211	-5.98	88.1	82WE 2-322

TABLE B.2. (contd)

WINTER Number	In 82WE Page ID Form	Compound	Units Q State	$\Delta H_f^0, 298$ (Q/mol)	$\Delta H_f^0, 298$ (Q/mol)	S_{298}^0 (Q/mol-K)	Data Sources
322	528	$\text{Na}_2\text{H}_2\text{Fe}(\text{CN})_6$ from $\text{H}_2\text{Fe}(\text{CN})_6^{2-}$	*C ai	32.18	-5.9	88.	81WE 48
322	538	$\text{Na}_2\text{H}_2\text{Fe}(\text{CN})_6$ from $\text{H}_2\text{Fe}(\text{CN})_6^{2-}$	*C ai	32.18	-5.9	88.	76WE 38
Summary data selected for reason 2							
322	548 A-1	$\text{Na}_2\text{H}_2\text{Fe}(\text{CN})_6$ from $\text{H}_2\text{Fe}(\text{CN})_6^{2-}$	*C ai	32.21	-5.9	88.1	82WE 2-322
322	558	$\text{Na}_3\text{HFe}(\text{CN})_6$ from $\text{H}_2\text{Fe}(\text{CN})_6^{3-}$	*J ai	-114.44	-284.8	351.	82WE 2-322
322	568	$\text{Na}_3\text{HFe}(\text{CN})_6$ from $\text{H}_2\text{Fe}(\text{CN})_6^{3-}$	!C ai	-27.362	-83.29	83.9	82WE 2-322
322	578	$\text{Na}_3\text{HFe}(\text{CN})_6$ from $\text{H}_2\text{Fe}(\text{CN})_6^{3-}$	*C ai	-27.38	-83.3	84.	81WE 48
322	588	$\text{Na}_3\text{HFe}(\text{CN})_6$ from $\text{H}_2\text{Fe}(\text{CN})_6^{3-}$	*C ai	-27.38	-83.3	84.	76WE 38322
Summary data selected for reason 2							
322	598 A-1	$\text{Na}_3\text{HFe}(\text{CN})_6$ from $\text{H}_2\text{Fe}(\text{CN})_6^{3-}$	*C ai	-27.36	-83.29	84.39	82WE 2-322
322	608	$\text{NaH}_2\text{FeCo}(\text{CN})_5$ from $\text{H}_2\text{FeCo}(\text{CN})_5^-$	*J ai	NA	-46.4	NA	82WE 2-322
322	618	$\text{NaH}_2\text{FeCo}(\text{CN})_5$ from $\text{H}_2\text{FeCo}(\text{CN})_5^-$	!C ai	NA	-11.1	NA	82WE 2-322
322	828	$\text{NaH}_2\text{FeCo}(\text{CN})_5$ from $\text{H}_2\text{FeCo}(\text{CN})_5^-$	*C ai	NA	-11.1	NA	81WE 48
322	838	$\text{NaH}_2\text{FeCo}(\text{CN})_5$ from $\text{H}_2\text{FeCo}(\text{CN})_5^-$	*C ai	NA	-11.1	NA	76WE 38
Summary data selected for reason 1							
322	648 A-2	$\text{NaH}_2\text{FeCo}(\text{CN})_5$ from $\text{H}_2\text{FeCo}(\text{CN})_5^-$	!C ai	NA	-11.1	NA	82WE 2-322
322	658	$\text{Na}_2\text{HFeCo}(\text{CN})_5$ from $\text{HFeCo}(\text{CN})_5^{2-}$	*J ai	NA	-287.9	NA	82WE 2-322
322	668	$\text{Na}_2\text{HFeCo}(\text{CN})_5$ from $\text{HFeCo}(\text{CN})_5^{2-}$	!C ai	NA	-88.81	NA	82WE 2-322
322	678	$\text{Na}_2\text{HFeCo}(\text{CN})_5$ from $\text{HFeCo}(\text{CN})_5^{2-}$	*C ai	NA	-88.8	NA	81WE 48
322	688	$\text{Na}_2\text{HFeCo}(\text{CN})_5$ from $\text{HFeCo}(\text{CN})_5^{2-}$	*C ai	NA	-88.8	NA	76WE 38
Summary data selected for reason 2							
322	698 A-2	$\text{Na}_2\text{HFeCo}(\text{CN})_5$ from $\text{HFeCo}(\text{CN})_5^{2-}$	*C ai	NA	-88.81	NA	82WE 2-322
322	708	$\text{Na}_2\text{Pd}(\text{CN})_4$	*J ai	184.7	NA	NA	82WE 2-322
322	718	$\text{Na}_2\text{Pd}(\text{CN})_4$	!C ai	25.82	NA	NA	82WE 2-322
322	728	$\text{Na}_2\text{Pd}(\text{CN})_4$	*C ai	25.8	NA	NA	81WE 48
322	738	$\text{Na}_2\text{Pd}(\text{CN})_4$	*C ai	25.8	NA	NA	76WE 39

TABLE B.2. (contd)

MINTeq	In 82WE				Units	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°	
Number	Page	ID	Form	Compound	Q State	(Q/mol)	(Q/mol)	(Q/mol·K)	Data Sources
Summary data selected for reason 2									
322	748	A-1		$\text{Na}_2\text{Pd}(\text{CN})_4$	*C ai	25.82	NA	NA	82WE 2-322
323	18			$\text{Na}_2\text{Pt}(\text{CN})_4$	*J ai	182.9	NA	NA	82WE 2-323
323	28			$\text{Na}_2\text{Pt}(\text{CN})_4$	!C ai	43.71	NA	NA	82WE 2-323
323	38			$\text{Na}_2\text{Pt}(\text{CN})_4$	*C ai	43.7	NA	NA	81WE 49
323	48			$\text{Na}_2\text{Pt}(\text{CN})_4$	*C ai	43.7	NA	NA	76WE 39
Summary data selected for reason 2									
328	58	A-1		$\text{Na}_2\text{Pt}(\text{CN})_4$	*C ai	43.71	NA	NA	82WE 2-323
323	68			$\text{Na}_4\text{Mn}(\text{CN})_6$	*J ai	NA	-486.	NA	82WE 2-323
323	78			$\text{Na}_4\text{Mn}(\text{CN})_6$	!C ai	NA	-97.8	NA	82WE 2-323
323	88			$\text{Na}_4\text{Mn}(\text{CN})_6$	!C ai	NA	-97.	NA	76WE 39
Summary data selected for reason 2									
323	98	A-2		$\text{Na}_4\text{Mn}(\text{CN})_6$	!C ai	NA	-97.8	NA	82WE 2-323
326	18			$\text{NaMgFe}(\text{CN})_6$	*J ai	-3.2	NA	NA	82WE 2-326
326	28			$\text{NaMgFe}(\text{CN})_6$	!C ai	-8.77	NA	NA	82WE 2-326
326	38			$\text{NaMgFe}(\text{CN})_6$	*C ai	-8.8	NA	NA	81WE 52
Summary data selected for reason 2									
326	48	A-1		$\text{NaMgFe}(\text{CN})_6$	*C ai	-8.71	NA	NA	82WE 2-326
326	58			$\text{Na}_2\text{MgFe}(\text{CN})_6$	*J ai	-385.3	NA	NA	82WE 2-326
326	68			$\text{Na}_2\text{MgFe}(\text{CN})_6$	!C ai	-72.97	NA	NA	82WE 2-326
326	78			$\text{Na}_2\text{MgFe}(\text{CN})_6$	*C ai	-73.8	NA	NA	81WE 52
Summary data selected for reason 2									
326	88	A-1		$\text{Na}_2\text{MgFe}(\text{CN})_6$	*C ai	-72.97	NA	NA	82WE 2-326
326	98			$\text{NaCaFe}(\text{CN})_6$	*J ai	-182.4	NA	NA	82WE 2-326
326	108			$\text{NaCaFe}(\text{CN})_6$	!C ai	-24.47	NA	NA	82WE 2-326
326	118			$\text{NaCaFe}(\text{CN})_6$	*C ai	-24.6	NA	NA	81WE 52
Summary data selected for reason 2									
326	128	A-1		$\text{NaCaFe}(\text{CN})_6$	*C ai	-24.47	NA	NA	82WE 2-326
326	138			$\text{Na}_2\text{CaFe}(\text{CN})_6$	*J ai	-484.1	NA	NA	82WE 2-326
326	148			$\text{Na}_2\text{CaFe}(\text{CN})_6$	!C ai	-96.58	NA	NA	82WE 2-326
326	158			$\text{Na}_2\text{CaFe}(\text{CN})_6$	*C ai	-96.6	NA	NA	81WE 52
Summary data selected for reason 2									
326	168	A-1		$\text{Na}_2\text{CaFe}(\text{CN})_6$	*C ai	-96.58	NA	NA	82WE 2-326

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
326	178	NaSrFe(CN) ₆	*J ai	-188.8	NA	NA	82WE 2-326
326	188	NaSrFe(CN) ₆	!C ai	-25.88	NA	NA	82WE 2-326
326	198	NaSrFe(CN) ₆	*C ai	-25.9	NA	NA	81WE 52
Summary data selected for reason 2							
326	208	A-1 NaSrFe(CN) ₆	*C ai	-25.88	NA	NA	82WE 2-326
342	18	KCN	*J cr	-181.88	-119.8	128.49	82WE 2-342
342	28	KCN	!C cr	-24.345	-27.81	38.718	82WE 2-342
342	38	KCN	*C cr	-24.35	-27.8	38.71	81WE 89
342	48	KCN I, cubic	*C cr	NA	-27.18	NA	78WE 53
Summary data selected for reason 2							
342	58	S-8 KCN	*C cr	-24.345	-27.81	38.71	82WE 2-342
1141882	342	51 S-8 $\text{CN}^- + \text{K}^+ \leftrightarrow \text{KCN}$					
	342	52 S-8 1141882 KCN					
	342	53	2	1.888 143	1.888 418		
342	68	KCN	*J ai	-118.9	-181.7	198.8	82WE 2-342
342	78	KCN	!C ai	-26.51	-24.31	46.99	82WE 2-342
342	88	KCN	*C ai	-26.5	-24.3	47.8	81WE 89
342	98	KCN	*C ai	-26.5	-24.3	47.8	78WE 53
Summary data selected for reason 2							
342	108	A-1 KCN	*C ai	-26.51	-24.31	46.99	82WE 2-342
342	118	KCN in 288 H ₂ O	*J	NA	-181.8	NA	82WE 2-342
342	128	KCN in 288 H ₂ O	!C	NA	-24.21	NA	82WE 2-342
342	138	KCN in 288 H ₂ O	*C	NA	-24.2	NA	81WE 89
342	148	KCN in 288 H ₂ O	*C	NA	-24.8	NA	78WE 53
Summary data selected for reason 2							
342	158	A-2 KCN in 288 H ₂ O	*C	NA	-24.21	NA	82WE 2-342
342	168	KCNO	*J cr	NA	-418.85	NA	82WE 2-342
342	178	KCNO	!C cr	NA	-188.86	NA	82WE 2-342
342	188	KCNO	*C cr	NA	-188.86	NA	81WE 89
342	198	KCNO	*C cr	NA	-188.84	NA	78WE 53

TABLE B.2. (contd)

WINTER	In 82WE				Units	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°	
Number	Page ID	Form	Compound		Q State	(Q/mol)	(Q/mol)	(Q/mol·K)	Data Sources
Summary data selected for reason 2									
342	200	S-2	KCNO	cyanogen	*C cr	NA	-105.84	NA	82WE 2-342
342	210		KCNO		*J ai	-388.7	-388.3	299.2	82WE 2-342
342	220		KCNO		!C ai	-95.99	-95.28	58.88	82WE 2-342
342	230		KCNO		*C a	-91.8	-95.2	58.8	81WE 69
342	240		KCNO		*C a	-91.8	-95.2	58.8	78WE 53
Summary data selected for reason 2									
342	250	A-1	KCNO	cyanogen	*C ai	-91.8	-95.2	58.8	82WE 2-342
345	10		K ₂ Zn(CN) ₄		*J cr	NA	-105.8	NA	82WE 2-345
345	20		K ₂ Zn(CN) ₄		!C cr	NA	-23.98	NA	82WE 2-345
345	30		K ₂ Zn(CN) ₄		*C cr	NA	-23.9	NA	81WE 72
Summary data selected for reason 2									
345	40	S-2	K ₂ Zn(CN) ₄		*C cr	NA	-23.9	NA	82WE 2-345
345	50		K ₂ Zn(CN) ₄		*J ai	-119.8	-102.3	431.	82WE 2-345
345	60		K ₂ Zn(CN) ₄		!C ai	-28.58	-38.79	183.	82WE 2-345
345	70		K ₂ Zn(CN) ₄		*C ai	-28.6	-38.8	183.	81WE 72
Summary data selected for reason 2									
345	80	A-1	K ₂ Zn(CN) ₄		*C ai	-28.58	-38.79	183.	82WE 2-345
345	90		K ₂ Zn(CN) ₄	in 400 H ₂ O	*J	NA	-102.3	NA	82WE 2-345
345	100		K ₂ Zn(CN) ₄	in 400 H ₂ O	!C	NA	-38.79	NA	82WE 2-345
345	110		K ₂ Zn(CN) ₄	in 400 H ₂ O	*C	NA	-38.8	NA	81WE 72
Summary data selected for reason 2									
345	120	A-2	K ₂ Zn(CN) ₄	in 400 H ₂ O	*C	NA	-38.79	NA	82WE 2-345
346	10		KHg(CN) ₃		*J ai	188.8	144.8	327.6	82WE 2-346
346	20		KHg(CN) ₃		!C ai	43.82	34.61	78.38	82WE 2-346
346	30		KHg(CN) ₃		*C ai	43.8	34.6	78.3	81WE 73
Summary data selected for reason 2									
346	40	A-1	KHg(CN) ₃		*C ai	43.82	34.61	78.38	82WE 2-346
346	50		KHg(CN) ₃	in 500 H ₂ O	*J	NA	144.8	NA	82WE 2-346
346	60		KHg(CN) ₃	in 500 H ₂ O	!C	NA	34.89	NA	82WE 2-346
346	70		KHg(CN) ₃	in 500 H ₂ O	*C	NA	34.9	NA	81WE 73
Summary data selected for reason 2									
346	80	A-2	KHg(CN) ₃	in 500 H ₂ O	*C	NA	34.89	NA	82WE 2-346

TABLE B.2. (contd)

WINTERQ Number	In 82WE Page ID Form	Compound	Units Q State	$\Delta H_f^0, 298$ (Q/mol)	$\Delta H_f^0, 298$ (Q/mol)	S_{298}^0 (Q/mol·K)	Data Sources
348 98		$K_2Hg(CN)_4$	*J cr	NA	-32.2	NA	82WE 2-348
348 100		$K_2Hg(CN)_4$	!C cr	NA	-7.7#	NA	82WE 2-348
348 110		$K_2Hg(CN)_4$	*C cr	NA	-7.7	NA	81WE 73
Summary data selected for reason 2							
348 120	S-2	$K_2Hg(CN)_4$	*C cr	NA	-7.7#	NA	82WE 2-348
348 130		$K_2Hg(CN)_4$	*J ai	51.9	21.8	51#.	82WE 2-348
348 140		$K_2Hg(CN)_4$	!C ai	12.4	5.21	122.	82WE 2-348
348 150		$K_2Hg(CN)_4$	*C ai	12.4	5.2	122.	81WE 73
Summary data selected for reason 2							
348 160	A-1	$K_2Hg(CN)_4$	*C ai	12.4	5.21	122.	82WE 2-348
348 170		$K_2Hg(CN)_4$ in 800 H ₂ O	*J	NA	27.2	NA	82WE 2-348
348 180		$K_2Hg(CN)_4$ in 800 H ₂ O	!C	NA	6.5#	NA	82WE 2-348
348 190		$K_2Hg(CN)_4$ in 800 H ₂ O	*C	NA	6.5	NA	81WE 73
Summary data selected for reason 2							
348 200	A-2	$K_2Hg(CN)_4$ in 800 H ₂ O	*C	NA	6.5#	NA	82WE 2-348
348 210		$KCl \cdot Hg(CN)_2$	*J cr	NA	-179.9	NA	82WE 2-348
348 220		$KCl \cdot Hg(CN)_2$	!C cr	NA	-43.0#	NA	82WE 2-348
348 230		$KCl \cdot Hg(CN)_2$	*C cr	NA	-43.0	NA	81WE 73
Summary data selected for reason 2							
348 240	S-2	$KCl \cdot Hg(CN)_2$	*C cr	NA	-43.0#	NA	82WE 2-348
348 250		$KCl \cdot Hg(CN)_2 \cdot H_2O$	*J cr	NA	-473.6	NA	82WE 2-348
348 260		$KCl \cdot Hg(CN)_2 \cdot H_2O$	!C cr	NA	-113.2	NA	82WE 2-348
348 270		$KCl \cdot Hg(CN)_2 \cdot H_2O$	*C cr	NA	-113.2	NA	81WE 73
Summary data selected for reason 1							
348 280	S-2	$KCl \cdot Hg(CN)_2 \cdot H_2O$	!C cr	NA	-113.2	NA	82WE 2-348
348 290		$KBr \cdot Hg(CN)_2$	*J cr	NA	-146.5	NA	82WE 2-348
348 300		$KBr \cdot Hg(CN)_2$	!C cr	NA	-35.49	NA	82WE 2-348
348 310		$KBr \cdot Hg(CN)_2$	*C cr	NA	-35.5	NA	81WE 73
Summary data selected for reason 2							
348 320	S-2	$KBr \cdot Hg(CN)_2$	*C cr	NA	-35.49	NA	82WE 2-348
348 330		$KBr \cdot Hg(CN)_2 \cdot 1.5H_2O$	*J cr	NA	-581.6	NA	82WE 2-348
348 340		$KBr \cdot Hg(CN)_2 \cdot 1.5H_2O$	!C cr	NA	-139.0	NA	82WE 2-348
348 350		$KBr \cdot Hg(CN)_2 \cdot 1.5H_2O$	*C cr	NA	-139.0	NA	81WE 73

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
Summary data selected for reason 1								
346	366	S-2	KBr·Hg(CN) ₂ ·1.5H ₂ O	!C cr	NA	-139.8	NA	82WE 2-346
346	378		KI·Hg(CN) ₂	*J cr	NA	-91.6	NA	82WE 2-346
346	366		KI·Hg(CN) ₂	!C cr	NA	-21.9	NA	82WE 2-346
346	398		KI·Hg(CN) ₂	*C cr	NA	-21.9	NA	81WE 73
Summary data selected for reason 1								
346	408	S-2	KI·Hg(CN) ₂	!C cr	NA	-21.9	NA	82WE 2-346
346	418		KI·Hg(CN) ₂ ·0.25H ₂ O	*J cr	NA	-184.4	NA	82WE 2-346
346	428		KI·Hg(CN) ₂ ·0.25H ₂ O	!C cr	NA	-39.29	NA	82WE 2-346
346	438		KI·Hg(CN) ₂ ·0.25H ₂ O	*C cr	NA	-39.3	NA	81WE 73
Summary data selected for reason 2								
346	448	S-2	KI·Hg(CN) ₂ ·0.25H ₂ O	*C cr	NA	-39.29	NA	82WE 2-346
346	458		KCu(CN) ₂	*J ai	NA	-25.5	NA	82WE 2-346
346	468		KCu(CN) ₂	!C ai	NA	-6.89	NA	82WE 2-346
346	478		KCu(CN) ₂	*C ai	NA	-6.1	NA	81WE 73
Summary data selected for reason 2								
346	488	A-2	KCu(CN) ₂	*C ai	NA	-6.89	NA	82WE 2-346
346	498		K ₂ Cu(CN) ₃	*J ai	-162.7	NA	NA	82WE 2-346
346	508		K ₂ Cu(CN) ₃	!C ai	-38.89	NA	NA	82WE 2-346
346	518		K ₂ Cu(CN) ₃	*C ai	-38.9	NA	NA	81WE 73
Summary data selected for reason 2								
346	528	A-1	K ₂ Cu(CN) ₃	*C ai	-38.89	NA	NA	82WE 2-346
346	538		K ₃ Cu(CN) ₄	*J ai	-283.2	NA	NA	82WE 2-346
346	548		K ₃ Cu(CN) ₄	!C ai	-67.69	NA	NA	82WE 2-346
346	558		K ₃ Cu(CN) ₄	*C ai	-67.7	NA	NA	81WE 73
Summary data selected for reason 2								
346	568	A-1	K ₃ Cu(CN) ₄	*C ai	-67.69	NA	NA	82WE 2-346
347	18		KAg(CN) ₂	*J cr	NA	-18.7	NA	82WE 2-347
347	28		KAg(CN) ₂	!C cr	NA	-8.99	NA	82WE 2-347
347	38		KAg(CN) ₂	*C cr	NA	-4.6	NA	81WE 74

TABLE B.2. (contd)

MINTER Number	In 82WE Page ID Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
Summary data selected for reason 2							
347	48 S-2	KAg(CN) ₂	*C cr	NA	-3.99	NA	82WE 2-347
347	58	KAg(CN) ₂	*J ai	22.2	18.8	297.	82WE 2-347
347	68	KAg(CN) ₂	!C ai	5.31	4.38	71.8	82WE 2-347
347	78	KAg(CN) ₂	*C ai	5.3	4.3	71.	81WE 74
Summary data selected for reason 2							
347	88 A-1	KAg(CN) ₂	*C ai	5.3	4.38	71.	82WE 2-347
347	98	K ₂ Ni(CN) ₄	*J ai	-94.5	-136.8	423.	82WE 2-347
347	108	K ₂ Ni(CN) ₄	!C ai	-22.6	-32.7	181.	82WE 2-347
347	118	K ₂ Ni(CN) ₄	*C a	-22.6	-32.7	181.	81WE 74
Summary data selected for reason 1							
347	128 A-1	K ₂ Ni(CN) ₄	!C ai	-22.6	-32.7	181.	82WE 2-347
347	138	K ₂ Ni(CN) ₄	*J aq	NA	-128.4	NA	82WE 2-347
347	148	K ₂ Ni(CN) ₄	!C aq	NA	-38.69	NA	82WE 2-347
347	158	K ₂ Ni(CN) ₄	*C au	NA	-38.7	NA	81WE 74
Summary data selected for reason 2							
347	168 A-2	K ₂ Ni(CN) ₄	*C au	NA	-38.69	NA	82WE 2-347
347	178	K ₃ Co(CN) ₈	*J cr	NA	NA	481.86	82WE 2-347
347	188	K ₃ Co(CN) ₈	!C cr	NA	NA	95.999	82WE 2-347
347	198	K ₃ Co(CN) ₈	*C cr	NA	NA	95.88	81WE 74
Summary data selected for reason 2							
347	208 S-2	K ₃ Co(CN) ₈	*C cr	NA	NA	95.999	82WE 2-347
347	218	K ₃ Co(CN) ₈	*J ai	NA	NA	548.2	82WE 2-347
347	228	K ₃ Co(CN) ₈	!C ai	NA	NA	129.1	82WE 2-347
347	238	K ₃ Co(CN) ₈	*C ai	NA	NA	129.1	81WE 74
Summary data selected for reason 1							
347	248 A-2	K ₃ Co(CN) ₈	!C ai	NA	NA	129.1	82WE 2-347
347	258	KFe(CN) ₆ ²⁻	*C ao	-89.4	NA	NA	78WE 58
Summary data selected for reason 4							
347	268	KFe(CN) ₆ ²⁻	*C ao	-89.4	NA	NA	78WE 58
347	288	K ₃ Fe(CN) ₈	*J cr	-129.6	-249.8	426.86	82WE 2-347
347	281	K ₃ Fe(CN) ₈	!C cr	-38.98	-59.76	181.83	82WE 2-347

