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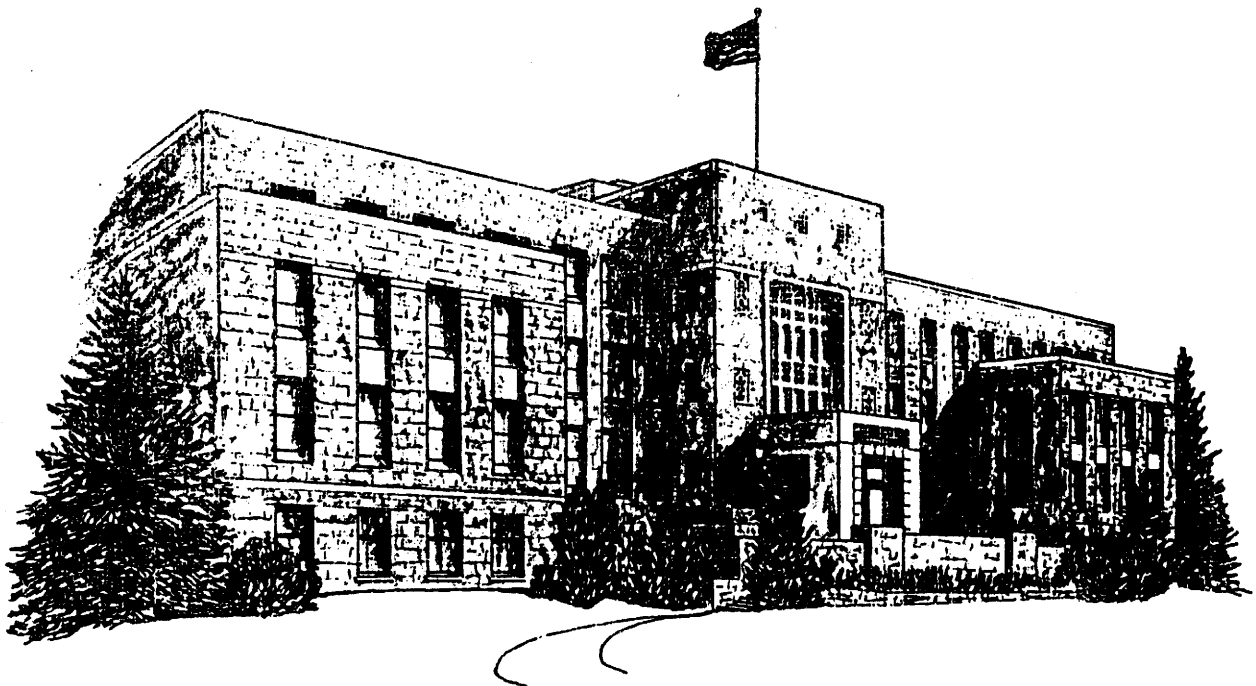
GEOCHEMICAL MODELING RESEARCH RELATED TO THE SURFACE DISPOSAL OF PROCESSED OIL SHALE SOLID WASTE

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GEOCHEMICAL MODELING RESEARCH RELATED TO THE SURFACE DISPOSAL
OF PROCESSED OIL SHALE SOLID WASTE

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ABSTRACT

Several geochemical codes are available in the literature to model

chemical processes such as oxidation-reduction, precipitation-dissolution,

formation of solution complex, adsorption, and ion exchange. However,

these models differ in the environments to which they apply. The objec-

tive of this research was to evaluate the applicability of existing

geochemical codes to predict water quality from an oil shale solid

waste environment. We selected EQ3/EQ6, GEOCHEM, MINTEQ, PHREEQE,

SOLMNEQ, and WATEQFC geochemical models for further evaluation. We

concluded that all these models lack thermodynamic data for minerals

and solution complexes which are important for oil shale solid waste

studies. Selection of any one of the models would require development

of a more reliable thermodynamic database, and this report describes

the initiation of that work. So far, critical evaluation of thermodynam-

ic data has been completed for Sr, F, Mo, and Se.

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INTRODUCTION

A major environmental issue associated with the disposal of pro-
cessed oil shale solid waste is the ability to understand and predict
the quality of water from oil shale solid waste disposal environments.
The behavior in water of potentially hazardous organic and inorganic
chemicals in oil shale solid waste is controlled by a number of chemical
processes such as oxidation-reduction, precipitation-dissolution, forma-
tion of organic and inorganic complexes, adsorption, and ion exchange.
It is necessary to understand these processes in detail to adequately
predict water quality.