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
	347 200		K ₃ Fe(CN) ₆	*C cr	-81.0	-59.7	101.83	81WE 74
	347 300		K ₃ Fe(CN) ₆	*C cr	-30.97	-59.7	101.8	76WE 58
Summary data selected for reason 2								
	347 310		K ₃ Fe(CN) ₆	*C cr	-30.00	-59.7	101.82	82WE 2-347
1141011	347 321	S-0	$6\text{CN}^- + 3\text{K}^+ + \text{Fe}^{3+} \leftrightarrow \text{K}_3\text{Fe}(\text{CN})_6$					
	347 322	S-0	1141011 K ₃ Fe(CN) ₆					
	347 323		3 6.000 143 3.000 410 1.000 201					
	347 330		K ₃ Fe(CN) ₆ from Fe(CN) ₆ ³⁻	*J ai	-120.4	-195.4	577.8	82WE 2-347
	347 331		K ₃ Fe(CN) ₆ from Fe(CN) ₆ ³⁻	IC ai	-28.78	-46.70	138.1	82WE 2-347
	347 340		K ₃ Fe(CN) ₆ from Fe(CN) ₆ ³⁻	*C a	-28.8	-46.7	138.1	81WE 74
	347 350		K ₃ Fe(CN) ₆ from Fe(CN) ₆ ³⁻	*C a	-28.8	-46.7	138.1	76WE 58
Summary data selected for reason 2								
	347 360	A-1	K ₃ Fe(CN) ₆ from Fe(CN) ₆ ³⁻	*C ai	-28.78	-46.7	138.1	82WE 2-347
	347 370		K ₃ Fe(CN) ₆ in 400 H ₂ O	*J	NA	-194.17	NA	82WE 2-347
	347 380		K ₃ Fe(CN) ₆ in 400 H ₂ O	IC	NA	-46.400	NA	82WE 2-347
	347 390		K ₃ Fe(CN) ₆ in 400 H ₂ O	*C	NA	-46.41	NA	81WE 74
Summary data selected for reason 2								
	347 400	A-2	K ₃ Fe(CN) ₆ in 400 H ₂ O	*C	NA	-46.00	NA	82WE 2-347
	347 410		K ₃ Fe(CN) ₆ in 200,000 H ₂ O	*J	NA	-194.97	NA	82WE 2-347
	347 420		K ₃ Fe(CN) ₆ in 200,000 H ₂ O	IC	NA	-46.500	NA	82WE 2-347
	347 430		K ₃ Fe(CN) ₆ in 200,000 H ₂ O	*C	NA	-46.00	NA	81WE 74
Summary data selected for reason 2								
	347 440	A-2	K ₃ Fe(CN) ₆ in 200,000 H ₂ O	*C	NA	-46.500	NA	82WE 2-347
	347 450		K ₃ Fe(CN) ₆ in 500,000 H ₂ O	*J	NA	-195.1	NA	82WE 2-347
	347 460		K ₃ Fe(CN) ₆ in 500,000 H ₂ O	IC	NA	-46.63	NA	82WE 2-347
	347 470		K ₃ Fe(CN) ₆ in 500,000 H ₂ O	*C	NA	-46.63	NA	81WE 74
Summary data selected for reason 1								
	347 480	A-2	K ₃ Fe(CN) ₆ in 500,000 H ₂ O	IC	NA	-46.63	NA	82WE 2-347
	347 490		K ₄ Fe(CN) ₆	*J cr	-453.0	-594.1	418.8	82WE 2-347
	347 500		K ₄ Fe(CN) ₆	IC cr	-100.3	-142.0	100.1	82WE 2-347

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
347	518	$K_4Fe(CN)_6$	*C cr	-188.3	-142.8	186.1	81WE 74
347	528	$K_4Fe(CN)_6$	*C cr	NA	-142.8	NA	78WE 58
Summary data selected for reason 1							
347	538	$K_4Fe(CN)_6$	!C cr	-188.3	-142.8	186.1	82WE 2-347
1141885	347	532 S-8 $6CN^- + 4K^+ + Fe^{2+} \leftrightarrow K_4Fe(CN)_6$					
347	533	S-8 1141885 $K_4Fe(CN)_6$					
347	534	3 8.888 143 4.888 418 1.888 288					
347	558	$K_4Fe(CN)_6$ from $Fe(CN)_6^{4-}$	*J ai	-438.81	-554.81	585.8	82WE 2-347
347	551	$K_4Fe(CN)_6$ from $Fe(CN)_6^{4-}$	!C ai	-184.89	-132.41	128.7	82WE 2-347
347	568	$K_4Fe(CN)_6$ from $Fe(CN)_6^{4-}$	*C a	-184.71	-132.4	128.7	81WE 75
347	578	$K_4Fe(CN)_6$ from $Fe(CN)_6^{4-}$	*C a	-184.71	-132.4	128.7	78WE 58
Summary data selected for reason 2							
347	588	A-1 $K_4Fe(CN)_6$ from $Fe(CN)_6^{4-}$	*C ai	-184.89	-132.41	128.7	82WE 2-347
348	18	$K_4Fe(CN)_6$ in 58,888 H ₂ O	*J	NA	-552.25	NA	82WE 2-348
348	28	$K_4Fe(CN)_6$ in 58,888 H ₂ O	!C	NA	-131.99	NA	82WE 2-348
348	38	$K_4Fe(CN)_6$ in 58,888 H ₂ O	*C	NA	-131.99	NA	81WE 75
Summary data selected for reason 1							
348	48	A-2 $K_4Fe(CN)_6$ in 58,888 H ₂ O	!C	NA	-131.99	NA	82WE 2-348
348	58	$K_4Fe(CN)_6$ in 588,888 H ₂ O	*J	NA	-553.33	NA	82WE 2-348
348	68	$K_4Fe(CN)_6$ in 588,888 H ₂ O	!C	NA	-132.25	NA	82WE 2-348
348	78	$K_4Fe(CN)_6$ in 588,888 H ₂ O	*C	NA	-132.25	NA	81WE 75
Summary data selected for reason 1							
348	88	A-2 $K_4Fe(CN)_6$ in 588,888 H ₂ O	!C	NA	-132.25	NA	82WE 2-348
348	98	$K_4Fe(CN)_6 \cdot 3H_2O$	*J cr	-1188.8	-1488.5	593.7	82WE 2-348
348	108	$K_4Fe(CN)_6 \cdot 3H_2O$	!C cr	-279.35	-358.58	141.9	82WE 2-348
348	118	$K_4Fe(CN)_6 \cdot 3H_2O$	*C cr	-279.4	-358.5	141.9	81WE 75
348	128	$K_4Fe(CN)_6 \cdot 3H_2O$	*C cr	-281.14	-358.5	148.	78WE 58
Summary data selected for reason 2							
348	138	$K_4Fe(CN)_6 \cdot 3H_2O$	*C cr	-279.35	-358.5	149.	82WE 2-348

TABLE B.2. (contd)

MINTeq Number	In B2WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
1141000	348 132	S-#	$6\text{CN}^- + 4\text{K}^+ + \text{Fe}^{2+} + 3\text{H}_2\text{O} \leftrightarrow \text{K}_4\text{Fe}(\text{CN})_6 \cdot 3\text{H}_2\text{O}$					
	348 183	S-#	1141000 $\text{K}_4\text{Fe}(\text{CN})_6 \cdot 3\text{H}_2\text{O}$					
	348 134		4 6.000 143 4.000 410 1.000 280 3.000 2					
	348 135.1		$\text{KFe}(\text{CN})_6^{3-}$	*C ao	95.43	47.63	30.75	76SM 21
	348 135.2		$\text{KFe}(\text{CN})_6^{3-}$	*C ao	89.42	NA	NA	87B
	348 135.3		$\text{KFe}(\text{CN})_6^{3-}$	*C ao	95.19	56.43	64.29	86CR
Summary data selected for reason 4								
	348 136	A-#	$\text{KFe}(\text{CN})_6^{3-}$	*C ao	95.19	56.43	64.29	86CR
4102801	348 137	A-#	$\text{K}^+ + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{KFe}(\text{CN})_6^{3-}$					
	348 138	A-#	4101433 $\text{KFe}(\text{CN})_6^{3-}$					
	348 139		3 1.000 410 1.000 280 6.000 143					
	348 145		$\text{K}_2\text{Fe}(\text{CN})_6^{2-}$	*C ao	26.51	-3.14	114.79	86CR
Summary data selected for reason 4								
	348 146	A-#	$\text{K}_2\text{Fe}(\text{CN})_6^{2-}$	*C ao	26.51	-3.14	114.79	86CR
4101434	348 147	A-#	$2\text{K}^+ + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{K}_2\text{Fe}(\text{CN})_6^{2-}$					
	348 148	A-#	4102803 $\text{K}_2\text{Fe}(\text{CN})_6^{2-}$					
	348 149		3 2.000 410 1.000 280 6.000 143					
	348 150		$\text{KHF}(\text{CN})_6^{2-}$	*C ao	90.62	56.33	99.41	86CR
Summary data selected for reason 4								
	348 151	A-#	$\text{KHF}(\text{CN})_6^{2-}$	*C ao	90.62	56.33	99.41	86CR
4101435	348 152	A-#	$\text{K}^+ + \text{H}^+ + \text{Fe}^{2+} + 6\text{CN}^- \leftrightarrow \text{KHF}(\text{CN})_6^{2-}$					
	348 153	A-#	4102814 $\text{KHF}(\text{CN})_6^{2-}$					
	348 154		4 1.000 410 1.000 330 1.000 280 6.000 143					
	348 155		$\text{KFe}(\text{CN})_6^{2-}$	*C ao	104.64	NA	NA	76SM 22

TABLE B.2. (contd)

MINTEQ Number	In 82WE Page ID Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
Summary data selected for reason 4							
348 156		$\text{KFe}(\text{CN})_6^{2-}$	*C ao	184.84	NA	NA	76SM 22
4181438 348 157		$\text{K}^+ + \text{Fe}^{3+} + \text{CN}^- \leftrightarrow \text{KFe}(\text{CN})_6^{2-}$					
348 158		4181438 $\text{KFe}(\text{CN})_6^{2-}$					
348 159		3 1.888 418 1.888 281 8.888 143					
348 166		$\text{K}_3\text{FeCo}(\text{CN})_5$	*J cr	NA	-583.2	NA	82WE 2-348
348 161		$\text{K}_3\text{FeCo}(\text{CN})_5$	!C cr	NA	-139.4	NA	82WE 2-348
348 162		$\text{K}_3\text{FeCo}(\text{CN})_5$	*C cr	NA	-139.4	NA	81WE 75
348 178		$\text{K}_3\text{FeCo}(\text{CN})_5$	*C cr	NA	-138.9	NA	76WE 58
Summary data selected for reason 2							
348 186	S-2	$\text{K}_3\text{FeCo}(\text{CN})_5$	*C cr	NA	-139.4	NA	82WE 2-348
348 198		$\text{K}_3\text{FeCo}(\text{CN})_5$ in 2,588 H_2O	*J	NA	-584.8	NA	82WE 2-348
348 208		$\text{K}_3\text{FeCo}(\text{CN})_5$ in 2,588 H_2O	!C	NA	-134.8	NA	82WE 2-348
348 218		$\text{K}_3\text{FeCo}(\text{CN})_5$ in 2,588 H_2O	*C	NA	-134.8	NA	81WE 75
Summary data selected for reason 1							
348 228	A-2	$\text{K}_3\text{FeCo}(\text{CN})_5$ in 2,588 H_2O	!C	NA	-134.8	NA	82WE 2-348
348 238		$\text{K}_3\text{FeCo}(\text{CN})_5 \cdot 3.5\text{H}_2\text{O}$	*J cr	NA	-1688.7	NA	82WE 2-348
348 248		$\text{K}_3\text{FeCo}(\text{CN})_5 \cdot 3.5\text{H}_2\text{O}$	!C cr	NA	-384.49	NA	82WE 2-348
348 258		$\text{K}_3\text{FeCo}(\text{CN})_5 \cdot 3.5\text{H}_2\text{O}$	*C cr	NA	-384.5	NA	81WE 75
348 268		$\text{K}_3\text{FeCo}(\text{CN})_5 \cdot 3.5\text{H}_2\text{O}$	*C cr	NA	-384.8	NA	76WE 58
Summary data selected for reason 2							
348 278	S-2	$\text{K}_3\text{FeCo}(\text{CN})_5 \cdot 3.5\text{H}_2\text{O}$	*C cr	NA	-384.49	NA	82WE 2-348
348 288		$\text{KH}_2\text{Fe}(\text{CN})_5$	*C au	NA	75.8	NA	76WE 59
Summary data selected for reason 4							
348 298	A-2	$\text{KH}_2\text{Fe}(\text{CN})_5$	*C au	NA	75.8	NA	76WE 59
348 308		$\text{KH}_3\text{Fe}(\text{CN})_5$	*C a	NA	48.8	NA	76WE 59
Summary data selected for reason 4							
348 318	A-2	$\text{KH}_3\text{Fe}(\text{CN})_5$	*C a	NA	48.8	NA	76WE 59
348 328		$\text{KH}_3\text{Fe}(\text{CN})_5$	*C au	NA	58.8	NA	76WE 59

TABLE B.2. (contd)

MINTeq	In 82WE				Units	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°		
Number	Page	ID	Form	Compound	Q	State	(Q/mol)	(Q/mol)	(Q/mol·K)	Data Sources
Summary data selected for reason 4										
348	338	A-2		$\text{KH}_3\text{Fe}(\text{CN})_6$	*C	au	NA	58.8	NA	78WE 59
348	348			$\text{K}_2\text{HFe}(\text{CN})_6$	*C	au	NA	14.8	NA	78WE 59
Summary data selected for reason 4										
348	358	A-2		$\text{K}_2\text{HFe}(\text{CN})_6$	*C	au	NA	14.8	NA	78WE 59
348	368			$\text{K}_2\text{H}_2\text{Fe}(\text{CN})_6$	*C	a	21.97	-11.7	181.	78WE 59
Summary data selected for reason 4										
348	378			$\text{K}_2\text{H}_2\text{Fe}(\text{CN})_6$	*C	a	21.97	-11.7	181.	78WE 59
4181431	348	372	A-8	$6\text{CN}^- + 2\text{K}^+ + 2\text{H}^+ + \text{Fe}^{2+} \leftrightarrow \text{K}_2\text{H}_2\text{Fe}(\text{CN})_6$						
348	373	A-8	4181431	$\text{K}_2\text{H}_2\text{Fe}(\text{CN})_6$						
348	374		4	6.888 143	2.888	418	2.888 338	1.888 288		
348	398			$\text{K}_2\text{H}_2\text{Fe}(\text{CN})_6$	*C	au	NA	-18.3	NA	78WE 59
Summary data selected for reason 4										
348	391	A-2		$\text{K}_2\text{H}_2\text{Fe}(\text{CN})_6$	*C	au	NA	-18.3	NA	78WE 59
348	408			$\text{K}_3\text{HFe}(\text{CN})_6$	*C	a	-42.78	-72.1	115.	78WE 59
Summary data selected for reason 4										
348	418			$\text{K}_3\text{HFe}(\text{CN})_6$	*C	a	-42.78	-72.1	115.	78WE 59
4181432	348	412	A-8	$6\text{CN}^- + 3\text{K}^+ + \text{H}^+ + \text{Fe}^{2+} \leftrightarrow \text{K}_3\text{HFe}(\text{CN})_6$						
348	413	A-8	4181432	$\text{K}_3\text{HFe}(\text{CN})_6$						
348	414		4	6.888 143	3.888	418	1.888 338	1.888 288		
348	438			$\text{K}_3\text{HFe}(\text{CN})_6$	*C	au	NA	-78.9	NA	78WE 59
Summary data selected for reason 4										
348	431	A-2		$\text{K}_3\text{HFe}(\text{CN})_6$	*C	au	NA	-78.9	NA	78WE 59
348	448			$\text{KH}_2\text{FeCo}(\text{CN})_5$	*C	a	NA	-14.8	NA	78WE 59
Summary data selected for reason 4										
348	458	A-2		$\text{KH}_2\text{FeCo}(\text{CN})_5$	*C	a	NA	-14.8	NA	78WE 59
348	468			$\text{KH}_2\text{FeCo}(\text{CN})_5$	*C	au	NA	-13.6	NA	78WE 59

TABLE B.2. (contd)

MINTEQ Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
Summary data selected for reason 4								
348	478	A-2	$\text{KH}_2\text{FeCo(CN)}_5$	*C au	NA	-13.6	NA	76WE 59
348	488		$\text{K}_2\text{HFeCo(CN)}_5$	*C a	NA	-74.6	NA	76WE 59
Summary data selected for reason 4								
348	498	A-2	$\text{K}_2\text{HFeCo(CN)}_5$	*C a	NA	-74.6	NA	76WE 59
348	508		$\text{K}_2\text{HFeCo(CN)}_5$	*C au	NA	-74.2	NA	76WE 59
Summary data selected for reason 4								
348	518	A-2	$\text{K}_2\text{HFeCo(CN)}_5$	*C au	NA	-74.2	NA	76WE 59
348	528		$\text{KZn}_{1.5}\text{Fe(CN)}_8$	*J cr	78.8	NA	NA	82WE 2-348
348	538		$\text{KZn}_{1.5}\text{Fe(CN)}_8$	!C cr	18.9	NA	NA	82WE 2-348
348	548		$\text{KZn}_{1.5}\text{Fe(CN)}_8$	*C cr	18.9	NA	NA	81WE 76
Summary data selected for reason 1								
348	558	S-8	$\text{KZn}_{1.5}\text{Fe(CN)}_8$	!C cr	18.9	NA	NA	82WE 2-348
1141818	348	S-8	$8\text{CN}^- + \text{K}^+ + 1.5\text{Zn}^{2+} + \text{Fe}^{2+} \leftrightarrow \text{KZn}_{1.5}\text{Fe(CN)}_8$					
348	562	S-8	1141818 $\text{KZn}_{1.5}\text{Fe(CN)}_8$					
348	563		4 8.886 143 1.888 418 1.588 958 1.888 288					
348	588		$\text{KZn}_{1.5}\text{Fe(CN)}_8$ from Fe(CN)_8^{4-}	*J ai	191.3	NA	NA	82WE 2-348
348	581		$\text{KZn}_{1.5}\text{Fe(CN)}_8$ from Fe(CN)_8^{4-}	!C ai	45.72	NA	NA	82WE 2-348
348	582		$\text{KZn}_{1.5}\text{Fe(CN)}_8$ from Fe(CN)_8^{4-}	*C ai	45.7	NA	NA	81WE 75
Summary data selected for reason 2								
348	598	A-1	$\text{KZn}_{1.5}\text{Fe(CN)}_8$ from Fe(CN)_8^{4-}	*C ai	45.72	NA	NA	82WE 2-348
348	608		$\text{K}_2\text{CdFe(CN)}_8$	*J cr	-48.8	NA	NA	82WE 2-348
348	618		$\text{K}_2\text{CdFe(CN)}_8$	!C cr	-11.2	NA	NA	82WE 2-348
348	628		$\text{K}_2\text{CdFe(CN)}_8$	*C cr	-11.2	NA	NA	81WE 75
Summary data selected for reason 1								
348	638	S-8	$\text{K}_2\text{CdFe(CN)}_8$	!C cr	-11.2	NA	NA	82WE 2-348
1141883	348	S-8	$8\text{CN}^- + 2\text{K}^+ + \text{Cd}^{2+} + \text{Fe}^{2+} \leftrightarrow \text{K}_2\text{CdFe(CN)}_8$					
348	632	S-8	1141883 $\text{K}_2\text{CdFe(CN)}_8$					

TABLE B.2. (contd)

WINTER	In 82WE			Units		$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°		
Number	Page	ID	Form	Compound	Q	State	(Q/mol)	(Q/mol)	(Q/mol·K)	Data Sources
348	833		4	8.888 143	2.888 418		1.888 188	1.888 288		
348	868			$K_2CdFe(CN)_8$	from $Fe(CN)_6^{4-}$	*J ai	58.7	NA	NA	82WE 2-348
348	861			$K_2CdFe(CN)_8$	from $Fe(CN)_6^{4-}$	!C ai	12.1	NA	NA	82WE 2-348
348	862			$K_2CdFe(CN)_8$	from $Fe(CN)_6^{4-}$	*C ai	12.1	NA	NA	81WE 75
Summary data selected for reason 1										
348	878	A-1		$K_2CdFe(CN)_8$	from $Fe(CN)_6^{4-}$	!C ai	12.1	NA	NA	82WE 2-348
348	888			$K_{12}Cd_8(Fe(CN)_8)_7$		*J cr	155.	NA	NA	82WE 2-348
348	898			$K_{12}Cd_8(Fe(CN)_8)_7$		!C cr	37.8	NA	NA	82WE 2-348
348	788			$K_{12}Cd_8(Fe(CN)_8)_7$		*C cr	37.	NA	NA	81WE 75
Summary data selected for reason 2										
348	718	S-8		$K_{12}Cd_8(Fe(CN)_8)_7$		*C cr	37.8	NA	NA	82WE 2-348
1141889	348	711	S-8	$42CN^- + 12K^+ + 8Cd^{2+} + 7Fe^{2+} \leftrightarrow K_{12}Cd_8(Fe(CN)_8)_7$						
348	712	S-8	1141889	$K_{12}Cd_8(Fe(CN)_8)_7$						
348	713		4	42.888 143	12.888 418		8.888 188	7.888 288		
348	748			$K_2Cu_2Fe(CN)_8$		*J cr	77.1	NA	NA	82WE 2-348
348	741			$K_2Cu_2Fe(CN)_8$		!C cr	18.4	NA	NA	82WE 2-348
348	742			$K_2Cu_2Fe(CN)_8$		*C cr	18.4	NA	NA	81WE 75
Summary data selected for reason 1										
348	758	S-8		$K_2Cu_2Fe(CN)_8$		!C cr	18.4	NA	NA	82WE 2-348
1141813	348	751	S-8	$8CN^- + 2K^+ + 2Cu^+ + Fe^{2+} \leftrightarrow K_2Cu_2Fe(CN)_8$						
348	752	S-8	1141813	$K_2Cu_2Fe(CN)_8$						
348	753		4	8.888 143	2.888 418		2.888 238	1.888 288		
348	788			$K_2Cu_2Fe(CN)_8$	from $Fe(CN)_6^{4-}$	*J ai	229.4	NA	NA	82WE 2-348
348	781			$K_2Cu_2Fe(CN)_8$	from $Fe(CN)_6^{4-}$	!C ai	54.83	NA	NA	82WE 2-348
348	782			$K_2Cu_2Fe(CN)_8$	from $Fe(CN)_6^{4-}$	*C ai	54.8	NA	NA	81WE 75

TABLE B.2. (contd)

MINTEQA	In 82WE				Units	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°	
Number	Page	ID	Form	Compound	Q State	(Q/mol)	(Q/mol)	(Q/mol·K)	Data Sources
Summary data selected for reason 2									
348	798	A-1		$K_2Cu_2Fe(CN)_6$ from $Fe(CN)_6^{4-}$	*C ai	54.83	NA	NA	82WE 2-348
348	806			$K_2Ni_3(Fe(CN)_6)_2$	*J cr	566.	NA	NA	82WE 2-348
348	816			$K_2Ni_3(Fe(CN)_6)_2$	!C cr	121.	NA	NA	82WE 2-348
348	826			$K_2Ni_3(Fe(CN)_6)_2$	*C cr	121.	NA	NA	81WE 75
Summary data selected for reason 1									
348	836	S-8		$K_2Ni_3(Fe(CN)_6)_2$	!C cr	121.	NA	NA	82WE 2-348
1141067	348	831	S-8	$12CN^- + 2K^+ + 3Ni^{2+} + 2Fe^{2+} \leftrightarrow K_2Ni_3(Fe(CN)_6)_2$					
348	832	S-8		1141067 $K_2Ni_3(Fe(CN)_6)_2$					
348	833		4	12.000 143	2.000 416	3.000 548	2.000 286		
348	856			$K_4Ni_4(Fe(CN)_6)_3$	*J cr	567.	NA	NA	82WE 2-348
348	861			$K_4Ni_4(Fe(CN)_6)_3$	!C cr	121.	NA	NA	82WE 2-348
348	862			$K_4Ni_4(Fe(CN)_6)_3$	*C cr	121.	NA	NA	81WE 75
Summary data selected for reason 1									
348	876	S-8		$K_4Ni_4(Fe(CN)_6)_3$	!C cr	121.	NA	NA	82WE 2-348
1141064	348	871	S-8	$18CN^- + 4K^+ + 4Ni^{2+} + 3Fe^{2+} \leftrightarrow K_4Ni_4(Fe(CN)_6)_3$					
348	872	S-8		1141064 $K_4Ni_4(Fe(CN)_6)_3$					
348	873		4	18.000 143	4.000 416	4.000 548	3.000 286		
348	906			$K_{12}Ni_8(Fe(CN)_6)_7$	*J cr	473.	NA	NA	82WE 2-348
348	901			$K_{12}Ni_8(Fe(CN)_6)_7$	!C cr	113.	NA	NA	82WE 2-348
348	902			$K_{12}Ni_8(Fe(CN)_6)_7$	*C cr	113.	NA	NA	81WE 75
Summary data selected for reason 1									
348	916	S-8		$K_{12}Ni_8(Fe(CN)_6)_7$	!C cr	113.	NA	NA	82WE 2-348
1141061	348	911	S-8	$42CN^- + 12K^+ + 8Ni^{2+} + 7Fe^{2+} \leftrightarrow K_{12}Ni_8(Fe(CN)_6)_7$					
348	912	S-8		1141061 $K_{12}Ni_8(Fe(CN)_6)_7$					
348	913		4	42.000 143	12.000 416	8.000 548	7.000 286		
348	946			$K_2Co_3(Fe(CN)_6)_2$	*J cr	562.	NA	NA	82WE 2-348
348	941			$K_2Co_3(Fe(CN)_6)_2$	!C cr	128.	NA	NA	82WE 2-348
348	942			$K_2Co_3(Fe(CN)_6)_2$	*C cr	128.	NA	NA	81WE 75

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (kJ/mol)	$\Delta H_f^\circ, 298$ (kJ/mol)	S_{298}° (J/mol·K)	Data Sources
Summary data selected for reason 1							
348	958 S-1	$K_2Co_3(Fe(CN)_6)_2$	IC cr	128.	NA	NA	82WE 2-848
348	958	$K_4Co_4(Fe(CN)_6)_3$	*J cr	477.	NA	NA	82WE 2-848
348	978	$K_4Co_4(Fe(CN)_6)_3$	IC cr	114.	NA	NA	82WE 2-848
348	958	$K_4Co_4(Fe(CN)_6)_3$	*C cr	114.	NA	NA	81WE 75
Summary data selected for reason 1							
348	998 S-1	$K_4Co_4(Fe(CN)_6)_3$	IC cr	114.	NA	NA	82WE 2-848
349	18	$K_2Pt(CN)_4$	*C a	NA	33.5	NA	78WE 68
Summary data selected for reason 4							
349	28 A-2	$K_2Pt(CN)_4$	*C a	NA	33.5	NA	78WE 68
358	18	$K_2Mn_3(Fe(CN)_6)_2$	*J cr	-29.	NA	NA	82WE 2-358
358	28	$K_2Mn_3(Fe(CN)_6)_2$	IC cr	-8.9	NA	NA	82WE 2-358
358	38	$K_2Mn_3(Fe(CN)_6)_2$	*C cr	-7.	NA	NA	81WE 77
Summary data selected for reason 2							
358	48 S-8	$K_2Mn_3(Fe(CN)_6)_2$	*C cr	-8.9	NA	NA	82WE 2-358
1141886	358 41 S-8	$12CN^- + 2K^+ + 3Mn^{2+} + 2Fe^{2+} \leftrightarrow K_2Mn_3(Fe(CN)_6)_2$					
	358 42 S-8	1141886 $K_2Mn_3(Fe(CN)_6)_2$					
358	43	4 12.888 143 2.888 418 3.888 478 2.888 288					
358	78	$K_8Mn_8(Fe(CN)_6)_5$	*J cr	-527.	NA	NA	82WE 2-358
358	71	$K_8Mn_8(Fe(CN)_6)_5$	IC cr	-126.	NA	NA	82WE 2-358
358	72	$K_8Mn_8(Fe(CN)_6)_5$	*C cr	-126.	NA	NA	81WE 77
Summary data selected for reason 1							
358	88 S-8	$K_8Mn_8(Fe(CN)_6)_5$	IC cr	-126.	NA	NA	82WE 2-358
1141812	358 81 S-8	$38CN^- + 8K^+ + 8Mn^{2+} + 5Fe^{2+} \leftrightarrow K_8Mn_8(Fe(CN)_6)_5$					
	358 82 S-8	1141812 $K_8Mn_8(Fe(CN)_6)_5$					
358	83	4 38.888 143 8.888 418 8.888 478 5.888 288					
352	18	$K_4Y_8(Fe(CN)_6)_7 \cdot 38H_2O$	*J cr	-9488.	NA	NA	82WE 2-352
352	28	$K_4Y_8(Fe(CN)_6)_7 \cdot 38H_2O$	IC cr	-2249.	NA	NA	82WE 2-352
352	38	$K_4Y_8(Fe(CN)_6)_7 \cdot 38H_2O$	*C cr	-2249.	NA	NA	81WE 79

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID Form	Compound	Units Q State	$\Delta G_f^0, 298$ (Q/mol)	$\Delta H_f^0, 298$ (Q/mol)	S_{298}^0 (Q/mol·K)	Data Sources
Summary data selected for reason 1							
352	48 S-1	$K_4Yg(Fe(CN)_6)7 \cdot 30H_2O$	!C cr	-2249.	NA	NA	82WE 2-352
352	58	$KGdFe(CN)_6$	*J cr	-312.1	NA	NA	82WE 2-352
352	68	$KGdFe(CN)_6$	!C cr	-74.59	NA	NA	82WE 2-352
352	78	$KGdFe(CN)_6$	*C cr	-74.8	NA	NA	81WE 79
Summary data selected for reason 2							
352	88 S-1	$KGdFe(CN)_6$	*C cr	-74.59	NA	NA	82WE 2-352
353	18	$KCeFe(CN)_6 \cdot 2H_2O$	*J cr	-796.9	NA	NA	82WE 2-353
353	28	$KCeFe(CN)_6 \cdot 2H_2O$	!C cr	-196.4	NA	NA	82WE 2-353
353	38	$KCeFe(CN)_6 \cdot 2H_2O$	*C cr	-196.5	NA	NA	81WE 86
Summary data selected for reason 2							
353	48 S-1	$KCeFe(CN)_6 \cdot 2H_2O$	*C cr	-196.4	NA	NA	82WE 2-353
353	58	$KLFe(CN)_6$	*J cr	-328.8	NA	NA	82WE 2-353
353	68	$KLFe(CN)_6$	!C cr	-76.67	NA	NA	82WE 2-353
353	78	$KLFe(CN)_6$	*C cr	-76.7	NA	NA	81WE 86
Summary data selected for reason 2							
353	88 S-1	$KLFe(CN)_6$	*C cr	-76.67	NA	NA	82WE 2-353
354	18	$KCeFe(CN)_6 \cdot 5H_2O$	*J cr	NA	-4863.	NA	82WE 2-354
354	28	$KCeFe(CN)_6 \cdot 5H_2O$	!C cr	NA	-971.1	NA	82WE 2-354
354	38	$KCeFe(CN)_6 \cdot 5H_2O$	*C cr	NA	-971.	NA	81WE 81
Summary data selected for reason 2							
354	48 S-2	$KCeFe(CN)_6 \cdot 5H_2O$	*C cr	NA	-971.1	NA	82WE 2-354
361	18	RbCN	*J cr	NA	NA	146.88	82WE 2-361
361	28	RbCN	!C cr	NA	NA	33.871	82WE 2-361
361	38	RbCN	*C cr	NA	NA	33.67	81WE 89
361	48	RbCN	*C cr	NA	NA	33.67	76WE 78
Summary data selected for reason 2							
361	58 S-2	RbCN	*C cr	NA	NA	33.67	82WE 2-361
361	68	RbCN	*J ai	-111.7	-186.4	215.5	82WE 2-361
361	78	RbCN	!C ai	-26.78	-24.86	51.51	82WE 2-361
361	88	RbCN	*C ai	-26.7	-24.8	51.5	81WE 89

TABLE B.2. (contd)

WINTER	In 82WE				Units	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°	
Number	Page	ID	Form	Compound	Q State	(Q/mol)	(Q/mol)	(Q/mol·K)	Data Sources
Summary data selected for reason 2									
361	98	A-1		RbCN	*C ai	-26.78	-24.88	51.51	82WE 2-361
362	18			Rb ₂ Zn(CN) ₄	*J ai	-128.9	-168.2	489.	82WE 2-362
362	28			Rb ₂ Zn(CN) ₄	!C ai	-28.98	-36.29	112.	82WE 2-362
362	38			Rb ₂ Zn(CN) ₄	*C ai	-28.9	-38.3	112.	81WE 98
Summary data selected for reason 2									
362	48	A-1		Rb ₂ Zn(CN) ₄	*C ai	-28.98	-38.29	112.	82WE 2-362
362	18			RbCd(CN) ₃	*J ai	78.8	NA	NA	82WE 2-362
362	28			RbCd(CN) ₃	!C ai	18.9	NA	NA	82WE 2-362
362	38			RbCd(CN) ₃	*C ai	18.9	NA	NA	81WE 91
Summary data selected for reason 1									
362	48	A-1		RbCd(CN) ₃	!C ai	18.9	NA	NA	82WE 2-362
362	58			Rb ₂ Cd(CN) ₄	*J ai	-86.2	-74.5	585.	82WE 2-362
362	68			Rb ₂ Cd(CN) ₄	!C ai	-14.4	-17.8	135.	82WE 2-362
362	78			Rb ₂ Cd(CN) ₄	*C ai	-14.4	-17.8	135.	81WE 91
Summary data selected for reason 1									
362	88	A-1		Rb ₂ Cd(CN) ₄	!C ai	-14.4	-17.8	135.	82WE 2-362
362	98			RbHg(CN) ₃	*J ai	179.1	148.8	346.4	82WE 2-362
362	108			RbHg(CN) ₃	!C ai	42.81	34.89	82.79	82WE 2-362
362	118			RbHg(CN) ₃	*C ai	42.8	34.9	82.8	81WE 91
Summary data selected for reason 2									
362	128	A-1		RbHg(CN) ₃	*C ai	42.1	34.89	82.79	82WE 2-362
362	138			Rb ₂ Hg(CN) ₄	*J ai	58.7	23.8	548.	82WE 2-362
362	148			Rb ₂ Hg(CN) ₄	!C ai	12.1	5.89	131.	82WE 2-362
362	158			Rb ₂ Hg(CN) ₄	*C ai	12.1	5.7	131.	81WE 91
Summary data selected for reason 2									
362	168	A-1		Rb ₂ Hg(CN) ₄	*C ai	12.1	5.89	131.	82WE 2-362
363	18			RbCu(CN) ₂	*J ai	-26.3	NA	NA	82WE 2-363
363	28			RbCu(CN) ₂	!C ai	-8.29	NA	NA	82WE 2-363
363	38			RbCu(CN) ₂	*C ai	-8.3	NA	NA	81WE 91

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
Summary data selected for reason 2								
363	48	A-1	RbCu(CN) ₂	*C ai	-6.29	NA	NA	82WE 2-363
363	66		Rb ₂ Cu(CN) ₃	*J ai	-164.8	NA	NA	82WE 2-363
363	68		Rb ₂ Cu(CN) ₃	!C ai	-39.26	NA	NA	82WE 2-363
363	76		Rb ₂ Cu(CN) ₃	*C ai	-39.2	NA	NA	81WE 91
Summary data selected for reason 2								
363	88	A-1	Rb ₂ Cu(CN) ₃	*C ai	-39.2	NA	NA	82WE 2-363
363	96		Rb ₃ Cu(CN) ₄	*J ai	-265.3	NA	NA	82WE 2-363
363	106		Rb ₃ Cu(CN) ₄	!C ai	-68.19	NA	NA	82WE 2-363
363	116		Rb ₃ Cu(CN) ₄	*C ai	-68.2	NA	NA	81WE 91
Summary data selected for reason 2								
363	126	A-1	Rb ₃ Cu(CN) ₄	*C ai	-68.19	NA	NA	82WE 2-363
363	136		RbAg(CN) ₂	*J ai	21.4	19.2	314.	82WE 2-363
363	146		RbAg(CN) ₂	!C ai	5.12	4.59	75.6	82WE 2-363
363	156		RbAg(CN) ₂	*C ai	5.1	4.6	75.	81WE 91
Summary data selected for reason 2								
363	166	A-1	RbAg(CN) ₂	*C ai	5.12	4.59	75.6	82WE 2-363
363	176		RbAu(CN) ₂	*J ai	1.7	-8.8	293.	82WE 2-363
363	186		RbAu(CN) ₂	!C ai	8.41	-2.1	78.6	82WE 2-363
363	196		RbAu(CN) ₂	*C ai	8.4	-2.1	78.	81WE 92
Summary data selected for reason 2								
363	206	A-1	RbAu(CN) ₂	*C ai	8.41	-2.1	78.	82WE 2-363
363	216		Rb ₂ Ni(CN) ₄	*J ai	-95.7	-134.7	468.	82WE 2-363
363	226		Rb ₂ Ni(CN) ₄	!C ai	-22.9	-32.19	116.	82WE 2-363
363	236		Rb ₂ Ni(CN) ₄	*C ai	-22.9	-32.2	116.	81WE 92
Summary data selected for reason 2								
363	246	A-1	Rb ₂ Ni(CN) ₄	*C ai	-22.9	-32.19	116.	82WE 2-363
363	256		Rb ₃ Co(CN) ₆	*J ai	NA	NA	597.1	82WE 2-363
363	266		Rb ₃ Co(CN) ₆	!C ai	NA	NA	142.7	82WE 2-363
363	276		Rb ₃ Co(CN) ₆	*C ai	NA	NA	142.7	81WE 92

TABLE B.2. (contd)

WINTER	In 82WE				Units	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°	
Number	Page	ID	Form	Compound	Q State	(J/mol)	(J/mol)	(J/mol-K)	Data Sources
Summary data selected for reason 1									
363	286	A-2		Rb ₃ Co(CN) ₆	IC ai	NA	NA	142.7	82WE 2-363
363	290			Rb ₃ Fe(CN) ₆	*J ai	-122.5	-191.6	634.7	82WE 2-363
363	300			Rb ₃ Fe(CN) ₆	IC ai	-29.28	-45.79	151.7	82WE 2-363
363	310			Rb ₃ Fe(CN) ₆	*C ai	-29.8	-45.8	151.7	81WE 92
Summary data selected for reason 2									
363	320	A-1		Rb ₃ Fe(CN) ₆	*C ai	-29.28	-45.79	151.7	82WE 2-363
363	330			Rb ₄ Fe(CN) ₆	*J ai	-448.85	-548.9	581.2	82WE 2-363
363	340			Rb ₄ Fe(CN) ₆	IC ai	-105.37	-131.19	138.9	82WE 2-363
363	350			Rb ₄ Fe(CN) ₆	*C ai	-105.39	-131.2	138.9	81WE 92
Summary data selected for reason 2									
363	360	A-1		Rb ₄ Fe(CN) ₆	*C ai	-105.37	-131.19	138.9	82WE 2-363
363	370			Rb ₃ FeCo(CN) ₅ from FeCo(CN) ₅ ³⁻	*J ai	NA	-568.7	NA	82WE 2-363
363	380			Rb ₃ FeCo(CN) ₅ from FeCo(CN) ₅ ³⁻	IC ai	NA	-134.8	NA	82WE 2-363
363	390			Rb ₃ FeCo(CN) ₅ from FeCo(CN) ₅ ³⁻	*C ai	NA	-134.8	NA	81WE 92
Summary data selected for reason 1									
363	400	A-2		Rb ₃ FeCo(CN) ₅ from FeCo(CN) ₅ ³⁻	IC ai	NA	-134.8	NA	82WE 2-363
363	410			RbH ₃ Fe(CN) ₆ from H ₃ Fe(CN) ₆ ⁻	*J ai	NA	284.6	NA	82WE 2-363
363	420			RbH ₃ Fe(CN) ₆ from H ₃ Fe(CN) ₆ ⁻	IC ai	NA	48.98	NA	82WE 2-363
363	430			RbH ₃ Fe(CN) ₆ from H ₃ Fe(CN) ₆ ⁻	*C ai	NA	48.9	NA	81WE 92
Summary data selected for reason 2									
363	440	A-2		RbH ₃ Fe(CN) ₆ from H ₃ Fe(CN) ₆ ⁻	*C ai	NA	48.98	NA	82WE 2-363
363	450			Rb ₂ H ₂ Fe(CN) ₆ from H ₂ Fe(CN) ₆ ²⁻	*J ai	98.63	48.9	460.	82WE 2-363
363	460			Rb ₂ H ₂ Fe(CN) ₆ from H ₂ Fe(CN) ₆ ²⁻	IC ai	21.66	11.2	110.	82WE 2-363
363	470			Rb ₂ H ₂ Fe(CN) ₆ from H ₂ Fe(CN) ₆ ²⁻	*C ai	21.63	11.2	110.	81WE 92

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
Summary data selected for reason 2								
363	488	A-1	$\text{Rb}_2\text{H}_2\text{Fe}(\text{CN})_6$ from $\text{H}_2\text{Fe}(\text{CN})_6^{2-}$	*C ai	21.66	11.2	118.	82WE 2-363
363	498		$\text{Rb}_3\text{HFe}(\text{CN})_6$ from $\text{HFe}(\text{CN})_6^{3-}$	*J ai	-186.68	-297.9	548.	82WE 2-363
363	508		$\text{Rb}_3\text{HFe}(\text{CN})_6$ from $\text{HFe}(\text{CN})_6^{3-}$	!C ai	-43.184	-71.28	129.	82WE 2-363
363	518		$\text{Rb}_3\text{HFe}(\text{CN})_6$ from $\text{HFe}(\text{CN})_6^{3-}$	*C ai	-43.21	-71.2	129.	81WE 92
Summary data selected for reason 2								
363	528	A-1	$\text{Rb}_3\text{HFe}(\text{CN})_6$ from $\text{HFe}(\text{CN})_6^{3-}$	*C ai	-43.184	-71.28	129.	82WE 2-363
364	18		$\text{RbH}_2\text{FeCo}(\text{CN})_5$ from $\text{H}_2\text{FeCo}(\text{CN})_5^-$	*J ai	NA	-57.3	NA	82WE 2-364
364	28		$\text{RbH}_2\text{FeCo}(\text{CN})_5$ from $\text{H}_2\text{FeCo}(\text{CN})_5^-$	!C ai	NA	-13.78	NA	82WE 2-364
364	38		$\text{RbH}_2\text{FeCo}(\text{CN})_5$ from $\text{H}_2\text{FeCo}(\text{CN})_5^-$	*C ai	NA	-13.7	NA	81WE 92
Summary data selected for reason 2								
364	48	A-2	$\text{RbH}_2\text{FeCo}(\text{CN})_5$ from $\text{H}_2\text{FeCo}(\text{CN})_5^-$	*C ai	NA	-13.7	NA	82WE 2-364
364	58		$\text{Rb}_2\text{HFeCo}(\text{CN})_5$ from $\text{HFeCo}(\text{CN})_5^{2-}$	*J ai	NA	-318.8	NA	82WE 2-364
364	68		$\text{Rb}_2\text{HFeCo}(\text{CN})_5$ from $\text{HFeCo}(\text{CN})_5^{2-}$	!C ai	NA	-74.89	NA	82WE 2-364
364	78		$\text{Rb}_2\text{HFeCo}(\text{CN})_5$ from $\text{HFeCo}(\text{CN})_5^{2-}$	*C ai	NA	-74.1	NA	81WE 92
Summary data selected for reason 2								
364	88	A-2	$\text{Rb}_2\text{HFeCo}(\text{CN})_5$ from $\text{HFeCo}(\text{CN})_5^{2-}$	*C ai	NA	-74.89	NA	82WE 2-364
364	98		$\text{Rb}_2\text{Pb}(\text{CN})_4$	*J ai	59.	NA	NA	82WE 2-364
364	108		$\text{Rb}_2\text{Pb}(\text{CN})_4$	*C ai	14.	NA	NA	82WE 2-364
364	118		$\text{Rb}_2\text{Pb}(\text{CN})_4$	*C ai	14.	NA	NA	81WE 92
Summary data selected for reason 1								
364	128	A-1	$\text{Rb}_2\text{Pb}(\text{CN})_4$	*C ai	14.	NA	NA	82WE 2-364
364	138		$\text{Rb}_2\text{Pt}(\text{CN})_4$	*J ai	142.7	NA	NA	82WE 2-364
364	148		$\text{Rb}_2\text{Pt}(\text{CN})_4$	!C ai	34.11	NA	NA	82WE 2-364
364	158		$\text{Rb}_2\text{Pt}(\text{CN})_4$	*C ai	34.1	NA	NA	81WE 92

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
Summary data selected for reason 2								
384	168	A-1	Rb ₂ Pt(CN) ₄	*C ai	34.11	NA	NA	82WE 2-384
384	178		Rb ₄ Mn(CN) ₈	*J aq	NA	-448.	NA	82WE 2-384
384	188		Rb ₄ Mn(CN) ₈	!C aq	NA	-187.	NA	82WE 2-384
384	198		Rb ₄ Mn(CN) ₈	*C aq	NA	-187.	NA	81WE 93
Summary data selected for reason 1								
384	208	A-2	Rb ₄ Mn(CN) ₈	!C aq	NA	-187.	NA	82WE 2-384
385	18		RbGd(Fe(CN) ₆)	*J cr	-317.5	NA	NA	82WE 2-385
385	28		RbGd(Fe(CN) ₆)	!C cr	-75.88	NA	NA	82WE 2-385
385	38		RbGd(Fe(CN) ₆)	*C cr	-75.9	NA	NA	81WE 94
Summary data selected for reason 2								
385	48	S-1	RbGd(Fe(CN) ₆)	*C cr	-75.88	NA	NA	82WE 2-385
385	58		RbCe(Fe(CN) ₆)·2H ₂ O	*J cr	-886.5	NA	NA	82WE 2-385
385	68		RbCe(Fe(CN) ₆)·2H ₂ O	!C cr	-192.6	NA	NA	82WE 2-385
385	78		RbCe(Fe(CN) ₆)·2H ₂ O	*C cr	-192.8	NA	NA	81WE 94
Summary data selected for reason 2								
385	88	S-1	RbCe(Fe(CN) ₆)·2H ₂ O	*C cr	-192.6	NA	NA	82WE 2-385
386	18		RbMgFe(CN) ₈ from MgFe(CN) ₆ ⁻	*J ai	-25.4	NA	NA	82WE 2-386
386	28		RbMgFe(CN) ₈ from MgFe(CN) ₆ ⁻	!C ai	-8.87	NA	NA	82WE 2-386
386	38		RbMgFe(CN) ₈ from MgFe(CN) ₆ ⁻	*C ai	-8.1	NA	NA	81WE 94
Summary data selected for reason 2								
386	48	A-1	RbMgFe(CN) ₈ from MgFe(CN) ₆ ⁻	*C ai	-8.87	NA	NA	82WE 2-386
386	58		Rb ₂ MgFe(CN) ₈ from MgFe(CN) ₆ ²⁻	*J ai	-349.3	NA	NA	82WE 2-386
386	68		Rb ₂ MgFe(CN) ₈ from MgFe(CN) ₆ ²⁻	!C ai	-83.48	NA	NA	82WE 2-386
386	78		Rb ₂ MgFe(CN) ₈ from MgFe(CN) ₆ ²⁻	*C ai	-83.5	NA	NA	81WE 94

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta H_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
Summary data selected for reason 2								
366	88	A-1	Rb ₂ MgFe(CN) ₆ from MgFe(CN) ₆ ²⁻	*C ai	-83.48	NA	NA	82WE 2-366
366	98		RbCaFe(CN) ₆ from CaFe(CN) ₆ ⁻	*J ai	NA	-124.6	NA	82WE 2-366
366	108		RbCaFe(CN) ₆ from CaFe(CN) ₆ ⁻	!C ai	NA	-29.78	NA	82WE 2-366
366	118		RbCaFe(CN) ₆ from CaFe(CN) ₆ ⁻	*C ai	NA	-29.8	NA	81WE 94
Summary data selected for reason 2								
366	128	A-2	RbCaFe(CN) ₆ from CaFe(CN) ₆ ⁻	*C ai	NA	-29.78	NA	82WE 2-366
366	138		Rb ₂ CaFe(CN) ₆ from CaFe(CN) ₆ ²⁻	*J ai	-448.8	NA	NA	82WE 2-366
366	148		Rb ₂ CaFe(CN) ₆ from CaFe(CN) ₆ ²⁻	!C ai	-187.1	NA	NA	82WE 2-366
366	158		Rb ₂ CaFe(CN) ₆ from CaFe(CN) ₆ ²⁻	*C ai	-187.1	NA	NA	81WE 94
Summary data selected for reason 1								
366	168	A-1	Rb ₂ CaFe(CN) ₆ from CaFe(CN) ₆ ²⁻	!C ai	-187.1	NA	NA	82WE 2-366
366	178		RbSrFe(CN) ₆ from SrFe(CN) ₆ ⁻	*J ai	-138.4	NA	NA	82WE 2-366
366	188		RbSrFe(CN) ₆ from SrFe(CN) ₆ ⁻	!C ai	-31.17	NA	NA	82WE 2-366
366	198		RbSrFe(CN) ₆ from SrFe(CN) ₆ ⁻	*C ai	-31.2	NA	NA	81WE 94
Summary data selected for reason 2								
366	208	A-1	RbSrFe(CN) ₆ from SrFe(CN) ₆ ⁻	*C ai	-31.17	NA	NA	82WE 2-366
373	18		CaCN	*J cr	NA	NA	139.75	82WE 2-373
373	28		CaCN	!C cr	NA	NA	33.841	82WE 2-373
373	38		CaCN	*C cr	NA	NA	33.48	81WE 182
Summary data selected for reason 2								
373	48	S-2	CaCN	*C cr	NA	NA	33.841	82WE 2-373
373	58		CaCN	*J ai	-119.6	-187.5	227.2	82WE 2-373
373	68		CaCN	!C ai	-28.58	-25.89	54.38	82WE 2-373
373	78		CaCN	*C ai	-28.6	-25.7	54.3	81WE 182
Summary data selected for reason 2								
373	88	A-1	CaCN	*C ai	-28.58	-25.89	54.3	82WE 2-373

TABLE B.2. (contd)

WINTER	In 82WE			Units	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°	Data Sources	
Number	Page	ID	Form	Compound	Q State (Q/mol)	(Q/mol)	(Q/mol·K)		
374	18			$\text{Ca}_2\text{Zn}(\text{CN})_4$	*J ai	-137.2	-174.5	494.	82WE 2-374
374	28			$\text{Ca}_2\text{Zn}(\text{CN})_4$	!C ai	-32.79	-41.71	118.	82WE 2-374
374	38			$\text{Ca}_2\text{Zn}(\text{CN})_4$	*C ai	-32.8	-41.7	118.	81WE 183
Summary data selected for reason 2									
374	48	A-1		$\text{Ca}_2\text{Zn}(\text{CN})_4$	*C ai	-32.79	-41.71	118.	82WE 2-374
375	18			$\text{CaCd}(\text{CN})_3$	*J ai	82.8	NA	NA	82WE 2-375
375	28			$\text{CaCd}(\text{CN})_3$	!C ai	15.8	NA	NA	82WE 2-375
375	38			$\text{CaCd}(\text{CN})_3$	*C ai	15.8	NA	NA	81WE 183
Summary data selected for reason 1									
375	48	A-1		$\text{CaCd}(\text{CN})_3$	!C ai	15.8	NA	NA	82WE 2-375
375	58			$\text{Ca}_2\text{Cd}(\text{CN})_4$	*J ai	-78.5	-88.7	598.	82WE 2-375
375	68			$\text{Ca}_2\text{Cd}(\text{CN})_4$	!C ai	-18.3	-21.2	141.	82WE 2-375
375	78			$\text{Ca}_2\text{Cd}(\text{CN})_4$	*C ai	-18.3	-21.2	141.	81WE 183
Summary data selected for reason 1									
375	88	A-1		$\text{Ca}_2\text{Cd}(\text{CN})_4$	!C ai	-18.3	-21.2	141.	82WE 2-375
375	98			$\text{CaHg}(\text{CN})_3$	*J ai	171.2	138.9	358.2	82WE 2-375
375	108			$\text{CaHg}(\text{CN})_3$	!C ai	48.92	33.28	85.61	82WE 2-375
375	118			$\text{CaHg}(\text{CN})_3$	*C ai	48.9	33.2	85.6	81WE 183
Summary data selected for reason 2									
375	128	A-1		$\text{CaHg}(\text{CN})_3$	*C ai	48.92	33.2	85.61	82WE 2-375
375	138			$\text{Ca}_2\text{Hg}(\text{CN})_4$	*J ai	94.4	9.8	573.	82WE 2-375
375	148			$\text{Ca}_2\text{Hg}(\text{CN})_4$	!C ai	8.22	2.3	137.	82WE 2-375
375	158			$\text{Ca}_2\text{Hg}(\text{CN})_4$	*C ai	8.2	2.3	137.	81WE 183
Summary data selected for reason 2									
375	168	A-1		$\text{Ca}_2\text{Hg}(\text{CN})_4$	*C ai	8.22	2.3	137.	82WE 2-375
375	178			$\text{CaCu}(\text{CN})_2$	*J ai	-94.3	NA	NA	82WE 2-375
375	188			$\text{CaCu}(\text{CN})_2$	!C ai	-8.28	NA	NA	82WE 2-375
375	198			$\text{CaCu}(\text{CN})_2$	*C ai	-8.2	NA	NA	81WE 184
Summary data selected for reason 2									
375	208	A-1		$\text{CaCu}(\text{CN})_2$	*C ai	-8.2	NA	NA	82WE 2-375
375	218			$\text{Ca}_2\text{Cu}(\text{CN})_3$	*J ai	-188.3	NA	NA	82WE 2-375
375	228			$\text{Ca}_2\text{Cu}(\text{CN})_3$	!C ai	-43.89	NA	NA	82WE 2-375
375	238			$\text{Ca}_2\text{Cu}(\text{CN})_3$	*C ai	-43.1	NA	NA	81WE 184

TABLE B.2. (contd)

MINTeq Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
Summary data selected for reason 2								
375	248	A-1	$\text{Ca}_2\text{Cu}(\text{CN})_3$	*C ai	-48.89	NA	NA	82WE 2-375
375	268		$\text{Ca}_3\text{Cu}(\text{CN})_4$	*J ai	-389.8	NA	NA	82WE 2-375
375	268		$\text{Ca}_3\text{Cu}(\text{CN})_4$	!C ai	-74.88	NA	NA	82WE 2-375
375	278		$\text{Ca}_3\text{Cu}(\text{CN})_4$	*C ai	-74.8	NA	NA	81WE 184
Summary data selected for reason 2								
375	288	A-1	$\text{Ca}_3\text{Cu}(\text{CN})_4$	*C ai	-74.8	NA	NA	82WE 2-375
375	298		$\text{CaAg}(\text{CN})_2$	*J ai	13.4	12.1	326.	82WE 2-375
375	308		$\text{CaAg}(\text{CN})_2$	!C ai	8.28	2.89	77.9	82WE 2-375
375	318		$\text{CaAg}(\text{CN})_2$	*C ai	3.2	2.9	78.	81WE 184
Summary data selected for reason 2								
375	328	A-1	$\text{CaAg}(\text{CN})_2$	*C ai	3.2	2.89	77.9	82WE 2-375
375	338		$\text{CaAu}(\text{CN})_2$	*J ai	-8.2	-15.9	385.	82WE 2-375
375	348		$\text{CaAu}(\text{CN})_2$	!C ai	-1.5	-3.88	72.9	82WE 2-375
375	358		$\text{CaAu}(\text{CN})_2$	*C ai	-1.5	-3.8	73.	81WE 184
Summary data selected for reason 2								
375	368	A-1	$\text{CaAu}(\text{CN})_2$	*C ai	-1.5	-3.8	72.9	82WE 2-375
375	378		$\text{Ca}_2\text{Ni}(\text{CN})_4$	*J ai	-112.1	-149.8	485.	82WE 2-375
375	388		$\text{Ca}_2\text{Ni}(\text{CN})_4$	!C ai	-26.79	-35.81	118.	82WE 2-375
375	398		$\text{Ca}_2\text{Ni}(\text{CN})_4$	*C ai	-26.8	-35.8	118.	81WE 184
Summary data selected for reason 2								
375	408	A-1	$\text{Ca}_2\text{Ni}(\text{CN})_4$	*C ai	-26.79	-35.81	118.	82WE 2-375
378	18		$\text{Ca}_3\text{Co}(\text{CN})_8$	*J ai	NA	NA	831.8	82WE 2-378
378	28		$\text{Ca}_3\text{Co}(\text{CN})_8$	!C ai	NA	NA	151.8	82WE 2-378
378	38		$\text{Ca}_3\text{Co}(\text{CN})_8$	*C ai	NA	NA	151.8	81WE 184
Summary data selected for reason 1								
378	48	A-2	$\text{Ca}_3\text{Co}(\text{CN})_8$	*C ai	NA	NA	151.8	82WE 2-378
378	58		$\text{Ca}_3\text{Fe}(\text{CN})_8$	*J ai	-148.8	-213.8	669.4	82WE 2-378
378	68		$\text{Ca}_3\text{Fe}(\text{CN})_8$	!C ai	-35.89	-58.91	188.8	82WE 2-378
378	78		$\text{Ca}_3\text{Fe}(\text{CN})_8$	*C ai	-35.1	-58.9	188.8	81WE 184

TABLE B.2. (contd)

MINTeq	In 82WE				Units	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°	
Number	Page	ID	Form	Compound	Q State	(Q/mol)	(Q/mol)	(Q/mol·K)	Data Sources
Summary data selected for reason 2									
376	86	A-1		$\text{Ca}_3\text{Fe}(\text{CN})_8$	*C ai	-35.89	-58.91	168.8	82WE 2-376
376	96			$\text{Ca}_4\text{Fe}(\text{CN})_8$	*J ai	-472.99	-577.4	827.2	82WE 2-376
376	106			$\text{Ca}_4\text{Fe}(\text{CN})_8$	!C ai	-113.85	-138.8	149.9	82WE 2-376
376	116			$\text{Ca}_4\text{Fe}(\text{CN})_8$	*C ai	-113.87	-138.8	149.9	81WE 184
Summary data selected for reason 2									
376	126	A-1		$\text{Ca}_4\text{Fe}(\text{CN})_8$	*C ai	-113.85	-138.8	149.9	82WE 2-376
376	136			$\text{CaH}_3\text{Fe}(\text{CN})_8$ from $\text{H}_3\text{Fe}(\text{CN})_8^-$	*J ai	NA	197.5	NA	82WE 2-376
376	146			$\text{CaH}_3\text{Fe}(\text{CN})_8$ from $\text{H}_3\text{Fe}(\text{CN})_8^-$	!C ai	NA	47.28	NA	82WE 2-376
376	156			$\text{CaH}_3\text{Fe}(\text{CN})_8$ from $\text{H}_3\text{Fe}(\text{CN})_8^-$	*C ai	NA	47.2	NA	81WE 184
Summary data selected for reason 2									
376	166	A-2		$\text{CaH}_3\text{Fe}(\text{CN})_8$ from $\text{H}_3\text{Fe}(\text{CN})_8^-$	*C ai	NA	47.2	NA	82WE 2-376
376	176			$\text{Ca}_2\text{H}_2\text{Fe}(\text{CN})_8$ from $\text{H}_2\text{Fe}(\text{CN})_8^{2-}$	*J ai	74.58	-81.1	485.	82WE 2-376
376	186			$\text{Ca}_2\text{H}_2\text{Fe}(\text{CN})_8$ from $\text{H}_2\text{Fe}(\text{CN})_8^{2-}$	!C ai	17.82	-14.6	116.	82WE 2-376
376	196			$\text{Ca}_2\text{H}_2\text{Fe}(\text{CN})_8$ from $\text{H}_2\text{Fe}(\text{CN})_8^{2-}$	*C ai	17.79	-14.6	116.	81WE 184
Summary data selected for reason 2									
376	206	A-1		$\text{Ca}_2\text{H}_2\text{Fe}(\text{CN})_8$ from $\text{H}_2\text{Fe}(\text{CN})_8^{2-}$	*C ai	17.82	-14.6	116.	82WE 2-376
376	216			$\text{Ca}_3\text{HFe}(\text{CN})_8$ from $\text{HFe}(\text{CN})_8^{3-}$	*J ai	-284.78	-319.2	573.	82WE 2-376
376	226			$\text{Ca}_3\text{HFe}(\text{CN})_8$ from $\text{HFe}(\text{CN})_8^{3-}$	!C ai	-48.944	-76.29	137.	82WE 2-376
376	236			$\text{Ca}_3\text{HFe}(\text{CN})_8$ from $\text{HFe}(\text{CN})_8^{3-}$	*C ai	-48.97	-76.3	137.	81WE 184
Summary data selected for reason 2									
376	246	A-1		$\text{Ca}_3\text{HFe}(\text{CN})_8$ from $\text{HFe}(\text{CN})_8^{3-}$	*C ai	-48.44	-76.29	137.	82WE 2-376
376	256			$\text{CaH}_2\text{FeCo}(\text{CN})_5$ from $\text{H}_2\text{FeCo}(\text{CN})_5^-$	*J ai	NA	-84.4	NA	82WE 2-376
376	266			$\text{CaH}_2\text{FeCo}(\text{CN})_5$ from $\text{H}_2\text{FeCo}(\text{CN})_5^-$	!C ai	NA	-15.4	NA	82WE 2-376
376	276			$\text{CaH}_2\text{FeCo}(\text{CN})_5$ from $\text{H}_2\text{FeCo}(\text{CN})_5^-$	*C ai	NA	-15.4	NA	81WE 184

TABLE B.2. (contd)

MINTER Number	In 82WE Page ID	Form	Compound	Units Q State	$\Delta G_f^\circ, 298$ (Q/mol)	$\Delta H_f^\circ, 298$ (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
Summary data selected for reason 1								
376	288	A-2	$\text{CaH}_2\text{FeCo}(\text{CN})_5$ from $\text{H}_2\text{FeCo}(\text{CN})_5^-$	!C ai	NA	-16.4	NA	82WE 2-376
376	298		$\text{Ca}_2\text{HFeCo}(\text{CN})_5$ from $\text{HFeCo}(\text{CN})_5^{2-}$	*J ai	NA	-324.3	NA	82WE 2-376
376	308		$\text{Ca}_2\text{HFeCo}(\text{CN})_5$ from $\text{HFeCo}(\text{CN})_5^{2-}$	!C ai	NA	-77.51	NA	82WE 2-376
376	318		$\text{Ca}_2\text{HFeCo}(\text{CN})_5$ from $\text{HFeCo}(\text{CN})_5^{2-}$	*C ai	NA	-77.5	NA	81WE 184
Summary data selected for reason 2								
376	328	A-2	$\text{Ca}_2\text{HFeCo}(\text{CN})_5$ from $\text{HFeCo}(\text{CN})_5^{2-}$	*C ai	NA	-77.51	NA	82WE 2-376
376	338		$\text{Ca}_2\text{Pd}(\text{CN})_4$	*J ai	43.6	NA	NA	82WE 2-376
376	348		$\text{Ca}_2\text{Pd}(\text{CN})_4$	!C ai	18.4	NA	NA	82WE 2-376
376	358		$\text{Ca}_2\text{Pd}(\text{CN})_4$	*C ai	18.4	NA	NA	81WE 186
Summary data selected for reason 1								
376	368	A-1	$\text{Ca}_2\text{Pd}(\text{CN})_4$	!C ai	18.4	NA	NA	82WE 2-376
376	378		$\text{Ca}_2\text{Pu}(\text{CN})_4$	*J ai	126.4	NA	NA	82WE 2-376
376	388		$\text{Ca}_2\text{Pu}(\text{CN})_4$	!C ai	38.21	NA	NA	82WE 2-376
376	398		$\text{Ca}_2\text{Pu}(\text{CN})_4$	*C ai	38.2	NA	NA	81WE 184
Summary data selected for reason 2								
376	408	A-1	$\text{Ca}_2\text{Pu}(\text{CN})_4$	*C ai	38.21	NA	NA	82WE 2-376
377	18		$\text{Ca}_4\text{Mn}(\text{CN})_8$	*J ai	NA	-477.	NA	82WE 2-377
377	28		$\text{Ca}_4\text{Mn}(\text{CN})_8$	!C ai	NA	-114.	NA	82WE 2-377
377	38		$\text{Ca}_4\text{Mn}(\text{CN})_8$	*C ai	NA	-114.	NA	81WE 186
Summary data selected for reason 1								
377	48	A-2	$\text{Ca}_4\text{Mn}(\text{CN})_8$	!C ai	NA	-114.	NA	82WE 2-377
378	18		$\text{CaY}(\text{Fe}(\text{CN})_6) \cdot 2\text{H}_2\text{O}$	*J cr	-838.3	NA	NA	82WE 2-378
378	28		$\text{CaY}(\text{Fe}(\text{CN})_6) \cdot 2\text{H}_2\text{O}$	!C cr	-288.4	NA	NA	82WE 2-378
378	38		$\text{CaY}(\text{Fe}(\text{CN})_6) \cdot 2\text{H}_2\text{O}$	*C cr	-288.4	NA	NA	81WE 186
Summary data selected for reason 1								
378	48	S-1	$\text{CaY}(\text{Fe}(\text{CN})_6) \cdot 2\text{H}_2\text{O}$	!C cr	-288.4	NA	NA	82WE 2-378
378	58		$\text{CaGd}(\text{Fe}(\text{CN})_6)$	*J cr	-318.	NA	NA	82WE 2-378
378	68		$\text{CaGd}(\text{Fe}(\text{CN})_6)$	!C cr	-76.8	NA	NA	82WE 2-378
378	78		$\text{CaGd}(\text{Fe}(\text{CN})_6)$	*C cr	-76.	NA	NA	81WE 186

TABLE B.2. (contd)

WINTER	In 82WE				Units	$\Delta G_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°		
Number	Page	ID	Form	Compound	Q	State	(Q/mol)	(Q/mol)	(Q/mol·K)	Data Sources
Summary data selected for reason 2										
378	88	S-1		$\text{CaO}(\text{Fe}(\text{CN})_6)$	*C	cr	-76.	NA	NA	82WE 2-378
378	98			$\text{CaCe}(\text{Fe}(\text{CN})_6) \cdot 2\text{H}_2\text{O}$	*J	cr	-888.	NA	NA	82WE 2-378
378	106			$\text{CaCe}(\text{Fe}(\text{CN})_6) \cdot 2\text{H}_2\text{O}$	!C	cr	-193.	NA	NA	82WE 2-378
378	118			$\text{CaCe}(\text{Fe}(\text{CN})_6) \cdot 2\text{H}_2\text{O}$	*C	cr	-193.1	NA	NA	81WE 186
Summary data selected for reason 2										
378	128	S-1		$\text{CaCs}(\text{Fe}(\text{CN})_6) \cdot 2\text{H}_2\text{O}$	*C	cr	-193.	NA	NA	82WE 2-378
378	138			$\text{CaMgFe}(\text{CN})_6$ from $\text{MgFe}(\text{CN})_6^{2-}$	*J	ai	-33.4	NA	NA	82WE 2-378
378	148			$\text{CaMgFe}(\text{CN})_6$ from $\text{MgFe}(\text{CN})_6^{2-}$	!C	ai	-7.98	NA	NA	82WE 2-378
378	158			$\text{CaMgFe}(\text{CN})_6$ from $\text{MgFe}(\text{CN})_6^{2-}$	*C	ai	-8.8	NA	NA	81WE 187
Summary data selected for reason 2										
378	168	A-1		$\text{CaMgFe}(\text{CN})_6$ from $\text{MgFe}(\text{CN})_6^{2-}$	*C	ai	-7.98	NA	NA	82WE 2-378
378	178			$\text{Ca}_2\text{MgFe}(\text{CN})_6$ from $\text{MgFe}(\text{CN})_6^{2-}$	*J	ai	-365.8	NA	NA	82WE 2-378
378	188			$\text{Ca}_2\text{MgFe}(\text{CN})_6$ from $\text{MgFe}(\text{CN})_6^{2-}$	!C	ai	-87.38	NA	NA	82WE 2-378
378	198			$\text{Ca}_2\text{MgFe}(\text{CN})_6$ from $\text{MgFe}(\text{CN})_6^{2-}$	*C	ai	-87.4	NA	NA	81WE 187
Summary data selected for reason 2										
378	208	A-1		$\text{Ca}_2\text{MgFe}(\text{CN})_6$ from $\text{MgFe}(\text{CN})_6^{2-}$	*C	ai	-87.38	NA	NA	82WE 2-378
378	218			$\text{CaCaFe}(\text{CN})_6$ from $\text{CaFe}(\text{CN})_6^{2-}$	*J	ai	-192.5	NA	NA	82WE 2-378
378	228			$\text{CaCaFe}(\text{CN})_6$ from $\text{CaFe}(\text{CN})_6^{2-}$	!C	ai	-31.67	NA	NA	82WE 2-378
378	238			$\text{CaCaFe}(\text{CN})_6$ from $\text{CaFe}(\text{CN})_6^{2-}$	*C	ai	-31.7	NA	NA	81WE 187
Summary data selected for reason 2										
378	248	A-1		$\text{CaCaFe}(\text{CN})_6$ from $\text{CaFe}(\text{CN})_6^{2-}$	*C	ai	-31.67	NA	NA	82WE 2-378
378	258			$\text{Ca}_2\text{CaFe}(\text{CN})_6$ from $\text{CaFe}(\text{CN})_6^{2-}$	*J	ai	-484.3	NA	NA	82WE 2-378
378	268			$\text{Ca}_2\text{CaFe}(\text{CN})_6$ from $\text{CaFe}(\text{CN})_6^{2-}$	!C	ai	-111.8	NA	NA	82WE 2-378
378	278			$\text{Ca}_2\text{CaFe}(\text{CN})_6$ from $\text{CaFe}(\text{CN})_6^{2-}$	*C	ai	-111.8	NA	NA	81WE 187

TABLE B.2. (contd)

MINTeq	In 82WE				Units	$\Delta H_f^\circ, 298$	$\Delta H_f^\circ, 298$	S_{298}°	
Number	Page ID	Form	Compound		Q State	(Q/mol)	(Q/mol)	(Q/mol·K)	Data Sources
Summary data selected for reason 1									
378	288	A-1	$\text{Ca}_2\text{CaFe}(\text{CN})_6$	from $\text{CaFe}(\text{CN})_6^{2-}$	!C ai	-111.0	NA	NA	82WE 2-378
378	298		$\text{CaSrFe}(\text{CN})_6$	from $\text{SrFe}(\text{CN})_6^-$	*J ai	-138.4	NA	NA	82WE 2-378
378	308		$\text{CaSrFe}(\text{CN})_6$	from $\text{SrFe}(\text{CN})_6^-$	!C ai	-33.88	NA	NA	82WE 2-378
378	318		$\text{CaSrFe}(\text{CN})_6$	from $\text{SrFe}(\text{CN})_6^-$	*C ai	-33.1	NA	NA	81WE 187
Summary data selected for reason 2									
378	328	A-1	$\text{CaSrFe}(\text{CN})_6$	from $\text{SrFe}(\text{CN})_6^-$	*C ai	-33.88	NA	NA	82WE 2-378

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APPENDIX C

COMPLETE SUMMARY FOR THERMODYNAMIC DATA OF ANTIMONY

APPENDIX C

COMPLETE SUMMARY FOR THERMODYNAMIC DATA OF ANTIMONY

The data tabulation follows the order of data presentation for compounds in the most complete reference for the thermodynamic data reviewed, i.e., the National Bureau of Standards publication by Wagman et al. (1982) (82WE). The order of data tabulation by element in Wagman et al. (1982) is shown in Table C.1, along with the MINTEQ number for the element. In addition, the page number where the element is first referenced in the thermodynamic tabulation for antimony, Table C.2, is included.

The thermodynamic data are listed in Table C.2. The column heading "Location In 82" refers to Wagman et al. (1982) [82WE]. Under this heading, the page number and order of presentation of antimony on the pages in 82WE are listed under the heading column "ID". This expansion of the numerical order facilitates the following:

- All data are listed or converted to units of kilocalorie because the database for MINTEQ is reported in units of kilocalorie
- Data reported in the units of kilojoule are listed on one line, and then the same data are listed on the following line in units of kilocalorie
- Additional data of up to nine lines from other sources can be inserted without disturbing the ID sequence
- An ID number is used for a summary line for each compound
- The MINTEQ identification number on the summary line for selected compounds to include in MINTEQ can be easily referenced to the citation in Wagman et al. (1982).

TABLE C.1. Data Tabulation by NBS Order Number of Elements

NBS Order No.	Element	MINTEQ Number	Data Start on page	NBS Order No.	Element	MINTEQ Number	Data Start on page
1	O	56		49	Tc	83	
2	H	33		50	Re	69	
3	He	34		51	Cr	21	
4	Ne	53		52	Mo	48	
5	Ar	5		53	W	91	
6	Kr	42		54	V	90	
7	Xe	92		55	Nb	51	
8	Rn	71		56	Ta	81	
9	F	27	C.11	57	Ti	86	C.22
10	Cl	18	C.12	58	Zr	96	
11	Br	13	C.13	59	Hf	35	
12	I	38	C.13	60	Sc	75	
13	At	7		61	Y	93	
14	S	73	C.14	62	Lu	45	
15	Se	76	C.15	63	Yb	94	
16	Te	84	C.16	64	Tm	88	
17	Po	63		65	Er	25	
18	N	49		66	Ho	37	
19	P	58		67	Dy	24	
20	As	6		68	Tb	82	
21	Sb	74	C.22	69	Gd	31	
22	Bi	12		70	Eu	26	
23	C	14		71	Sm	78	
24	Si	77		72	Pm	62	
25	Ge	32		73	Nd	52	
26	Sn	79		74	Pr	64	C.22
27	Pb	60	C.17	75	Ce	17	
28	B	9		76	La	43	C.22
29	Al	3	C.18	84	Cm	19	
30	Ga	30	C.17	85	Am	4	
31	In	39	C.17	86	Pu	66	
32	Tl	87		87	Np	55	
33	Zn	95	C.17	88	U	89	C.22
34	Cd	16	C.18	89	Pa	59	
35	Hg	36		90	Th	85	
36	Cu	23	C.19	91	Ac	1	
37	Ag	2	C.18	92	Be	11	
38	Au	8	C.19	93	Mg	46	C.23
39	Ni	54	C.20	94	Ca	15	C.24
40	Co	20	C.20	95	Sr	80	C.24
41	Fe	28	C.21	96	Ba	10	
42	Pd	61		97	Ra	67	
43	Rh	70		98	Li	44	C.24
44	Ru	72		99	Na	50	C.25
45	Pt	65		100	K	41	C.26
46	Ir	40		101	Rb	68	C.27
47	Os	57		102	Cs	22	C.28
48	Mn	47	C.21	103	Fr	29	

TABLE C.2. Complete Summary for Thermodynamic Data of Antimony(a)

MINTeq Number	Location		Form (b)	Compound	Energy (Q)		$\Delta G_{f,298}^{\circ}$ (Q/kcal)	$\Delta H_{f,298}^{\circ}$ (Q/kcal)	S_{298}° (Q/mol·K)	Data Sources(e)
	In 82WE	Page ID			Units	State				
					(c)	(d)				
79	78#		Sb(OH) ₃	equivalent to HSbO ₂ (ao)+H ₂ O(l)	+J	a ₀	-844.7	-773.6	116.3	82WE 2-79
79	79#		Sb(OH) ₃		!C	a ₀	-154.1	-184.9	27.6#	82WE 2-79
79	80#		Sb(OH) ₃	undissoc.; std. state, m=1	+C	a ₀	-154.1	-184.9	27.8	88WE 10#
79	81#		Sb(OH) ₃ ⁰	equivalent to HSbO ₂ (ao)+H ₂ O(l)	+C		-154.7	-184.9	38.8	74NR 19#

(a) Values indicated by "NA" are not available in the literature reviewed in this study.

(b) S = solid, A = aqueous. Additional codes under the general form for the compound include the following:

A-# and S-# indicate that the compound was selected for the MINTeq database, i.e.,

A-# for aqueous compounds selected, and S-# for solids selected;

A-1 and S-1 indicate that elements are not in the MINTeq database, or that "ai" and "aq" forms of aqueous solutions are not in the MINTeq database;

A-2 and S-2 indicate that ΔG is not available and hence cannot be included in the MINTeq database.

(c) "+C" = data reported in units of kcal; "+J" = data reported in units of joule; "!C" = data in units of kcal calculated from the "+J" data; i.e., !C = +J/4.184. The summary line for each chemical formulation is listed in units of kcal since the database for MINTeq is conventionally assembled in units of kcal. Approximate data listed by Bard et al. (1985) are enclosed in parentheses.

(d) Symbols used in the table for physical states follow the convention of Wagman et al. (1982). Symbols used in earlier NBS reports are listed after those in Wagman et al. (1982).

ai, a = aqueous solution, ionized substance standard, m = 1 mol/kg.

a₀ = aqueous solution, un-ionized substance, standard state, m = 1 mol/kg, or an ion for which here no further ionization is considered.

aq, au = aqueous solution, concentration unspecified - Such solutions may be assumed to be "dilute".

cr = crystalline solid - The symbols above occasionally are modified by number to distinguish two substances in the same state: a numeral is appended to the physical state designation, e.g., cr2, cr3, etc. A more general designation is i2, i3, etc.

(e) The reference code lists in order

1) the last two digits of the year when the reference was published,

2) the first letter of the surnames of the first two authors listed for the reference, and

3) the page number in the reference on which the data is listed.

A secondary source of the data is provided in parentheses, which uses the data in the first reference. The number of significant figures in the data listed in this table is taken from the first reference. Semicolons separate additional references (as well as multiple references for $\Delta G_{f,298}^{\circ}$, $\Delta H_{f,298}^{\circ}$, and S_{298}°).

TABLE C.2. (contd)

MINTeq Number	in 82WE Page ID Form	Compound	Units Q State	ΔG_f° (Q/mol)	ΔH_f° (Q/mol)	S° (Q/mol-K)	Data Sources
Summary data selected for reasons 3 and 4, equivalent to $\text{HSbO}_2(\text{aq}) + \text{H}_2\text{O}(\text{l})$ (a)							
79 820	A-8	$\text{Sb}(\text{OH})_3^{\circ}$	MINTeq component Sb (III) +C a ₀	-164.1	-184.9	27.8	82WE 2-79 (88WE 188)748
79 821	A-8	$\text{Sb}(\text{OH})_3^{\circ}$	Basis species for the +3 valence state of Sb				
79 822	A-8	748 $\text{Sb}(\text{OH})_3^{\circ}$					
79 928		$\text{Sb}(\text{OH})_6^-$	+J a ₀	-1188.7	NA	NA	87PD 7 (76BM)
79 935		$\text{Sb}(\text{OH})_6^-$	+C a ₀	-284.11	NA	NA	87PD 7 (76BM)
79 931		$\text{Sb}(\text{OH})_6^-$	+C a ₀	-288.76	NA	NA	88SC (76BM)
Summary data selected for reason 4. Value from 76PD could not be reproduced. The value calculated in this report, from 76BM is -288.76. (Appendix I)							
79 948	A-8	$\text{Sb}(\text{OH})_6^-$	+C a ₀	-288.76	NA	NA	88SC 7 (76BM)
741	79 941	A-8 $\text{Sb}(\text{OH})_6^-$	Basis species for the +5 valence state of Sb				
7487418	79 942	A-8 $\text{Sb}(\text{OH})_3^{\circ} + 3\text{H}_2\text{O} \leftrightarrow \text{Sb}(\text{OH})_6^- + 3\text{H}^+ + 2\text{e}^-$	Redox reaction				
79 943	A-8	7487418 $\text{Sb}(\text{OH})_6^-/\text{Sb}(\text{OH})_3^{\circ}$					
79 944		5 1.888 748 3.888 842 -2.888 881 -3.888 338 -1888 741					45.18 81VQ

(a) Summary line selected to represent the data listed in the prior lines for this compound.

The reasons used to select the data included in the summary line follow:

1. After change of energy units, the significant figures for data in 82WE are the same as earlier NBS publications.
2. Significant figures for data taken from earlier NBS document, or other document, with energy units reported in kcal.
3. Data in NBS documentation selected as commonly accepted value.
4. Only data found.
5. Errata revision from earlier National Bureau of Standards publication.
6. More recent documentation than Wagman et al. (1982), or other early documentation.

There are three additional summary lines for each compound that is selected for the MINTeq database.

First line: Chemical reaction selected to represent the formation of the compound.

Second line: Number selected for MINTeq followed by the chemical compound.

Third line: The first number in the compound column represents the number of basis species used. This is followed by several groups of paired entries that represent the contribution from each basis species. In each group, the first entry is the number of basis species required; the second entry is the identification number used to represent the basis species.

TABLE C.2. (contd)

WINTER Number	in 82WE Page ID Form	Compound	Units Q State	ΔG_f° (Q/mol)	ΔH_f° (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
	79 10	Sb III	*J cr	0.0	0.0	45.69	82WE 2-79
	79 20	Sb III	!C cr	0.0	0.0	10.92	82WE 2-79
	79 30	Sb III	*C cr	0.0	0.0	10.92	88WE 99
	79 40	Sb	*C	0.0	0.0	10.26	81VG 916
	79 50	Sb	*C cr			10.92	74NR 49
	79 60	Sb	*C cr			10.9	78BS 79
							from NBS docs.
Summary data selected for reason 1							
	79 70 S-0	Sb III	!C cr	0.0	0.0	10.92	82WE 2-79
0074001	79 71 S-0	$\text{Sb}(\text{OH})_3^- + 3\text{H}^+ + 3\text{e}^- \leftrightarrow \text{Sb} + 3\text{H}_2\text{O}$					
	79 72 S-0	0074001 Sb					
	79 73	4 1.000 740 3.000 330 3.000 1 -3.000 2					
	79 80	SbO^+	*J a ₀	-177.11	NA	NA	82WE 2-79
	79 90	SbO^+	!C a ₀	-42.330	NA	NA	82WE 2-79
	79 100	SbO^+ std. state, n = 1	*C a _q	-42.33	NA	NA	88WE 99
	79 111	SbO^+	*C	-42.0	NA	NA	74P 525
	79 110	SbO^+	*J	-175.64	-193.7	22.33	85BP 173
	79 120	SbO^+	!C	-41.979	-46.30	5.34	85BP 173
Summary data selected for reasons 4 and 6							
	79 130 A-0	SbO^+	!C a ₀	-41.979	-46.30	5.34	85BP 173 (82WE 2-79)
7403300	79 131 A-0	$\text{Sb}(\text{OH})_3^0 + \text{H}^+ \leftrightarrow \text{SbO}^+ + 2\text{H}_2\text{O}$					
	79 132 A-0	7403300 SbO^+					
	79 133	3 1.000 740 1.000 330 -2.000 2					
	79 140	SbO_2	*C cr	-100.2	-113.5	15.2	78BS 79 from 71CR
Summary data selected for reason 4							
	79 150 S-0	SbO_2	*C cr	-100.2	-113.5	15.2	78BS 79 from 71CR
2074102	79 151 S-0	$\text{Sb}(\text{OH})_6^- + \text{e}^- + 2\text{H}^+ \leftrightarrow \text{SbO}_2 + 4\text{H}_2\text{O}$					
	79 152 S-0	2074102 SbO_2					
	79 153	4 1.000 741 1.000 1 2.000 330 -4.000 2					
	79 160	SbO_2^+	*C a _q	-65.50	NA	NA	74P 525

TABLE C.2. (contd)

MINTeq Number	in 82WE Page ID Form	Compound	Units Q State	ΔG_f° (Q/mol)	ΔH_f° (Q/mol)	S° (Q/mol·K)	Data Sources
Summary data selected for reason 4							
79	170 A-0	SbO_2^+	*C aq	-85.50	NA	NA	74P 525 (86IN 40)
7413300	79 171 A-0	$\text{Sb(OH)}_6^- + 2\text{H}^+ \leftrightarrow \text{SbO}_2^+ + 4\text{H}_2\text{O}$					
79	172 A-0	7413300 SbO_2^+					
79	180	SbO_2^-	*J aq	-340.19	NA	NA	82WE 2-79
79	190	SbO_2^-	!C aq	-81.307	NA	NA	82WE 2-79
79	200	SbO_2^- std. state, m = 1	*C aq	-81.32	NA	NA	88WE 90
79	201	SbO_2^-	*C aq	-82.5	NA	NA	74P 525 (86IN 40)
79	210	SbO_2^-	*J	-339.74	-417.6	55.2	85BP 173 from NBS docs.
79	220	SbO_2^-	!C	-81.20	-99.81	13.2	85BP 173 from NBS docs.
Summary data selected for reasons 8 and 4							
79	230 A-0	SbO_2^-	!C aq	-81.31	-99.81	13.2	85BP 173 (82WE 2-79)
7403301	79 231 A-0	$\text{Sb(OH)}_3^0 \leftrightarrow \text{SbO}_2^- + \text{H}_2\text{O} + \text{H}^+$					
79	232 A-0	7403301 SbO_2^-					
79	233	3 1.000 740 -1.000 2 -1.000 330					
79	240	SbO_3^-	*C aq	-122.93	NA	NA	74P 525 (86IN 40)
Summary data selected for reason 4							
79	250 A-0	SbO_3^-	*C aq	-122.93	NA	NA	74P 525 (86IN 40)
7410021	79 251 A-0	$\text{Sb(OH)}_6^- \leftrightarrow \text{SbO}_3^- + 3\text{H}_2\text{O}$					
79	252 A-0	7410021 SbO_3^-					
79	253	2 1.000 741 -3.000 2					

TABLE C.2. (contd)

WINTER Number	in 82WE			Units		ΔG_f° (Q/mol)	ΔH_f° (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
	Page	ID	Form	Compound	Q State				
	79	268	Sb ₂ O ₃	oxide, tri-	*J aq	NA	-689.9	NA	82WE 2-79
	79	278	Sb ₂ O ₃		!C aq	NA	-164.9	NA	82WE 2-79
	79	288	Sb ₂ O ₃		*C aq	NA	-164.9	NA	88WE 99
Summary data selected for reason 1									
	79	298	A-2	Sb ₂ O ₃	!C aq	NA	-164.9	NA	82WE 2-79
	79	291	Sb ₂ O ₃		*C	-149.83	NA	NA	76SM -12
	79	292	Sb ₂ O ₃		*C	-149.896	NA	NA	76EM -375
	79	308	Sb ₂ O ₃	valentinite	*J	-826.3	-788.8	123.	79RH 21
	79	318	Sb ₂ O ₃	valentinite	!C	-149.7	-169.4	29.4	79RH 21
	79	328	Sb ₂ O ₃	valentinite	*C cr	-151.8	-169.4	33.71	74NR 58
	79	338	Sb ₂ O ₃	valentinite	*C cr	-147.8	NA	NA	74P 525
	79	348	Sb ₂ O ₃		*C cr	-149.7	-169.4	29.4	78BS 79
									from 71CR
	79	358	Sb ₂ O ₃	orthorhombic	*C cr	-149.75	NA	NA	86IN 48
									from NBS docs.
Summary data selected for reason 6									
	79	368	S-8	Sb ₂ O ₃ valentinite, orthorhombic	*C cr	-149.7	-169.4	29.4	79RH 21
2874887	79	381	S-8	2Sb(OH) ₃ ⁰ ↔ Sb ₂ O ₃ + 3H ₂ O valentinite, orthorhombic					
	79	382	S-8	2874887 Sb ₂ O ₃ was 2874888 in 87P0					
	79	383		2 2.888 748 -3.888 2					
	79	378	Sb ₂ O ₃	senarmontite	*C cr	-153.2	-172.18	31.65	74NR 58
	79	371	Sb ₂ O ₃	senarmontite	*C cr	-149.8	NA	NA	74P 525
	79	372	Sb ₂ O ₃	cubic	*C cr	-155.55	NA	NA	86IN 48
									from NBS docs.
Summary data selected for reasons 3 and 4. Cubic, dimorphous with valentinite. No NBS data.									
	79	373	Sb ₂ O ₃	senarmontite, cubic	*C cr	-155.	-172.18	31.65	74NR 58
2874888	79	375	S-8	2Sb(OH) ₃ ⁰ ↔ Sb ₂ O ₃ + 3H ₂ O senarmontite, cubic					
	79	376	S-8	2874888 Sb ₂ O ₃					
	79	377		2 2.888 748 -3.888 2					
	79	388	Sb ₂ O ₄	oxide, tetra-	*J cr	-754.52	-888.55	NA	87 PS
	79	381	Sb ₂ O ₄	oxide, tetra-	*C cr	-188.34	-218.46	NA	87 PS
	79	382	Sb ₂ O ₄	oxide, tetra-	*J cr	-795.7	-987.5	127.2	82WE 2-79
	79	398	Sb ₂ O ₄	oxide, tetra-	!C cr	-198.1	-218.9	38.48	82WE 2-79
	79	488	Sb ₂ O ₄	oxide, tetra-	*C cr	-198.1	-218.9	38.4	88WE 99

TABLE C.2. (contd)

MINTeq Number	in 82WE Page ID Form	Compound	Units Q State	ΔG_f° (Q/mol)	ΔH_f° (Q/mol)	S° (Q/mol·K)	Data Sources
79 410	Sb ₂ O ₄	oxide, tetra-	*C cr	-198.2	-218.9	38.4	78BS 79 from NBS docs.
79 411	Sb ₂ O ₄	anhydrous orthorhombic	*C cr	-185.9	NA	NA	74P 525
Summary data selected for reasons 2 and 3							
79 420	Sb ₂ O ₄	oxide, tetra-	*C cr	-198.1	-218.9	38.4	82WE 2-79
2874881	79 422 S-8	2Sb(OH) ₃ ⁰ ↔ Sb ₂ O ₄ + 2H ₂ O + 2H ⁺ + 2e ⁻	oxide, tetra-				
79 423 S-8	2874881	Sb ₂ O ₄					
79 424	4	2.888 748	-2.888 2	-2.888 338	-2.888	1	
79 438	Sb ₂ O ₅	oxide, pent-	*J cr	-829.2	-971.9	125.1	82WE 2-79
79 448	Sb ₂ O ₅		!C cr	-198.2	-232.3	29.98	82WE 2-79
79 458	Sb ₂ O ₅		*C cr	-198.2	-232.3	29.9	88WE 99
79 468	Sb ₂ O ₅		*C cr	-198.2	-232.3	29.9	78BS 79 from NBS docs.
79 481	Sb ₂ O ₅		*C cr	-288.83	-248.8	29.91	74NR 58
79 482	Sb ₂ O ₅	anhydrous, cubic	*C cr	-288.5	NA	NA	74P 525
Summary data selected for reasons 2 and 3							
79 478 S-8	Sb ₂ O ₅		*C cr	-198.2	-232.3	29.9	82WE 2-79
2874188	79 471 S-8	2Sb(OH) ₅ ⁻ + 2H ⁺ ↔ Sb ₂ O ₅ + 7H ₂ O					
79 472 S-8	2874188	Sb ₂ O ₅					
79 473	3	2.888 741	2.888 338	-7.888	2		
79 498	Sb ₂ O ₅		*J aq	NA	-958.9	NA	82WE 2-79
79 588	Sb ₂ O ₅		!C aq	NA	-228.7	NA	82WE 2-79
Summary data selected for reason 4							
79 518 A-2	Sb ₂ O ₅		!C aq	NA	-228.7	NA	82WE 2-79
79 548	Sb ₄ O ₈	II, cubic	*J cr	-1288.1	-1448.8	228.9	82WE 2-79
79 558	Sb ₄ O ₈	II, cubic	!C cr	-383.88	-344.31	52.88	82WE 2-79
79 588	Sb ₄ O ₈	II, cubic	*C cr	-383.1	-344.3	52.8	88WE 99
79 578	Sb ₄ O ₈	II, cubic	*J	-1284.4	-1423.2	285.3	85BP 173
79 588	Sb ₄ O ₈	II, cubic	!C	-382.28	-348.15	83.41	85BP 173
Summary data selected for reason 8							
79 598 S-8	Sb ₄ O ₈	II, cubic	!C cr	-383.88	-344.31	52.88	82WE 2-79

TABLE C.2. (contd)

MINTeq Number	in 82WE Page ID Form	Compound	Units q State	ΔG_f° (Q/mol)	ΔH_f° (Q/mol)	S° (Q/mol-K)	Data Sources
2074002	79 591 S-0	$4\text{Sb}(\text{OH})_3^{\circ} \leftrightarrow \text{Sb}_4\text{O}_6 + 6\text{H}_2\text{O}$	II, cubic				
	79 592 S-0	2074002 Sb_4O_6	II, cubic				
	79 593	2 4.000 740 -6.000	2				
	79 600	Sb_4O_6	I, orthorhombic	*J cr	-1263.0	-1417.1	246.0 82WE 2-79
	79 610	Sb_4O_6	I, orthorhombic	!C cr	-299.5	-338.70	58.80 82WE 2-79
	79 620	Sb_4O_6	I, orthorhombic	*C cr	-299.5	-338.7	58.8 68WE 100
	79 630	Sb_4O_6	I, orthorhombic	*J	-1249.34	-1403.15	282.0 85BP 173
	79 640	Sb_4O_6	I, orthorhombic	!C	-298.60	-335.96	67.40 85BP 173
Summary data selected for reason 8							
	79 650 S-0	Sb_4O_6	I, orthorhombic	!C cr	-299.5	-338.70	58.8 82WE 2-79
2074003	79 651 S-0	$4\text{Sb}(\text{OH})_3^{\circ} \leftrightarrow \text{Sb}_4\text{O}_6 + 6\text{H}_2\text{O}$	I, orthorhombic				
	79 652 S-0	2074003 Sb_4O_6	I, orthorhombic				
	79 653	2 4.000 740 -6.000	2				
	79 660	Sb_6O_{13}		*J cr	NA	-2885.8	NA 82WE 2-79
	79 670	Sb_6O_{13}		!C cr	NA	-870.60	NA 82WE 2-79
	79 680	Sb_6O_{13}		*C cr	NA	-870.6	68WE 100
Summary data selected for reason 2							
	79 690 S-2	Sb_6O_{13}		*C cr	NA	-870.6	NA 82WE 2-79
	79 700	HSbO_2		*J a ₀	-487.5	-487.9	46.4 82WE 2-79
	79 710	HSbO_2		!C a ₀	-97.40	-116.6	11.1 82WE 2-79
	79 711	HSbO_2		*C a ₀	-97.5	NA	NA 74P 525
Summary data selected for reasons 3 and 4							
	79 720 A-0	HSbO_2		!C a ₀	-97.40	-116.6	11.1 82WE 2-79
7400021	79 721 A-0	$\text{Sb}(\text{OH})_3 \leftrightarrow \text{HSbO}_2 + \text{H}_2\text{O}$					
	79 722 A-0	7400021 HSbO_2					
	79 723	2 1.000 740 -1.000	2				
	79 730	$\text{Sb}(\text{OH})_3$		*J cr	-885.2	NA	NA 82WE 2-79
	79 740	$\text{Sb}(\text{OH})_3$		!C cr	-163.8	NA	NA 82WE 2-79
	79 750	$\text{Sb}(\text{OH})_3$		*C cr	-163.8	NA	NA 68WE 100
	79 760	$\text{Sb}(\text{OH})_3$		*C cr	-160.7	-192.1	25.8 74NR 60

TABLE C.2. (contd)

MINTEQA	in 82WE		Units		ΔG_f°	ΔH_f°	S_{298}°	
Number	Page ID	Form	Compound	Q State	(Q/mol)	(Q/mol)	(Q/mol·K)	Data Sources
Summary data selected for reasons 3 and 4								
79	770	S-0	Sb(OH) ₃	*C cr	-183.8	-192.1	calc	82WE 2-79; 74NR 86
2874004	79	771 S-0	Sb(OH) ₃ ⁰ ↔ Sb(OH) ₃ (s)					
	79	772 S-0	2874004 Sb(OH) ₃ (s)					
	79	773	1 1.000 740					
	79	774	Sb(OH) ₂ ⁺	*C aq	-99.333	NA	NA	76BM -375
	79	775	Sb(OH) ₂ ⁺	*C	-99.847	NA	NA	76SM -12
	79	830	Sb(OH) ₂ ⁺	*C	-99.8	NA	NA	74NR 190
Summary data selected for reason 4								
	79	840 A-0	Sb(OH) ₂ ⁺	*C	-99.3	NA	NA	76BM -375
7403302	79	841 A-0	Sb(OH) ₃ ⁰ + H ⁺ ↔ Sb(OH) ₂ ⁺ + H ₂ O					
	79	841 A-0	3 1.000 740 1.000 330 -1.000 002					
	79	842 A-0	7403302 Sb(OH) ₂ ⁺					
	79	850	Sb(OH) ₄ ⁻	*C aq	-194.868	NA	NA	76BM -375
	79	850	Sb(OH) ₄ ⁻	*C aq	-194.895	NA	NA	76SM -12
	79	850	Sb(OH) ₄ ⁻	*J aq	-813.20	-989.80	190.4	85BP 174
	79	860	Sb(OH) ₄ ⁻	!C aq	-194.36	-238.52	45.51	85BP 174
	79	870	Sb(OH) ₄ ⁻	*C	-195.3	NA	NA	74NR 190
Summary data selected for reason 4								
	79	880 A-0	Sb(OH) ₄ ⁻	!C aq	-194.36	-238.52	45.51	85BP 174
7400020	79	881 A-0	Sb(OH) ₃ ⁰ + H ₂ O ↔ Sb(OH) ₄ ⁻ + H ⁺					
	79	882 A-0	7400020 Sb(OH) ₄ ⁻					
	79	883	3 1.000 740 1.000 2 -1.000 330					
	79	890	Sb(OH) ₅ ⁰	*C aq	-235.76	NA	NA	76BM -375
	79	891	Sb(OH) ₅ ⁰	*C aq	-235.76	NA	NA	76SM -133

TABLE C.2. (contd)

MINTeq Number	in 82WE Page ID	Form	Compound	Units Q State	ΔG_f° (Q/mol)	ΔH_f° (Q/mol)	S° (Q/mol·K)	Data Sources
Summary data selected for reason 4								
79 892			$\text{Sb}(\text{OH})_5^\circ$	C aq	-235.78	NA	NA	78SM 133
7418828	79 893		$\text{Sb}(\text{OH})_6^- + \text{H}^+ \rightarrow \text{Sb}(\text{OH})_5^\circ + \text{H}_2\text{O}$					
79 894		3	1.000 741	1.000 336	-1.000 882			
79 958			H_3SbO_4	*J aq	NA	-987.1	NA	82WE 2-79
79 968			H_3SbO_4	!C aq	NA	-218.8	NA	82WE 2-79
79 978			H_3SbO_4	*C aq	NA	-218.8	NA	88WE 188
79 988			H_3SbO_4	*C	NA	-218.8	NA	74NR 198
Summary data selected for reason 1								
79 998 A-2			H_3SbO_4	!C aq	NA	-218.8	NA	82WE 2-79
79 1008			$\text{HSb}(\text{OH})_6$	*J aq	NA	-1478.6	NA	82WE 2-79
79 1018			$\text{HSb}(\text{OH})_6$	!C aq	NA	-353.39	NA	82WE 2-79
79 1028			$\text{HSb}(\text{OH})_6$	*C aq	NA	-353.4	NA	88WE 188
Summary data selected for reason 2								
79 1038 A-2			$\text{HSb}(\text{OH})_6$	*C aq	NA	-353.39	NA	82WE 2-79
79 1048			SbF_3 fluoride, tri-	*J cr	NA	-915.5	NA	82WE 2-79
79 1058			SbF_3	!C cr	NA	-218.8	NA	82WE 2-79
79 1068			SbF_3	*C cr	NA	-218.8	NA	88WE 188
79 1078			SbF_3	*J c	-838.	-915.5	185.4	85BP 174
79 1088			SbF_3	!C c	-288.	-218.8	25.19	85BP 174
Summary data selected for reasons 1 and 4								
79 1098			SbF_3 fluoride, tri-	!C cr	-288.	-218.8	25.19	85BP 174
4274888	79 1092 S-8		$\text{Sb}(\text{OH})_3^\circ + 3\text{H}^+ + 3\text{F}^- \leftrightarrow \text{SbF}_3 + 3\text{H}_2\text{O}$					
79 1093 S-8			4274888 SbF_3					
79 1094		4	1.000 748	3.000 338	3.000 278	-3.000	2	
79 1108			SbF_3 in 288 H_2O	*J aq	NA	-918.9	NA	82WE 2-79
79 1128			SbF_3	!C	NA	-217.7	NA	82WE 2-79
79 1121			SbF_3	*J aq	NA	-918.9	NA	85BP 1749
79 1121			SbF_3	*C aq	NA	-217.7	NA	85BP 1749
79 1138			SbF_3 in 288 H_2O	*C	NA	-217.7	NA	88WE 188

TABLE C.2. (contd)

MINTEQA	in 82WE			Units	ΔG_f°	ΔH_f°	S°	
Number	Page ID	Form	Compound	Q State	(Q/mol)	(Q/mol)	(Q/mol·K)	Data Sources
Summary data selected for reason 1								
	79 1140 A-2	SbF ₃	in 200 H ₂ O	!C aq	NA	-217.7	NA	82WE 2-79
	79 1150	SbOF undiss.		*J a ₀	-487.4	NA	NA	82WE 2-79
	79 1160	SbOF		!C a ₀	-116.5	NA	NA	82WE 2-79
Summary data selected for reason 4								
	79 1170 A-0	SbOF ₀ undiss.		!C a ₀	-116.5	NA	NA	82WE 2-79
7402700	79 1171 A-0	$\text{Sb(OH)}_3^0 + \text{F}^- + \text{H}^+ \leftrightarrow \text{SbOF}^0 + 2\text{H}_2\text{O}$						
	79 1172 A-0	7402700 SbOF ⁰						
	79 1173	4	1.000 740	1.000 270	1.000 330	-2.000	2	
	79 1180	H ₃ SbF ₆		*J aq	NA	-1876.1	NA	82WE 2-79
	79 1190	H ₃ SbF ₆		!C aq	NA	-448.40	NA	82WE 2-79
Summary data selected for reason 4								
	79 1200 A-2	H ₃ SbF ₆		!C aq	NA	-448.40	NA	82WE 2-79
	79 1210	Sb(OH) ₂ F		*J a ₀	-724.6	NA	NA	82WE 2-79
	79 1220	Sb(OH) ₂ F		!C a ₀	-173.2	NA	NA	82WE 2-79
	79 1230	Sb(OH) ₂ F undissoc.; std state, m=1		*C aq	-173.2	NA	NA	68WE 100
Summary data selected for reason 1								
	79 1240 A-0	Sb(OH) ₂ F ⁰		!C a ₀	-173.2	NA	NA	82WE 2-79
7402702	79 1241 A-0	$\text{Sb(OH)}_3^0 + \text{F}^- + \text{H}^+ \leftrightarrow \text{Sb(OH)}_2\text{F}^0 + \text{H}_2\text{O}$						
	79 1242 A-0	7402702 Sb(OH) ₂ F ⁰						
	79 1243	4	1.000 740	1.000 270	1.000 330	-1.000	2	
	79 1250	SbCl ₃	chloride, tri-	*J cr	-323.67	-382.17	184.1	82WE 2-79
	79 1260	SbCl ₃		!C cr	-77.359	-91.341	44.00	82WE 2-79
	79 1270	SbCl ₃		*C cr	-77.36	-91.34	44.0	68WE 100
	79 1280	SbCl ₃		*C cr	-77.37	-91.34	44.0	74MR 54
	79 1281	SbCl ₃ (C,L,G) Melt Pt 730C BP 2200C		*C cr	-77.4	-91.3	44.0	78BS 79 from NBS docs.
Summary data selected for reason 2								
	79 1290 S-0	SbCl ₃	chloride, tri-	*C cr	-77.36	-91.34	44.0	82WE 2-79
4174000	79 1291 S-0	$\text{Sb(OH)}_3^0 + 3\text{H}^+ + 3\text{Cl}^- \leftrightarrow \text{SbCl}_3 + 3\text{H}_2\text{O}$						
	79 1292 S-0	4174000 SbCl ₃						

TABLE C.2. (contd)

MINTEQA Number	in 82WE Page ID Form	Compound	Units Q State	ΔG_f° (Q/mol)	ΔH_f° (Q/mol)	S° (Q/mol·K)	Data Sources
79 1293	4	1.000 746	3.000 180	3.000 330	-3.000	2	
79 1300	SbCl ₄ ⁻		*J aq	-471.79	-552.0	288.0	84VS 1643
79 1310	SbCl ₄ ⁻		*C	-112.76	-131.9	88.83	84VS 1643
79 1320	SbCl ₄ ⁻		*C	-113.73	NA	NA	74NR 190
Summary data selected for reasons 4 and 6							
79 1330 A-1	SbCl ₄ ⁻		*C aq	-112.76	-131.9	88.83	84VS 1643
79 1340	SbOCl		*J cr	NA	-374.0	NA	82WE 2-79
79 1350	SbOCl		IC cr	NA	-89.39	NA	82WE 2-79
79 1360	SbOCl		*C cr	NA	-89.4	NA	88WE 101
79 1370	SbOCl		*C cr	NA	-89.4	NA	74NR 54
Summary data selected for reason 2							
79 1380 S-2	SbOCl		*C cr	NA	-89.39	NA	82WE 2-79
79 1390	Sb ₄ O ₅ Cl ₂	III oxychloride (ous)	*J cr	NA	-1451.4	NA	82WE 2-79
79 1400	Sb ₄ O ₅ Cl ₂		IC cr	NA	-346.89	NA	82WE 2-79
79 1410	Sb ₄ O ₅ Cl ₂		*C cr	NA	-346.9	NA	88WE 101
Summary data selected for reason 2							
79 1420 S-2	Sb ₄ O ₅ Cl ₂	III oxychloride (ous)	*C cr	NA	-346.89	NA	82WE 2-79
79 1430	SbBr ₃		*J cr	-239.3	-259.4	207.1	82WE 2-79
79 1440	SbBr ₃		IC cr	-57.19	-82.00	49.50	82WE 2-79
79 1450	SbBr ₃		*C cr	-57.2	-82.0	49.5	88WE 101
79 1460	SbBr ₃		*C cr	-57.2	-82.0	49.5	74NR 55
79 1470	SbBr ₃ (C,L,G) Melt Pt 95°C BP 289°C		*C cr	-57.2	-82.0	49.5	70BS 79 from NBS docs.
Summary data selected for reason 2							
79 1500 S-0	SbBr ₃		*C cr	-57.19	-82.0	49.5	82WE 2-79
4074000	79 1501 S-0	Sb(OH) ₃ ⁰ + 3H ⁺ + 3Br ⁻ ↔ SbBr ₃ + 3H ₂ O					
79 1502 S-0	4074000	SbBr ₃					
79 1503	4	1.000 746	3.000 130	3.000 330	-3.000	2	
79 1504	SbI ₃		*J cr	NA	-100	213.	85AP
79 1505	SbI ₃		*C cr	NA	24	50.6	85AP
79 1510	SbI ₃	iodide, tri-	*J cr	NA	-100.4	NA	82WE 2-79
79 1520	SbI ₃		IC cr	NA	-24.00	NA	82WE 2-79
79 1530	SbI ₃	ΔH_f° , 298 from NBS docs.	*J c	-94.	-100.4	(212).*	85BP 175

TABLE C.2. (contd)

MINTED Number	in 82WE Page ID	Form	Compound	Units Q State	ΔG_f° (Q/mol)	ΔH_f° (Q/mol)	S° (Q/mol·K)	Data Sources
	79 1540		SbI ₃	!C c	-22.	-24.00	(50.7)*	85BP 175
	79 1490		SbI ₃ (C,L,G) Melt Pt 730C	*C cr	-22.7	-23.0	51.5	78BS 79 from NBS docs.
Summary data selected for reasons 2 and 4					*(approximate data listed by 85BP in parentheses)			
	79 1550		SbI ₃	!C cr	-22.	-24.0	51.5	85BP 175 (82WE 2-79)
4374000	79 1552 S-0		$\text{Sb}(\text{OH})_3^{\circ} + 3\text{H}^+ + 3\text{I}^- \leftrightarrow \text{SbI}_3 + 3\text{H}_2\text{O}$					
	79 1553 S-0		4374000 SbI ₃					
	79 1554	4	1.000 740	3.000 330	3.000 300	-3.000	2	
	79 1560		SbI ₃	*J aq	NA	-98.7	NA	82WE 2-79
	79 1570		SbI ₃	!C aq	NA	-23.6	NA	82WE 2-79
	79 1580		SbI ₃	*C aq	NA	-23.6	NA	88WE 101
Summary data selected for reason 1								
	79 1600 A-1		SbI ₃	!C aq	NA	-23.6	NA	82WE 2-79
				*C	-33.005	NA	NA	78SM -77
	79 1610		Sb ₂ S ₃ stibnite	*J	-173.6	-174.9	102.	79RH 17
	79 1620		Sb ₂ S ₃ black	*J cr	-173.6	-174.9	102.0	82WE 2-79
	79 1630		Sb ₂ S ₃ stibnite	*C cr	-37.30	-37.7	43.5	74NR 02
	79 1640		Sb ₂ S ₃ stibnite	!C	-41.49	-41.80	43.5	79RH 17
	79 1650		Sb ₂ S ₃ black	!C cr	-41.49	-41.80	43.50	82WE 2-79
	79 1660		Sb ₂ S ₃ black	*C cr	-41.5	-41.8	43.5	88WE 101
	79 1670		Sb ₂ S ₃	*C cr	-41.5	NA	NA	86IN 40 from NBS docs.
	79 1680		Sb ₂ S ₃	*C cr	-89.9	-87.8	43.5	78BS 79 from NBS docs.
Summary data selected for reason 2								
	79 1690		Sb ₂ S ₃ black, stibnite	*C cr	-41.49	-41.80	43.50	82WE 2-79
1074000	79 1692 S-0		$2\text{Sb}(\text{OH})_3^{\circ} + 3\text{HS}^- + 3\text{H}^+ \leftrightarrow \text{Sb}_2\text{S}_3 + 6\text{H}_2\text{O}$					
	79 1693 S-0		1074000 Sb ₂ S ₃					
	79 1694	4	2.000 740	3.000 730	3.000 330	-6.000	2	
	79 1700		Sb ₂ S ₃ orange, amorphous	*J am	NA	-147.3	NA	82WE 2-79
	79 1710		Sb ₂ S ₃ orange, amorphous	!C	NA	-35.21	NA	82WE 2-79
	79 1720		Sb ₂ S ₃ amorphous	*C cr		-30.2		74NR 02
	79 1730		Sb ₂ S ₃ orange, amorphous	*C	NA	-35.2	NA	88WE 101

TABLE C.2. (contd)

WINTER Number	in 82WE Page ID	Form	Compound	Units Q State	ΔG_f° (Q/mol)	ΔH_f° (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
Summary data selected for reasons 2 and 3								
79 1748	S-2	Sb ₂ S ₃	orange, amorphous	*C cr	NA	-35.2	NA	68WE 161 (82WE 2-79)
79 1758		SbS ₃ ²⁻	orange, amorphous	*C aq	-68.4	-58.8	188.8	78BS from 52L
Summary data selected for reason 4								
79 1768	A-1	SbS ₃ ²⁻		*C aq	-68.4	-58.8	188.8	78BS from 52L
88 18		Sb ₂ S ₄ ²⁻		*J a ₀	-99.5	-219.2	-52.3	82WE 2-88
88 28		Sb ₂ S ₄ ²⁻		!C a ₀	-23.8	-52.39	-12.5	82WE 2-88
88 38		Sb ₂ S ₄ ²⁻	std. state, n = 1	*C a ₀	-23.8	-52.4	-12.5	68WE 161
88 48		Sb ₂ S ₄ ²⁻		*C aq	-23.8	NA	NA	88IN 48 from NBS docs.
88 58		Sb ₂ S ₄ ²⁻		*C aq	-61.7*	-113.8*	-2.5*	78BS 79 from NBS docs.
Summary data selected for reason 2 *(refers to NBS publications, NBS sources used in this table)								
88 68		Sb ₂ S ₄ ²⁻	std. state, n = 1	*C a ₀	-23.8	-52.39	-12.5	82WE 2-88
7487388	88 62	A-8	$2\text{Sb}(\text{OH})_3^0 + 4\text{HS}^- + 2\text{H}^+ \leftrightarrow \text{Sb}_2\text{S}_4^{2-} + 6\text{H}_2\text{O}$					
88 63	A-8	7487388	Sb ₂ S ₄ ²⁻					
88 64		4	2.888 748	4.888 738	2.888 338	-6.888	2	
88 78		Sb ₂ (SO ₄) ₃	III sulfate	*J cr	NA	-2482.5	NA	82WE 2-88
88 88		Sb ₂ (SO ₄) ₃		!C cr	NA	-574.21	NA	82WE 2-88
88 98		Sb ₂ (SO ₄) ₃		*C cr	NA	-574.2	NA	68WE 161
88 108		Sb ₂ (SO ₄) ₃		*C cr	NA	-574.2	NA	74NR 67
Summary data selected for reason 2								
88 118	S-2	Sb ₂ (SO ₄) ₃	III sulfate	*C cr	NA	-574.21	NA	82WE 2-88
88 128		Sb ₂ Se ₃		*C cr	-29.8	-38.5	47.1	74NR 63
Summary data selected for reason 4								
88 138	S-8	Sb ₂ Se ₃		*C cr	-29.8	-38.5	47.1	74NR 63
1274888	88 131	S-8	$2\text{Sb}(\text{OH})_3^0 + 3\text{HS}^- + 3\text{H}^+ \leftrightarrow \text{Sb}_2\text{Se}_3 + 6\text{H}_2\text{O}$					
88 132	S-8	1274888	Sb ₂ Se ₃					

TABLE C.2. (contd)

MINTeq Number	in 82WE		Compound	Units		ΔG_f° (Q/mol)	ΔH_f° (Q/mol)	S° (Q/mol·K)	Data Sources
	Page	ID Form		Q	State				
88 133		4	2.000 740	3.000 760	3.000 330	-6.000	2		
88 140		Sb ₂ Te ₃		*J	cr	-55.2	-58.5	234.	82WE 2-80
88 150		Sb ₂ Te ₃		*C	cr	-13.2	-13.5	55.9	82WE 2-80
88 160		Sb ₂ Te ₃		*C	cr	-13.2	-13.5	58.	68WE 101
88 170		Sb ₂ Te ₃		*C	cr	-13.2	-13.5	58.8	74NR 63
Summary data selected for reason 2									
88 180	S-1	Sb ₂ Te ₃		*C	cr	-13.2	-13.5	55.9	82WE 2-80
88 190		NH ₄ SbO ₂		*J	aj	-419.50	NA	NA	82WE 2-80
88 200		NH ₄ SbO ₂		!C	aj	-100.26	NA	NA	82WE 2-80
88 210		NH ₄ SbO ₂	std. state, n = 1	*C	aq	-100.9	NA	NA	68WE 102
Summary data selected for reason 1									
88 220	A-1	NH ₄ SbO ₂		!C	aj	-100.26	NA	NA	82WE 2-80
88 230		SbF ₃ ·NH ₃		*J	cr	NA	-1018.8	NA	82WE 2-80
88 240		SbF ₃ ·NH ₃		!C	cr	NA	-243.50	NA	82WE 2-80
88 250		SbF ₃ ·NH ₃		*C	cr	NA	-243.5	NA	68WE 102
Summary data selected for reason 2									
88 260	S-2	SbF ₃ ·NH ₃		*C	cr	NA	-243.5	NA	82WE 2-80
88 270		SbF ₃ ·2NH ₃		*J	cr	NA	-1115.5	NA	82WE 2-80
88 280		SbF ₃ ·2NH ₃		!C	cr	NA	-260.61	NA	82WE 2-80
88 290		SbF ₃ ·2NH ₃		*C	cr	NA	-260.6	NA	68WE 102
Summary data selected for reason 2									
88 300	S-2	SbF ₃ ·2NH ₃		*C	cr	NA	-260.61	NA	82WE 2-80
88 310		SbF ₃ ·3NH ₃		*J	cr	NA	-1260.4	NA	82WE 2-80
88 320		SbF ₃ ·3NH ₃		!C	cr	NA	-260.00	NA	82WE 2-80
88 330		SbF ₃ ·3NH ₃		*C	cr	NA	-260.9	NA	68WE 102
Summary data selected for reason 2									
88 340	S-2	SbF ₃ ·3NH ₃		*C	cr	NA	-260.9	NA	82WE 2-80
88 350		SbF ₃ ·4NH ₃		*J	cr	NA	-1278.2	NA	82WE 2-80
88 360		SbF ₃ ·4NH ₃		!C	cr	NA	-305.50	NA	82WE 2-80
88 370		SbF ₃ ·4NH ₃		*C	cr	NA	-305.5	NA	68WE 102
Summary data selected for reason 2									
88 380	S-2	SbF ₃ ·4NH ₃		*C	cr	NA	-305.5	NA	82WE 2-80
88 390		SbF ₃ ·6NH ₃		*J	cr	NA	-1433.0	NA	82WE 2-80
88 400		SbF ₃ ·6NH ₃		!C	cr	NA	-342.5	NA	82WE 2-80
88 410		SbF ₃ ·6NH ₃		*C	cr	NA	-342.5	NA	68WE 1-2

TABLE C.2. (contd)

MINTeq Number	in 82WE Page ID Form	Compound	Units Q State	ΔG_f° (Q/mol)	ΔH_f° (Q/mol)	S° (Q/mol·K)	Data Sources
Summary data selected for reason 1							
88	428 S-2	SbF ₃ ·6NH ₃	IC cr	NA	-342.5	NA	82WE 2-88
88	438	(NH ₄) ₂ Sb ₂ S ₄	*J aj	-258.8	-484.1	174.5	82WE 2-88
88	448	(NH ₄) ₂ Sb ₂ S ₄	IC aj	-81.7	-115.7	41.71	82WE 2-88
88	458	(NH ₄) ₂ Sb ₂ S ₄	*C aj	-81.7	-115.7	41.7	88WE 182
Summary data selected for reason 2							
88	488 A-1	(NH ₄) ₂ Sb ₂ S ₄	*C aj	-81.7	-115.7	41.7	88WE 182
121	18	(PbI ₂) ₃ ·SbI ₃	*J cr	NA	-537.2	NA	82WE 2-121
121	28	(PbI ₂) ₃ ·SbI ₃	IC cr	NA	-128.4	NA	82WE 2-121
Summary data selected for reason 4							
121	38 S-2	(PbI ₂) ₃ ·SbI ₃	IC cr	NA	-128.4	NA	82WE 2-121
121	48	(PbI ₂) ₃ ·SbI ₃ ·12H ₂ O	*J cr	NA	-4889.8	NA	82WE 2-121
121	58	(PbI ₂) ₃ ·SbI ₃ ·12H ₂ O	IC cr	NA	-977.29	NA	82WE 2-121
Summary data selected for reason 4							
121	88 S-2	(PbI ₂) ₃ ·SbI ₃ ·12H ₂ O	IC cr	NA	-977.29	NA	82WE 2-121
132	18	GaSb	*J cr	-38.9	-41.8	76.87	82WE 2-132
132	28	GaSb	IC cr	-9.38	-9.99	18.18	82WE 2-132
132	38	GaSb	*C cr	-9.3	-18.8	18.18	88WE 122
132	48	GaSb	*C cr	-9.3	-18.7	18.18	74NR 84
132	58	GaSb	*C cr	-9.3	NA	NA	88IN 48 from NBS docs.
Summary data selected for reason 2							
132	88 S-1	GaSb	*C cr	-9.3	-9.99	18.18	82WE 2-132
134	18	InSb	*J cr	-25.5	-38.5	86.2	82WE 2-134
134	28	InSb	IC cr	-8.18	-7.29	28.6	82WE 2-134
134	38	InSb	*C cr	-8.1	-7.3	28.6	88WE 226
134	48	InSb	*C cr	-8.1	NA	NA	88IN 48 (82WE 2-134)
134	58	InSb cubic	*C cr	-3.88	-3.89	28.6	74NR 84
Summary data selected for reasons 2 and 3							
134	88 S-1	InSb	*C cr	-8.1	-7.3	28.6	88WE 226
142	18	ZnSb	*J cr	NA	-14.6	NA	82WE 2-142
142	28	ZnSb	IC cr	NA	-3.49	NA	82WE 2-142
142	38	ZnSb	*C cr	NA	-3.5	NA	88WE 246
142	48	ZnSb	*C cr	-4.2	NA	NA	88IN 48 (from 77BK)

TABLE C.2. (contd)

MINTeq Number	in 82WE Page ID Form	Compound	Units Q State	ΔG_f° (Q/mol)	ΔH_f° (Q/mol)	S° (Q/mol·K)	Data Sources
Summary data selected for reasons 2 and 4							
142	50 S-0	ZnSb	*C cr	-4.2	-3.5	Calc.	88IN (77BK); 88WE 245
1474002	142 51 S-0	$\text{Sb}(\text{OH})_3^0 + 5e^- + \text{Zn}^{2+} + 3\text{H}^+ \leftrightarrow \text{ZnSb} + 3\text{H}_2\text{O}$					
142	52 S-0	1474002 ZnSb					
142	53	5 1.000 740 5.000 001 1.000 950 3.000 3300 -3.000 2					
148	10	CdSb	*J cr	-13.01	-14.39	92.9	82WE 2-148
148	20	CdSb	!C cr	-3.11	-3.439	22.2	82WE 2-148
148	30	CdSb	*C cr	-3.11	-3.44	22.2	88WE 250
148	40	CdSb	*C cr	-3.11	NA	NA	88IN 40 from NBS docs.
Summary data selected for reason 2							
148	50 S-0	CdSb	*C cr	-3.11	-3.44	22.2	82WE 2-148
1474004	148 51 S-0	$\text{Sb}(\text{OH})_3^0 + 5e^- + \text{Cd}^{2+} + 3\text{H}^+ \leftrightarrow \text{CdSb} + 3\text{H}_2\text{O}$					
148	52 S-0	1474004 CdSb					
148	53	5 1.000 740 5.000 1 1.000 100 3.000 330 -3.000 2					
148	60	Cd ₃ Sb ₂	*J cr	NA	-50.2	NA	82WE 2-148
148	70	Cd ₃ Sb ₂	!C cr	NA	-13.9	NA	82WE 2-148
148	80	Cd ₃ Sb ₂	*C cr	NA	-13.9	NA	88WE 250
Summary data selected for reason 2							
148	90 S-2	Cd ₃ Sb ₂	!C cr	NA	-13.9	NA	82WE 2-148
148	1100	AlSb	*C cr	-11.4	NA	NA	88IN 40 (from 77BK)
Summary data selected for reason 4							
148	1200 S-0	AlSb	*C cr	-11.4	NA	NA	88IN 40 (from 77BK)
1474003	148 1201 S-0	$\text{Sb}(\text{OH})_3^0 + 6e^- + \text{Al}^{3+} + 3\text{H}^+ \leftrightarrow \text{AlSb} + 3\text{H}_2\text{O}$					
148	1202 S-0	1474003 AlSb					
148	1203	5 1.000 740 6.000 1 1.000 30 3.000 330 -3.000 2					
148	1300	Ag ₃ Sb	*C cr	-5.4	NA	NA	88IN 40 (from 77BK)

TABLE C.2. (contd)

MINTeq Number	in 82WE Page ID	Form	Compound	Units Q State	ΔG_f° (Q/mol)	ΔH_f° (Q/mol)	S° (Q/mol·K)	Data Sources
Summary data selected for reason 4								
148 1400	S-0		Ag ₃ Sb	*C cr	-5.4	NA	NA	86IN 40 (from 77BK)
1474006	148 1401	S-0	$\text{Sb}(\text{OH})_3^0 + 6e^- + 3\text{Ag}^+ + 3\text{H}^+ \leftrightarrow \text{Ag}_3\text{Sb} + 3\text{H}_2\text{O}$					
	148 1402	S-0	1474006 Ag ₃ Sb					
148 1403		5	1.000 740	0.000 1	3.000 20	3.000 330	-3.000 2	
148 1500			AuSb ₂ -alpha	*C cr	NA	-3.12	NA	74NR 04
148 1600			AuSb ₂	*C cr	-3.3	NA	NA	86IN 40 (from 77BK)
Summary data selected for reason 4								
148 1700	S-1		AuSb ₂	*C cr	-3.3	-3.12	Calc.	86IN 40 (77BK); 74NR 04
150 10			Cu ₂ Sb	*J cr	NA	-11.7	NA	82WE 2-158
150 20			Cu ₂ Sb	!C cr	NA	-2.00	NA	82WE 2-158
150 30			Cu ₂ Sb	*C cr	NA	-2.0	NA	89WE 23
150 40			Cu ₂ Sb	*C cr	-3.9	NA	NA	86IN 40 (from 77BK)
Summary data selected for reason 4								
150 50	S-0		Cu ₂ Sb	*C cr	-3.9	-2.0	Calc.	86IN 40 (77BK); 89WE 23
1474012	150 51	S-0	$\text{Sb}(\text{OH})_3^0 + 6e^- + 3\text{H}^+ + \text{Cu}^{2+} + \text{Cu}^+ \leftrightarrow \text{Cu}_2\text{Sb} + 3\text{H}_2\text{O}$					
	150 52	S-0	1474012 Cu ₂ Sb					
150 53		6	1.000 740	0.000 1	3.000 330	1.000 230	1.000 231	-3.000 2
150 60			Cu ₃ Sb	*J cr	NA	-0.	NA	82WE 2-158
150 70			Cu ₃ Sb	!C cr	NA	-3.	NA	82WE 2-158
150 80			Cu ₃ Sb	*C cr	NA	-2.	NA	89WE 23
150 90			Cu ₃ Sb	*C cr	-6.14	NA	NA	86IN 40 from 79LS
Summary data selected for reasons 2 and 4								
150 100	S-0		Cu ₃ Sb	*C cr	-6.14	-2.	Calc.	86IN from 79LS; 89WE 23

TABLE C.2. (contd)

MINTeq Number	in 82WE			Compound	Units		ΔG_f° (Q/401)	ΔH_f° (Q/401)	S° (Q/401-K)	Data Sources
	Page	ID	Form		Q	State				
1474014	158	101	S-0	$\text{Sb}(\text{OH})_3^0 + 5e^- + 3H^+ + 3Cu^+ \leftrightarrow \text{Cu}_3\text{Sb} + 3H_2O$						
	158	102	S-0	1474014 Cu ₃ Sb						
	158	103		5 1.000 740 0.000	1		3.000 330	3.000 230	-3.000	2
	158	1100		Cu(SbO ₃) ₂	*C	cr	-230.8	NA	NA	88IN 40 from 79LS
Summary data selected for reason 4										
	158	1200	S-0	Cu(SbO ₃) ₂	*C	cr	-230.8	NA	NA	88IN 40 from 79LS
2074005	158	1201	S-0	$2\text{Sb}(\text{OH})_3^0 + \text{Cu}^{+2} \leftrightarrow \text{Cu}(\text{SbO}_3)_2 + 8H^+ + 4e^-$						
	158	1202	S-0	2074005 Cu(SbO ₃) ₂						
	158	1203		5 2.000 740 1.000	231		-6.000 330	6.000 330	-4.000 001	
	168	10		NiSb	*J	cr	NA	-80.1	NA	82WE 2-168
	168	20		NiSb	!C	cr	NA	-15.8	NA	82WE 2-168
	168	30		NiSb	*C	cr	NA	-15.8	NA	89WE 50
	168	40		NiSb breithauptite	*C	cr	-15.8	-15.8	17.5	74NR 84
	168	50		NiSb	*C	cr	-20.2	NA	NA	88IN 40 from 77BK
Summary data selected for reasons 1 and 4										
	168	00	S-0	NiSb breithauptite	*C	cr	-20.2	-15.8	Calc.	74NR 84
1474001	168	01	S-0	$\text{Sb}(\text{OH})_3^0 + 5e^- + 3H^+ + \text{Ni}^{2+} \leftrightarrow \text{NiSb} + 3H_2O$						
	168	02	S-0	1474001 NiSb						
	168	03		5 1.000 740 5.000	1		3.000 330	1.000 540	-3.000	2
	174	10		CoSb	*J	cr	NA	-42.	NA	82WE 2-174
	174	20		CoSb	!C	cr	NA	-10.	NA	82WE 2-174
	174	30		CoSb	*C	cr	NA	-10.	NA	89WE 00
	174	40		CoSb	*C	cr	-9.7	NA	NA	88IN 40 from 77BK
Summary data selected for reasons 1 and 4										
	174	50	S-1	CoSb	!C	cr	-9.7	-10.	Calc.	88IN 40; 82WE 2-174
	174	60		CoSb ₂	*J	cr	NA	-54.	NA	82WE 2-174
	174	70		CoSb ₂	!C	cr	NA	-13.	NA	82WE 2-174

TABLE C.2. (contd)

MINTeq Number	in 82WE Page ID	Form	Compound	Units Q State	ΔG_f^{298} (kJ/mol)	ΔH_f^{298} (kJ/mol)	S^{298} (J/mol·K)	Data Sources
174	88		CoSb ₂	*C cr	NA	-13.	NA	89WE 88
174	98		CoSb ₂	*C cr	-11.9	NA	NA	86IN 48 from 77BK
Summary data selected for reasons 1 and 4								
174	188	S-1	CoSb ₂	!C cr	-11.9	-13.	Calc.	86IN 48; 82WE 2-174
174	118		CoSb ₃	*J cr	NA	-87.	NA	82WE 2-174
174	128		CoSb ₃	!C cr	NA	-18.	NA	82WE 2-174
174	138		CoSb ₃	*C cr	NA	-18.	NA	89WE 88
174	148		CoSb ₃	*C cr	-14.7	NA	NA	86IN 48 from 77BK
Summary data selected for reasons 1 and 4								
174	158	S-1	CoSb ₃	!C cr	-14.7	-18.	Calc.	86IN 48; 82WE 2-174
188	18		FeSb	*J cr	NA	-18.8	NA	82WE 2-188
188	28		FeSb	!C cr	NA	-2.39	NA	82WE 2-188
188	38		FeSb	*C cr	NA	-2.4	NA	89WE 84
Summary data selected for reason 2								
188	48	S-2	FeSb	*C cr	NA	-2.4	NA	89WE 84 (82WE 2-188)
188	58		FeSb ₂	*J cr	NA	-15.1	NA	82WE 2-188
188	68		FeSb ₂	!C cr	NA	-3.61	NA	82WE 2-188
188	78		FeSb ₂	*C cr	NA	-3.6	NA	89WE 84
Summary data selected for reason 2								
188	88	S-2	FeSb ₂	*C cr	NA	-3.6	NA	89WE 84 (82WE 2-188)
193	98		MnSb	*J cr	NA	-58.	NA	82WE 2-193
193	108		MnSb	!C cr	NA	-12.	NA	82WE 2-193
193	118		MnSb	*C cr	NA	-12.	NA	89WE 112
193	128		MnSb	*C cr	-7.6	NA	NA	86IN 48 from 77BK
193	138		MnSb	*C cr	NA	-12.6	NA	74NR 64
Summary data selected for reasons 1 and 4								
193	148	S-8	MnSb	*C cr	-7.6	-12.	Calc.	86IN 48; 82WE 2-193

TABLE C.2. (contd)

MINTeq Number	in 82WE Page ID	Form	Compound	Units Q State	ΔG_f° (Q/mol)	ΔH_f° (Q/mol)	S° (Q/mol.K)	Data Sources
1474013	193 141 S-0		$Mn^{3+} + Sb(OH)_3^0 + 8e^- + 3H^+ \leftrightarrow MnSb + 3H_2O$					
	193 142 S-0		1474013 MnSb					
	193 143		5 1.000 471 1.000 740 6.000 1 3.000 330 -3.000 2					
	193 1600		Mn2Sb	*C cr	-9.7	NA	NA	86IN 40 from 77BK
Summary data selected for reason 4								
	193 1600 S-0		Mn2Sb	*C cr	-9.7	NA	NA	86IN 40 from 77BK
1474009	193 1601 S-0		$2Mn^{2+} + Sb(OH)_3^0 + 7e^- + 3H^+ \leftrightarrow Mn_2Sb + 3H_2O$					
	193 1602 S-0		1474009 Mn2Sb					
	193 1603		5 2.000 470 1.000 740 7.000 1 3.000 330 -3.000 2					
	210 10		TiSb	*J cr	NA	-281.2	NA	82WE 2-210
	210 20		TiSb	!C cr	NA	-67.21	NA	82WE 2-210
Summary data selected for reason 4								
	210 30 S-2		TiSb	!C cr	NA	-67.21	NA	82WE 2-210
	240 10		PrSb	*J cr	NA	NA	105.00	82WE 2-240
	240 20		PrSb	!C cr	NA	NA	25.110	82WE 2-240
Summary data selected for reason 4								
	240 30 S-2		PrSb	!C cr	NA	NA	25.110	82WE 2-240
	244 10		LaSb	*J cr	NA	NA	80.70	82WE 2-244
	244 20		LaSb	!C cr	NA	NA	21.22	82WE 2-244
Summary data selected for reason 4								
	244 30 S-2		LaSb	!C cr	NA	NA	21.22	82WE 2-244
	250 10		USb	*J cr	NA	130.	NA	82WE 2-250
	250 20		USb	!C cr	NA	33.0	NA	82WE 2-250
	250 30		USb	*C cr	NA	33.	NA	81WE 6
Summary data selected for reason 2								
	250 40 S-2		USb	*C cr	NA	33.	NA	82WE 2-250
	250 50		USb2	*J cr	-170.	-170.	141.40	82WE 2-250
	250 60		USb2	!C cr	-42.1	-42.1	33.810	82WE 2-250
	250 70		USb2	*C cr	-42.	-42.	33.81	81WE 6

TABLE C.2. (contd)

MINTeq Number	in 82WE			Compound	Units Q State	ΔG_f° (Q/mol)	ΔH_f° (Q/mol)	S° (Q/mol·K)	Data Sources
256	80			USb ₂	*C cr	-42.	NA	NA	88IN 48 from NBS docs.
Summary data selected for reason 2									
256	90	S-8		USb ₂	*C cr	-42.1	-42.1	33.81	82WE 2-256
1474811	256	91	S-8	$UO_2^{2+} + 2Sb(OH)_3^0 + 12e^- + 18H^+ \leftrightarrow USb_2 + 8H_2O$					
256	92	S-8		1474811 USb ₂					
256	93			5	1.000 893	2.000 740	12.000	1	10.000 330 -8.000 2
256	100			U ₃ Sb ₄	*J cr	-456.	-452.	349.78	82WE 2-256
256	110			U ₃ Sb ₄	!C cr	-109.	-108.	83.600	82WE 2-256
256	120			U ₃ Sb ₄	*C cr	-109.	-108.	83.7	81WE 8
256	130			U ₃ Sb ₄	*C cr	-109.	NA	NA	88IN 48 from NBS docs.
Summary data selected for reasons 2 and 3									
256	140			U ₃ Sb ₄	*C cr	-109.	-108.	83.6	82WE 2-256
1474815	256	142	S-8	$3U^{4+} + 4Sb(OH)_3^0 + 24e^- + 12H^+ \leftrightarrow U_3Sb_4 + 12H_2O$					
256	143	S-8		1474815 U ₃ Sb ₄					
256	144			5	3.000 891	4.000 740	24.000	1	12.000 330 -12.000 2
256	150			Mg ₂ Sb ₃	*C cr	-87.6	NA	NA	88IN 48 from 77BK
Summary data selected for reason 4									
256	160	S-8		Mg ₂ Sb ₃	*C cr	-87.6	NA	NA	88IN 48 from 77BK
1474885	256	181	S-8	$2Mg^{2+} + 3Sb(OH)_3^0 + 9H^+ + 13e^- \leftrightarrow Mg_2Sb_3 + 9H_2O$					
256	182	S-8		1474885 Mg ₂ Sb ₃					
256	183			5	2.000 460	3.000 740	9.000	330	13.000 1 -9.000 2
284	18			Mg ₃ Sb ₂ alpha	*J cr	NA	-234.	NA	82WE 2-284
284	20			Mg ₃ Sb ₂	!C cr	NA	-55.9	NA	82WE 2-284
284	30			Mg ₃ Sb ₂	*C cr	NA	-56.	NA	71PW 22
Summary data selected for reason 2									
284	40	S-2		Mg ₃ Sb ₂ alpha	*C cr	NA	-55.9	NA	82WE 2-284

TABLE C.2. (contd)

WINTER	in 82WE			Units		ΔG_f°	ΔH_f°	S°		
Number	Page	ID	Form	Compound	Q	State	(Q/mol)	(Q/mol)	(Q/mol·K)	Data Sources
	272	18		Ca ₃ Sb ₂	*J	cr	NA	-728.	NA	82WE 2-272
	272	28		Ca ₃ Sb ₂	!C	cr	NA	-174.	NA	82WE 2-272
	272	38		Ca ₃ Sb ₂	*C	cr	-189.9	NA	NA	86IN 48 from 77BK
Summary data selected for reason 4										
	272	48	S-8	Ca ₃ Sb ₂	*C	cr	-189.9	-174.	Calc.	86IN 48; 82WE 2-272
1474818	272	41	S-8	$3\text{Ca}^{2+} + 2\text{Sb}(\text{OH})_3^\circ + 8\text{H}^+ + 12\text{e}^- \leftrightarrow \text{Ca}_3\text{Sb}_2 + 8\text{H}_2\text{O}$						
	272	42	S-8	1474818	Ca ₃ Sb ₂					
	272	43		5	3.000	231	2.000	746	8.000	336
									12.000	1
									-8.000	2
	279	18		SrSb	*J	cr	NA	-192.	NA	82WE 2-279
	279	28		SrSb	!C	cr	NA	-45.9	NA	82WE 2-279
	279	38		SrSb	*C	cr	NA	-48.	NA	71PW 78
Summary data selected for reason 2										
	279	48	S-2	SrSb	*C	cr	NA	-45.9	NA	82WE 2-279
	279	58		Sr ₂ Sb	*J	cr	NA	-322.	NA	82WE 2-279
	279	68		Sr ₂ Sb	!C	cr	NA	-77.8	NA	82WE 2-279
Summary data selected for reason 4										
	279	78	S-2	Sr ₂ Sb	!C	cr	NA	-77.8	NA	82WE 2-279
	279	88		Sr ₃ Sb ₂	*J	cr	NA	-565.	NA	82WE 2-279
	279	98		Sr ₃ Sb ₂	!C	cr	NA	-135.	NA	82WE 2-279
	279	108		Sr ₃ Sb ₂	*C	cr	NA	-135.	NA	71PW 78
Summary data selected for reason 1										
	279	118	S-2	Sr ₃ Sb ₂	!C	cr	NA	-135.	NA	82WE 2-279
	298	18		Li ₃ Sb	*J	cr	NA	-322.	NA	82WE 2-298
	298	28		Li ₃ Sb	!C	cr	NA	-77.8	NA	82WE 2-298
	298	38		Li ₃ Sb	*C	cr	NA	-77.	NA	81WE 18
Summary data selected for reason 2										
	298	48	S-2	Li ₃ Sb	*C	cr	NA	-77.	NA	82WE 2-298
	298	58		Li ₃ Sb ₂	*J	cr	NA	-182.8	NA	82WE 2-298
	298	68		Li ₃ Sb ₂	!C	cr	NA	-43.58	NA	82WE 2-298
	298	78		Li ₃ Sb ₂	*C	cr	NA	-43.5	NA	81WE 19

TABLE C.2. (contd)

MINTER Number	in 82WE Page ID Form	Compound	Units Q State	ΔG_f° (Q/mol)	ΔH_f° (Q/mol)	S_{298}° (Q/mol·K)	Data Sources
Summary data selected for reason 2							
298	88 S-2	LigSb ₂	*C cr	NA	-43.6	NA	82WE 2-298
313	18	NaSb	*J cr	-83.	-83.	98.	82WE 2-313
313	28	NaSb	!C cr	-15.	-15.	23.	82WE 2-313
313	38	NaSb	*C cr	-15.	-15.	23.	81WE 38
313	48	NaSb	*C cr	-15.	NA	NA	86IN 48 from NBS docs.
Summary data selected for reason 1							
313	58	NaSb	!C cr	-15.	-15.	23.	82WE 2-313
1474888	313	52 S-8	$\text{Na}^+ + \text{Sb}(\text{OH})_3^0 + 3\text{H}^+ + 4\text{e}^- \leftrightarrow \text{NaSb} + 3\text{H}_2\text{O}$				
	313	53 S-8	1474888 NaSb				
313	54	5	1.000 500	1.000 748	3.000 330	4.000 1	-3.000 2
313	68	Na ₃ Sb	*J cr	-188.	-285.	128.	82WE 2-313
313	78	Na ₃ Sb	!C cr	-43.8	-49.8	38.1	82WE 2-313
313	88	Na ₃ Sb	*C cr	-43.	-49.	38.	81WE 38
313	98	Na ₃ Sb	*C cr	-43.	NA	NA	86IN 48 from NBS docs.
Summary data selected for reason 2							
313	108	Na ₃ Sb	*C cr	-43.	-49.	38.	82WE 2-313
1474887	313	102 S-8	$3\text{Na}^+ + \text{Sb}(\text{OH})_3^0 + 3\text{H}^+ + 6\text{e}^- \leftrightarrow \text{Na}_3\text{Sb} + 3\text{H}_2\text{O}$				
	313	103 S-8	1474887 Na ₃ Sb				
313	104	5	3.000 500	1.000 748	3.000 330	8.000 1	-3.000 2
313	118	NaSbO ₂	*J a _i	-882.89	NA	NA	82WE 2-313
313	128	NaSbO ₂	!C a _i	-143.98	NA	NA	82WE 2-313
313	138	NaSbO ₂	*C a _i	-143.91	NA	NA	81WE 38
313	148	NaSbO ₂	*C a _i	-143.91	NA	NA	76WE 38
Summary data selected for reason 2							
313	158	A-1 NaSbO ₂	*C a _i	-143.98	NA	NA	82WE 2-313
313	168	Na ₂ Sb ₂ S ₄ in 400 H ₂ O	*J	NA	-899.6	NA	82WE 2-313
313	178	Na ₂ Sb ₂ S ₄	!C aq	NA	-187.2	NA	82WE 2-313
313	188	Na ₂ Sb ₂ S ₄	*C	NA	-187.2	NA	81WE 38
313	198	Na ₂ Sb ₂ S ₄	*C	NA	-187.2	NA	76WE 38

TABLE C.2. (contd)

MINTeq Number	in 82WE Page ID	Form	Compound	Units Q State	ΔG_f° (Q/mol)	ΔH_f° (Q/mol)	S°_{298} (Q/mol·K)	Data Sources
Summary data selected for reason 1								
313	288	A-1	$\text{Na}_2\text{Sb}_2\text{S}_4$ in 400 H ₂ O	!C aq	NA	-187.2	NA	82WE 2-313
313	218		Na_3SbS_3 in 900 H ₂ O	*J aq	NA	-799.1	NA	82WE 2-313
313	228		Na_3SbS_3	!C	NA	-191.8	NA	82WE 2-313
313	238		Na_3SbS_3	*C	NA	-191.8	NA	81WE 38
Summary data selected for reason 1								
313	248	A-1	Na_3SbS_3 in 900 H ₂ O	!C aq	NA	-191.8	NA	82WE 2-313
339	18		KSb	*J cr	NA	-82.42	NA	82WE 2-339
339	28		KSb	!C cr	NA	-19.78	NA	82WE 2-339
339	38		KSb	*C cr	NA	-19.78	NA	81WE 66
Summary data selected for reason 1								
339	48	S-2	KSb	!C cr	NA	-19.78	NA	82WE 2-339
339	58		KSb ₂	*J cr	NA	-187.11	NA	82WE 2-339
339	68		KSb ₂	!C cr	NA	-25.888	NA	82WE 2-339
339	78		KSb ₂	*C cr	NA	-25.88	NA	81WE 66
Summary data selected for reason 2								
339	88	S-2	KSb ₂	*C cr	NA	-25.88	NA	82WE 2-339
339	98		K ₃ Sb	*J cr	NA	-183.31	NA	82WE 2-339
339	108		K ₃ Sb	!C cr	NA	-43.812	NA	82WE 2-339
339	118		K ₃ Sb	*C cr	NA	-43.8	NA	81WE 66
Summary data selected for reason 2								
339	128	S-2	K ₃ Sb	*C cr	NA	-43.81	NA	82WE 2-339
339	138		K ₅ Sb ₄	*J cr	NA	-379.1	NA	82WE 2-339
339	148		K ₅ Sb ₄	!C cr	NA	-98.61	NA	82WE 2-339
339	158		K ₅ Sb ₄	*C cr	NA	-98.6	NA	81WE 66
Summary data selected for reason 2								
339	168	S-2	K ₅ Sb ₄	*C cr	NA	-98.61	NA	82WE 2-339
339	178		K ₂ Sb ₂ S ₄	*C a	-159.2	-173.8	38.5	78WE 58
Summary data selected for reason 4								
339	188	A-1	K ₂ Sb ₂ S ₄	*C a	-159.2	-173.8	38.5	78WE 58
339	198		3KBr·2SbBr ₃	*J cr	NA	-1742.2	NA	82WE 2-339
339	208		3KBr·2SbBr ₃	!C cr	NA	-416.48	NA	82WE 2-339
339	218		3KBr·2SbBr ₃	*C cr	NA	-416.4	NA	81WE 66

TABLE C.2. (contd)

MINTeq	in 82WE			Compound	Units	ΔG_f^{298}	ΔH_f^{298}	S^{298}	
Number	Page	ID	Form		Q State	(Q/mol)	(Q/mol)	(Q/mol·K)	Data Sources
Summary data selected for reason 2									
339	220	S-2	3KBr·2SbBr ₃		*C cr	NA	-418.4	NA	82WE 2-339
360	10		RbSb		*J cr	NA	-160.0	NA	82WE 2-360
360	20		RbSb		!C cr	NA	-23.90	NA	82WE 2-360
360	30		RbSb		*C cr	NA	-23.9	NA	81WE 89
360	40		RbSb		*C cr	NA	-23.9	NA	78WE 70
Summary data selected for reason 4									
360	50	S-2	RbSb		*C cr	NA	-23.9	NA	82WE 2-360
360	60		RbSb ₂		*J cr	NA	-102.5	NA	82WE 2-360
360	70		RbSb ₂		!C cr	NA	-24.50	NA	82WE 2-360
360	80		RbSb ₂		*C cr	NA	-24.5	NA	81WE 89
360	90		RbSb ₂		*C cr	NA	-24.5	NA	78WE 70
Summary data selected for reason 2									
360	100	S-2	RbSb ₂		*C cr	NA	-24.5	NA	82WE 2-360
360	110		Rb ₃ Sb		*J cr	NA	-173.0	NA	82WE 2-360
360	120		Rb ₃ Sb		!C cr	NA	-41.49	NA	82WE 2-360
360	130		Rb ₃ Sb		*C cr	NA	-41.5	NA	81WE 89
360	140		Rb ₃ Sb		*C cr	NA	-41.5	NA	78WE 70
Summary data selected for reason 2									
360	150	S-2	Rb ₃ Sb		*C cr	NA	-41.49	NA	82WE 2-360
360	160		Rb ₃ Sb ₇		*J cr	NA	-310.	NA	82WE 2-360
360	170		Rb ₃ Sb ₇		!C cr	NA	-74.1	NA	82WE 2-360
360	180		Rb ₃ Sb ₇		*C cr	NA	-74.1	NA	81WE 89
360	190		Rb ₃ Sb ₇		*C cr	NA	-74.1	NA	78WE 70
Summary data selected for reason 1									
360	200	S-2	Rb ₃ Sb ₇		!C cr	NA	-74.1	NA	82WE 2-360
360	210		Rb ₅ Sb ₄		*J cr	NA	-444.	NA	82WE 2-360
360	220		Rb ₅ Sb ₄		!C cr	NA	-100.	NA	82WE 2-360
360	230		Rb ₅ Sb ₄		*C cr	NA	-100.1	NA	81WE 89
360	240		Rb ₅ Sb ₄		*C cr	NA	-100.1	NA	78WE 70
Summary data selected for reason 2									
360	250	S-2	Rb ₅ Sb ₄		*C cr	NA	-100.2	NA	82WE 2-360
360	260		RbSbO ₂		*J aj	-624.18	NA	NA	82WE 2-360
360	270		RbSbO ₂		!C aj	-149.18	NA	NA	82WE 2-360
360	280		RbSbO ₂		*C aj	-149.19	NA	NA	81WE 89
360	290		RbSbO ₂		*C aj	-149.02	NA	NA	78WE 50

TABLE C.2. (contd)

MINTER Number	in 82WE Page ID Form	Compound	Units Q State	ΔG_f° (kJ/mol)	ΔH_f° (kJ/mol)	S_{298}° (J/mol·K)	Data Sources
Summary data selected for reason 2							
366	366 A-1	RbSbO ₂	*C aj	-149.18	NA	NA	82WE 2-366
366	316	SbCl ₃ ·3RbCl	*J cr	NA	-1716.3	NA	82WE 2-366
366	326	SbCl ₃ ·3RbCl	!C cr	NA	-416.2	NA	82WE 2-366
366	336	SbCl ₃ ·3RbCl	*C cr	NA	-416.2	NA	81WE 89
366	346	SbCl ₃ ·3RbCl	*C cr	NA	-416.2	NA	76WE 76
Summary data selected for reason 1							
366	356 S-2	SbCl ₃ ·3RbCl	!C cr	NA	-416.2	NA	82WE 2-366
366	366	7RbBr·3SbBr ₃	*J cr	NA	-3761.2	NA	82WE 2-366
366	376	7RbBr·3SbBr ₃	!C cr	NA	-884.61	NA	82WE 2-366
366	386	7RbBr·3SbBr ₃	*C cr	NA	-884.6	NA	81WE 89
366	396	7RbBr·3SbBr ₃	*C cr	NA	-884.6	NA	76WE 76
Summary data selected for reason 2							
366	406 S-2	7RbBr·3SbBr ₃	*C cr	NA	-884.6	NA	76WE 76 (82WE 2-366)
366	416	Rb ₂ Sb ₂ S ₄	*J aj	-667.3	-721.7	196.8	82WE 2-366
366	426	Rb ₂ Sb ₂ S ₄	!C aj	-159.5	-172.5	45.66	82WE 2-366
366	436	Rb ₂ Sb ₂ S ₄	*C aj	-159.5	-172.5	45.6	81WE 89
Summary data selected for reason 2							
366	446 A-1	Rb ₂ Sb ₂ S ₄	*C aj	-159.5	-172.5	45.6	82WE 2-366
373	16	CaSbO ₂	*J aj	-632.21	NA	NA	82WE 2-373
373	26	CaSbO ₂	!C aj	-151.16	NA	NA	82WE 2-373
Summary data selected for reason 4							
373	36 A-1	CaSbO ₂	!C aj	-151.16	NA	NA	82WE 2-373
373	46	Ca ₂ Sb ₂ S ₄	*J aj	-683.7	-736.6	213.8	82WE 2-373
373	56	Ca ₂ Sb ₂ S ₄	!C aj	-163.41	-175.9	51.16	82WE 2-373
Summary data selected for reason 4							
373	66 A-1	Ca ₂ Sb ₂ S ₄	!C aj	-163.41	-175.9	51.16	82WE 2-373

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APPENDIX D

CALCULATIONS FOR ANTIMONY BASIS SPECIE $\text{Sb}(\text{OH})_6^-$

APPENDIX D

CALCULATIONS FOR ANTIMONY BASIS SPECIE Sb(OH)_6^-

Similar to Peterson et al. (1987), Sb(OH)_6^- is selected as the basis specie for antimony. They list a value of -284.11 kcal/mol for $\Delta G_{f,298}^0$, but did not list their method of calculation from the data of Baes and Mesmer (1976). A value of -288.76 kcal/mol for $\Delta G_{f,298}^0$ for Sb(OH)_6^- was calculated in this study, as compared to the value of -284.11 reported by Peterson et al. (1987).

This appendix records the method we used to calculate $\Delta G_{f,298}^0$ from the data of Baes and Mesmer (1976). This method is based upon discussions with S. Peterson and on equations 16-14 and 16-13 from Baes and Mesmer, and the $\Delta G_{f,298}^0$ of S_2O_5 from Wagman et al. (1982). The first two equations are added:

The equilibrium constant, $\log K_r^0$, is converted to the free energy of reaction,

$$\Delta G_{r,298}^0 = - (2.303 \times R \times T) * \log K_r^0$$

After substitution, $\Delta G_{r,298}^0$ is 8.76 Kcal/mol.

(a) See Table 16.5 in Baes and Mesmer (1976).

Next, using $\Delta G_{f,298}^{\circ}$ for Sb_2O_5 from Wagman et al. (1982) to calculate $\Delta G_{f,298}^{\circ}, \text{Sb}(\text{OH})_6^-$,

$$\begin{aligned}
 8.76 &= \Delta G_{f,298}^{\circ}, \text{Sb}(\text{OH})_6^- + \Delta G_{f,298}^{\circ}, \text{H}^+ - \left[\frac{1}{2} \Delta G_{f,298}^{\circ} \text{Sb}_2\text{O}_5 \right. \\
 &\quad \left. + \frac{7}{2} \Delta G_{f,298}^{\circ}, \text{H}_2\text{O} \right] \\
 &= \Delta G_{f,298}^{\circ}, \text{Sb}(\text{OH})_6^- + 0 - \left[\frac{1}{2} (-198.2) + \frac{7}{2} (-56.69) \right] \\
 &= \Delta G_{f,298}^{\circ}, \text{Sb}(\text{OH})_6^- + 0 - [\quad 99.10 + \quad 198.42]
 \end{aligned}$$

After simplifying,

$$\Delta G_{f,298}^{\circ}, \text{Sb}(\text{OH})_6^- = -288.76 \text{ kcal/mol},$$

the value for $\Delta G_{f,298}^{\circ}, \text{Sb}(\text{OH})_6^-$ used in this report.

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APPENDIX E

MINTEQ THERMODYNAMIC DATA FILES FOR CYANIDE

MINTEQ THERMODYNAMIC DATA FILES FOR CYANIDE

File: SbComp.dat - Component

143 CN-	-1.0	0.0	0.0	26.018
144 OCN-	-1.0	0.0	0.0	42.017

File: SbAqs.dat - Aqueous

AQUEOUS	REVISION	13-OCT-8	13:32:15	
1001431 BAFe(CN)6-1	-69.6800	55.4356		-1.00 0.00 0.00 349.2804
0.00 3	1.000 100	1.000 281	6.000 143	
1501434 CAHFe(CN)6-	-82.0000	52.7097		-2.00 0.00 0.00 253.0394
0.00 5	1.000 150	1.000 330	1.000 280	6.000 143 1.000 1
4101433 KFe(CN)6-3	-84.0000	48.1204		-3.00 0.00 0.00 251.0517
0.00 3	1.000 410	1.000 280	6.000 143	
4101434 K2Fe(CN)6-2	-77.3000	48.9780		-2.00 0.00 0.00 290.1500
0.00 3	2.000 410	1.000 280	6.000 143	
4101435 KHFe(CN)6-	-78.1000	51.4702		-2.00 0.00 0.00 252.0597
0.00 4	1.000 410	1.000 330	1.000 280	6.000 143
4401432 Li2Fe(CN)6-	-83.4980	48.5338		-2.00 0.00 0.00 225.8354
0.00 3	2.000 440	1.000 280	6.000 143	
4401433 LiHFeCN6-2	-80.9990	51.2188		-2.00 0.00 0.00 219.9024
0.00 4	1.000 440	1.000 330	1.000 280	6.000 143
4901431 NH4Fe(CN)6-3	-84.5000	48.0684		-3.00 0.00 0.00 314.0324
0.00 3	1.000 490	1.000 280	6.000 143	
4901433 NH5Fe(CN)6-	-83.9000	51.4035		-2.00 0.00 0.00 315.0403
0.00 4	1.000 490	1.000 330	1.000 280	6.000 143
5001431 NAFc(CN)6-3	-84.9000	47.9885		-3.00 0.00 0.00 234.9432
0.00 3	1.000 500	1.000 280	6.000 143	
5001432 NA2Fe(CN)6-2	-85.0000	48.7435		-2.00 0.00 0.00 257.9330
0.00 3	2.000 500	1.000 280	6.000 143	
5001433 NAHFe(CN)6-2	-85.6000	51.4335		-2.00 0.00 0.00 235.9512
0.00 4	1.000 500	1.000 330	1.000 280	6.000 143
4901432 NH4)2FECN)6-2	-83.0000	48.8666		-2.00 0.00 0.00 332.0709
0.00 3	2.000 490	1.000 280	6.000 143	
201431 AG(CN)OH-	0.0000	-0.5600		-1.00 0.00 0.00 150.8933
0.00 4	1.000 143	1.000 20	1.000 2	-1.000 330

MINTEQ THERMODYNAMIC DATA FILES FOR CYANIDE (contd)

201432	AG(CN)2-	-32.6750	20.3814	-1.00	0.00	0.00	159.9037
0.00	2	2.000	143	1.000	20		
4101431	K2H2FE(CN)6	-85.8600	52.3058	0.00	0.00	0.00	292.1659
0.00	4	6.000	143	2.000	410	2.000	330
1501431	CAFE(CN)6-	-69.5000	55.4730	-1.00	0.00	0.00	252.0314
0.00	3	6.000	143	1.000	150	1.000	281
1501432	CAFE(CN)62-	-83.1000	49.6898	-2.00	0.00	0.00	252.0314
0.00	3	6.000	143	1.000	150	1.000	280
1501433	CA2FE(CN)6	-83.7000	50.9952	0.00	0.00	0.00	292.1094
0.00	3	6.000	143	2.000	150	1.000	280
1601431	CDCN+	0.0000	5.3200	1.00	0.00	0.00	138.4287
0.00	2	1.000	143	1.000	160		
1601432	CD(CN)20	-13.0000	10.3703	0.00	0.00	0.00	164.4465
0.00	2	2.000	143	1.000	160		
1601433	CD(CN)3-	-21.6000	14.8341	-1.00	0.00	0.00	190.4642
0.00	2	3.000	143	1.000	160		
1601434	CD(CN)42-	-23.5600	18.2938	-2.00	0.00	0.00	216.4820
0.00	2	4.000	143	1.000	160		
2301431	CU(CN)43-	-51.4000	30.3456	-3.00	0.00	0.00	167.6170
0.00	2	4.000	143	1.000	230		
2301432	CU(CN)2-	-29.1000	24.0272	-1.00	0.00	0.00	115.5815
0.00	2	2.000	143	1.000	230		
2301433	CU(CN)32-	-40.2000	28.6524	-2.00	0.00	0.00	141.5992
0.00	2	3.000	143	1.000	230		
2801431	FE(CN)64-	-85.8000	45.6063	-4.00	0.00	0.00	211.9534
0.00	2	6.000	143	1.000	280		
2801432	HFE(CN)63-	-84.1600	49.9969	-3.00	0.00	0.00	212.9614
0.00	3	6.000	143	1.000	280	1.000	330
2801433	H2FE(CN)62-	-83.1000	52.4450	-2.00	0.00	0.00	213.9693
0.00	3	6.000	143	2.000	330	1.000	280
2811431	FE(CN)63-	-70.1000	52.6283	-3.00	0.00	0.00	211.9534
0.00	2	6.000	143	1.000	281		
3301431	HCN	-10.4000	9.2356	0.00	0.00	0.00	27.0257
0.00	2	1.000	143	1.000	330		
3301441	HOCN	-2.0000	3.4450	0.00	0.00	0.00	43.0251
0.00	2	1.000	144	1.000	330		

MINTEQ THERMODYNAMIC DATA FILES FOR CYANIDE (contd)

3611431	HGCN+	-33.8300	24.1738			1.00	0.00	0.00	226.6077
0.00	4	1.000	143	1.000	361	2.000	330	-2.000	2
3611432	HG(CN)2	-57.2400	40.6513			0.00	0.00	0.00	252.6255
0.00	4	2.000	143	1.000	361	2.000	330	-2.000	2
3611433	HG(CN)3-	-64.8300	44.4042			-1.00	0.00	0.00	278.6432
0.00	4	3.000	143	1.000	361	2.000	330	-2.000	2
3611434	HG(CN)42-	-69.9300	47.4094			-2.00	0.00	0.00	304.6610
0.00	4	4.000	143	1.000	361	2.000	330	-2.000	2
3611435	HG(CN)2CL-	0.0000	40.3735			-1.00	0.00	0.00	288.0782
0.00	5	2.000	143	1.000	180	1.000	361	2.000	330
3611436	HG(CN)3CL2-	0.0000	43.8332			-2.00	0.00	0.00	314.0959
0.00	5	3.000	143	1.000	180	1.000	361	2.000	330
3611437	HG(CN)3BR2-	0.0000	44.9415			-2.00	0.00	0.00	358.5472
0.00	5	3.000	143	1.000	130	1.000	361	2.000	330
3801432	I2CN-	0.0000	-11.8480			-1.00	0.00	0.00	279.8267
0.00	3	1.000	143	2.000	380	-2.000	1		
3801433	I(CN)2-	0.0000	-11.4580			-1.00	0.00	0.00	178.9399
0.00	3	2.000	143	1.000	380	-2.000	1		
4101432	K3HFE(CN)6	-85.9900	50.2241			0.00	0.00	0.00	330.2563
0.00	4	6.000	143	3.000	410	1.000	330	1.000	280
4401431	LIFE(CN)63-	-80.1490	47.6858			-3.00	0.00	0.00	218.8944
0.00	3	6.000	143	1.000	440	1.000	280		
4601431	MGFE(CN)6-	-69.3100	55.3916			-1.00	0.00	0.00	236.2584
0.00	3	6.000	143	1.000	460	1.000	281		
4601432	MGFE(CN)62-	0.0000	49.4251			-2.00	0.00	0.00	236.2584
0.00	3	6.000	143	1.000	460	1.000	280		
5401431	NI(CN)42-	-43.1900	30.1257			-2.00	0.00	0.00	162.7610
0.00	2	4.000	143	1.000	540				
8001431	SRFE(CN)6-	-69.8300	55.6181			-1.00	0.00	0.00	299.5734
0.00	3	1.000	800	1.000	281	6.000	143		
8701431	TL(CN)4-	0.0000	-8.0189			-1.00	0.00	0.00	308.4543
0.00	3	4.000	143	1.000	870	-2.000	1		
8701432	TLFE(CN)63-	-84.8800	48.7508			-3.00	0.00	0.00	416.3367
0.00	3	6.000	143	1.000	870	1.000	280		
9501431	ZN(CN)42-	-25.5390	16.7150			-2.00	0.00	0.00	169.4610
0.00	2	4.000	143	1.000	950				

MINTEQ THERMODYNAMIC DATA FILES FOR CYANIDE (contd)

9501432	ZN(CN)3-	-20.1990	16.0480					-1.00	0.00	0.00	143.4432
0.00	2	3.000	143	1.000	950						
9501430	ZN(CN)2(AQ)	-10.9990	11.0710					0.00	0.00	0.00	117.4255
0.00	2	2.000	143	1.000	950						
5401436	NI(CN)3-	0.0000	22.6346					-1.00	0.00	0.00	136.7432
0.00	2	3.000	143	1.000	540						
5401432	NIH(CN)4-	0.0000	36.7482					-1.00	0.00	0.00	163.7689
0.00	3	4.000	143	1.000	540	1.000	330				
5401433	NIH2(CN)4(AQ)	0.0000	41.4576					0.00	0.00	0.00	164.7768
0.00	3	4.000	143	1.000	540	2.000	330				
5401434	NIH3(CN)4+	0.0000	43.9498					1.00	0.00	0.00	165.7848
0.00	3	4.000	143	1.000	540	3.000	330				
5401435	NI(CN)2(AQ)	0.0000	14.5864					0.00	0.00	0.00	110.7255
0.00	2	2.000	143	1.000	540						
2811432	FE2(CN)6(AQ)	0.0000	56.9822					0.00	0.00	0.00	267.8004
0.00	2	6.000	143	2.000	281						
201440	AG(OCN)2-	0.0000	5.0034					-1.00	0.00	0.00	191.9025
0.00	2	2.000	144	1.000	20						
201433	AG(CN)32-	-33.4950	21.4002					-2.00	0.00	0.00	185.9214
0.00	2	3.000	143	1.000	20						
1001430	BAFE(CN)62-	0.0000	49.4032					-2.00	0.00	0.00	349.2804
0.00	3	6.000	143	1.000	280	1.000	100				

File: SbSolid.dat - Solid

SOLIDS		REVISION		13-OCT-8 13:43:45		
1102001	AG4FECN)6.H2	0.0000	89.6909			661.4415
4	6.000 143	4.000	20	1.000 280	1.000 2	
1102002	AGCN	-26.3850	16.2180			133.8859
2	1.000 143	1.000	20			
1116001	CD2FECN)6.7H	0.0000	62.9824			562.8824
4	6.000 143	2.000	160	1.000 280	7.000 2	

MINTEQ THERMODYNAMIC DATA FILES FOR CYANIDE (contd)

1121001	CRCN	0.0000	-23.8880				78.0138
3	1.000 143	1.000 210	1.000 1				
1121002	CR2CN	0.0000	-56.6450				130.0099
3	1.000 143	2.000 210	3.000 1				
1123001	CUCN	-30.2000	19.4974				89.5637
2	1.000 143	1.000 230					
1123102	CU2FECN)6	0.0000	61.4168				339.0454
3	6.000 143	2.000 231	1.000 280				
1138001	CNI	17.3090	-11.3114				152.9222
3	1.000 143	1.000 380	-2.000 1				
1141001	K12NI8FECN67	0.0000	431.0902				2422.3737
4	42.000 143	12.000 410	8.000 540	7.000 280			
1141002	KCN I, CUB	-2.7400	-1.4403				65.1160
2	1.000 143	1.000 410					
1141003	K2CDFECN)6	0.0000	63.0279				402.5610
4	6.000 143	2.000 410	1.000 160	1.000 280			
1141004	K4NI4FECN63	0.0000	183.5467				1027.0135
4	18.000 143	4.000 410	4.000 540	3.000 280			
1141005	K4FECN)6	-95.6200	48.8241				368.3466
3	6.000 143	4.000 410	1.000 280				
1141006	K2MN3FECN62	0.0000	121.0011				666.9176
4	12.000 143	2.000 410	3.000 470	2.000 280			
1141007	K2NI3FECN62	0.0000	123.1267				678.1735
4	12.000 143	2.000 410	3.000 540	2.000 280			
1141008	K4FECN6.3H	-99.1750	49.5424				422.3925
4	6.000 143	4.000 410	1.000 280	3.000 2			
1141009	K12CD8FECN67	0.0000	441.9853				2852.1417
4	42.000 143	12.000 410	8.000 160	7.000 280			
1141010	KZN1.5FECN)6	0.0000	66.8086				349.1367
4	6.000 143	1.000 410	1.500 950	1.000 280			
1141011	K3FE(CN)6	-83.2900	54.6440				329.2483
3	6.000 143	3.000 410	1.000 281				
1141012	K8MN6FECN65	0.0000	293.6849				1702.1819
4	30.000 143	8.000 410	6.000 470	5.000 280			
1141013	K2CU2FECN)6	0.0000	72.5142				417.2420
4	6.000 143	2.000 410	2.000 230	1.000 280			

MINTEQ THERMODYNAMIC DATA FILES FOR CYANIDE (contd)

1147014	MN2FE(CN)6	0.0000	59.0272				321.8295
3	6.000 143	2.000	470	1.000	280		
1150001	NACN CRI,CUB	0.5200	-2.2869				49.0075
2	1.000 143	1.000	500				
1160001	PB2FECN6.3H	0.0000	63.6011				680.3993
4	6.000 143	2.000	600	1.000	280	3.000 2	
1187001	TL4FECN6.2H	0.0000	56.9162				1065.5172
4	6.000 143	4.000	870	1.000	280	2.000 2	
1195001	ZN2FECN6.2H	0.0000	61.2321				378.7640
4	6.000 143	2.000	950	1.000	280	2.000 2	
7714401	AGOCN	-13.1750	6.6159				149.8853
2	1.000 144	1.000	20				
1102002	AG4FE(CN)6	-260.9100	193.9140				133.8859
3	6.000 143	4.000	20	1.000	280		
1116002	CD2FE(CN)6	0.0000	28.2243				436.7754
3	6.000 143	2.000	160	1.000	280		
1136100	HG(CN)2	-60.7300	45.3791				252.6255
4	1.000 361	2.000	143	2.000	330	-2.000 2	
1160002	PB2FE(CN)6	0.0000	27.5895				626.3534
3	6.000 143	2.000	600	1.000	280		
1195002	ZN2FE(CN)6	0.0000	29.9263				342.7334
3	6.000 143	2.000	950	1.000	280		

APPENDIX F

MINTEQ THERMODYNAMIC DATA FILES FOR ANTIMONY

MINTEQ THERMODYNAMIC DATA FILES FOR ANTIMONY

File: SbComp.dat - Component

740 SbOH)3	0.0	0.0	0.0	172.7719
741 SBOH)6	1.0	0.0	0.0	223.7938

File: SbRedox.dat - REOX

7407410 SBOH6/SBOH3	0.0000	-223.5383							
0.00 5	-1.000	740	1.000	741	-3.000	2	3.000	330	3.000 1

File: SbAqs.dat - Aqueous

7400021 HSB02	-0.0150	-0.0073				0.00	0.00	0.00	154.7567
0.00 2	1.000	740	-1.000	2					
7402700 SBOFO(aq)	0.0000	6.1864				0.00	0.00	0.00	156.7478
0.00 4	1.000	740	1.000	270	1.000	330	-2.000	2	
7402702 SB(OH)2F	0.0000	6.1937				0.00	0.00	0.00	174.7631
0.00 4	1.000	740	1.000	270	1.000	330	-1.000	2	
7403300 SBO+	1.9700	0.9228				1.00	0.00	0.00	137.7494
0.00 3	1.000	740	1.000	330	-2.000	2			
7403301 SBO2-	16.7750	-11.8011				-1.00	0.00	0.00	153.7488
0.00 3	1.000	740	-1.000	2	-1.000	330			
7403302 SB(OH)2+	0.0000	-144.1854				1.00	0.00	0.00	155.7647
0.00 3	1.000	740	1.000	330	-1.000	2			
7407300 SB2S42-	-75.6800	49.3005				-2.00	0.00	0.00	371.7640
0.00 4	2.000	740	4.000	730	2.000	330	-6.000	2	
7410021 SBO3-	0.0000	2.9319				-1.00	0.00	0.00	169.7482
0.00 2	1.000	741	-3.000	2					
7413300 SBO2+	0.0000	2.3895				1.00	0.00	0.00	153.7488
0.00 3	1.000	741	2.000	330	-4.000	2			
7400020 SB(OH)4-1	16.6950	-12.0429				-1.00	0.00	0.00	189.7794
0.00 3	1.000	740	1.000	2	-1.000	330			

MINTEQ THERMODYNAMIC DATA FILES FOR ANTIMONY (contd)

File: SbSolid.dat - Solid

74001	SB	-20.0450	11.7058					121.7500	
4	1.000 740	3.000 330	3.000 1	-3.000 2					
1074000	SB2S3 STIB	-69.2900	60.1560					339.6980	SB2S3
4	2.000 740	3.000 730	3.000 330	-6.000 2					
1274000	SB2SE3	-81.9900	67.7571					480.3800	SB2SE3
4	2.000 740	3.000 760	3.000 330	-6.000 2					
1474001	NISB BREITHA	-22.9450	18.5225					180.4400	NISB
5	1.000 740	5.000 1	3.000 330	1.000 540	-3.000 2				
1474002	ZNSB	13.1160	-11.0138					187.1400	ZNSB
5	1.000 740	5.000 1	1.000 950	3.000 330	-3.000 2				
1474003	ALSB	0.0000	-65.6241					148.7315	ALSB
5	1.000 740	6.000 1	1.000 30	3.000 330	-3.000 2				
1474004	CDSB	-5.3450	0.3943					234.1610	CDSB
5	1.000 740	5.000 1	3.000 330	1.000 160	-3.000 2				
1474005	MG2SB3	0.0000	-74.6838					413.8600	MG2SB3
5	2.000 460	3.000 740	9.000 330	13.000 1	-9.000 2				
1474006	AG3SB	0.0000	56.1818					445.3546	AG3SB
5	1.000 740	6.000 1	3.000 20	3.000 330	-3.000 2				
1474007	NA3SB	103.2450	-94.4084					190.7193	NA3SB
5	3.000 500	1.000 740	3.000 330	6.000 1	-3.000 2				
1474008	NASB	22.3850	-23.1770					144.7398	NASB
5	1.000 500	1.000 740	3.000 330	4.000 1	-3.000 2				
1474009	MN2SB	0.0000	-61.0796					231.6261	MN2SB
5	2.000 470	1.000 740	7.000 1	3.000 330	-3.000 2				
1474010	CA3SB2	175.1300	-142.9738					363.7340	CA3SB2
5	3.000 150	2.000 740	6.000 330	12.000 1	-6.000 2				
1474011	USB2	24.6800	-29.5246					481.5289	USB2
5	1.000 893	2.000 740	12.000 1	10.000 330	-8.000 2				
1474012	CU2S8	-55.7450	34.8827					248.8420	CU2SB
6	1.000 740	6.000 1	3.000 330	1.000 230	1.000 231	-3.000 2			2
1474013	MNSB	-5.0450	2.9099					176.6881	MNSB
5	1.000 471	1.000 740	6.000 1	3.000 330	-3.000 2				
1474014	CU3SB	-73.6450	42.5937					312.3880	CU3SB
5	1.000 740	6.000 1	3.000 330	3.000 230	-3.000 2				

MINTEQ THERMODYNAMIC DATA FILES FOR ANTIMONY (contd)

1474015	U3SB4	235.7200	-152.3288					1201.0867	U3SB4
5	3.000 891	4.000 740	24.000 1	12.000 330	-12.000 2				
2074001	SB204	16.2700	-3.4597					307.4976	SB204
4	2.000 740	-2.000 2	-2.000 330	-2.000 1					
2074002	SB406 II,CU8	-14.6000	19.6586					582.9964	SB406 II, CUBIC
2	4.000 740	-6.000 2							
2074003	SB406 I,ORTHO	-8.9900	17.0346					582.9964	SB406 I, ORTHORHOM
2	4.000 740	-6.000 2							
2074004	SB(OH)3 SOLID	-7.2000	7.1099					172.7720	SB(OH)3
1	1.000 740								
2074005	CU(SB03)2	0.0000	-45.2105					403.0424	CU(SB03)2
4	2.000 740	1.000 231	-6.000 330	-4.000 1					
2074006	SB203 SENARMO	-7.3250	12.3654					291.4982	SB203
2	2.000 740	-3.000 2							
2074007	SB203 VALENTI	-4.5450	8.4806					291.4982	SB203
2	2.000 740	-3.000 2							
2074100	SB205	0.0000	12.4827					323.4970	SB205
3	2.000 741	2.000 330	-7.000 2						
2074102	SB02	0.0000	27.8241					153.7488	SB02
4	1.000 741	1.000 1	2.000 330	-4.000 2					
4074000	SBBR3	5.0720	-1.0562					361.4620	SBBR3
4	1.000 740	3.000 130	3.000 330	-3.000 2					
4174000	S8CL3	8.4140	-0.5915					228.1081	SBCL3
4	1.000 740	3.000 180	3.000 330	-3.000 2					
4274000	SBF3	1.6080	10.2251					178.7452	SBF3
4	1.000 740	3.000 330	3.000 270	-3.000 2					
4374000	SBI3	-3.2480	0.5380					502.4634	SBI3
4	1.000 740	3.000 330	3.000 380	-3.000 2					

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