Several geochemical codes are available in the literature to model
these chemical processes. However, these models differ in the environ-
ments to which they apply and in their numerical analysis techniques.
Thus, it was necessary to evaluate the applicability of existing geo-
chemical models to predict water quality from oil shale waste disposal
environments.

MATERIALS AND METHODS

In order to evaluate the applicability of existing geochemical
codes for oil shale solid waste, the following criteria were established
for preliminary screening of codes.

1) Is the code in the public domain?

2) Is the code well documented?

3) Is the code in use and being kept updated?

4) Is the code able to model processes of interest, or could it be
    readily modified to include such processes?

Having met these criteria, the following six geochemical codes were obtained and examined in detail:

1) EQ3/EQ6   (Worley, 1979)

2) GEOCHEM   (Sposito and Mattigod, 1980)

3) MINTEQ   (Felmy et al., 1984)

4) PHREEQE   (Parkhurst et al., 1980)

5) SOLMNEQ   (Kharaka and Barens, 1973)

6) WATEQFC   (Runnells and Lindberg, 1981)

RESULTS AND DISCUSSION

Table 1 summarizes the capability of each code to model important processes. The WATEQFC, GEOCHEM, SOLMNEQ, and MINTEQ are speciation/saturation codes. The EQ3/EQ6 and PHREEQE codes model mass transfer as well as speciation/saturation.

The models were difficult to compare with one another. We noted large differences between the equilibrium constants used in the models to make identical calculations (see Table 2). All models worked well for a pH range of 6 to 9. However, the pH of oil shale solid waste water ranges from 2 to 13. All the models lacked thermodynamic data for high temperature minerals (e.g., silicates) and solution complexes (both organic and inorganic) which are important for oil shale solid waste environment studies. It was decided that selection of any one of the models would require the development of a more reliable thermodynamic database.

The establishment of a reliable thermodynamic database requires critical evaluation of thermodynamic data, reviewing available literature, and selecting the most reliable thermodynamic data for minerals

Table 1. Capabilities of Selected Geochemical Codes.

CAPABILITY	1	2	CODE 3	4	5	6
Number of elements	18	44	32	19	24	34
Number of species	140	2000	373	120	181	500
Number of minerals	250	500	238	24	158	375
Speciation/saturation	Yes	Yes	Yes	Yes	Yes	Yes
Adsorption	No	Yes	Yes	No	No	No
Ion exchange	No	Yes	No	No	No	No
Organic complexation	No	Yes	No	No	No	No
Mass transfer	Yes	No	No	Yes	No	No
Temperature range ($°C$)	0-300	1	0-300	–	0-350	25
Pressure range (bars)	1-500	1	–	–	1-1000	1
Database						
easily modified	Yes	Yes	Yes	Yes	No	Yes

1. EQ3/EQ6 (Worley, 1979)

2. GEOCHEM (Sposito and Mattigod, 1980)

3. MINTEQ (Felmy et al. 1984)

4. PHREEQE (Parkhurst et al. 1980)

5. SOLMNEQ (Kharaka and Barnes, 1973)

6. WATEQFC (Runnells and Lindberg, 1981)

Table 2. Comparison of Equilibrium Constants of $SrCO_3(c)$, $BaCO_3(c)$, and $CaF_2(c)$ Used by Different Geochemical Models Along with Recently Reported Values.

Reaction	log equilibrium constant					Recently reported value
	WATEQFC	GEOCHEM	MINTEQ	EQ3/EQ6	PHREEQE	
$SrCO_3(c) \longrightarrow Sr^{2+} + CO_3^{2-}$	-11.41	-9.00	-9.25	-11.70	-9.25	-9.27[1]
$BaCO_3(c) \longrightarrow Ba^{2+} + CO_3^{2-}$	-13.22	-----	-8.58	-13.90	-----	-8.56[2]
$CaF_2(c) \longrightarrow Ca^{2+} + 2F^-$	-10.96	-9.00	-10.96	-10.96	-10.96	-10.41[3]

[1]Reported by Busenberg et al. (1981) in Geochimica Cosmochimica Acta.

[2]Reported by Busenberg et al. (1986) in Geochimica Cosmochimica Acta.

[3]Reported by Elrashidi and Lindsay (1986) in Soil Science Journal.

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and solution complexes that are important for oil shale solid waste
studies. So far, critical evaluations of thermodynamic data have been
completed for Sr, Mo, F, and Se solid phases and solution complexes.
These evaluations are given in Part II.

CONCLUSIONS

On the basis of progress made thus far in this research, the
following conclusions may be drawn:

1) In evaluating available geochemical codes, we noted large
differences between models in the equilibrium constants used to make
identical calculations.

2) All of the models lacked thermodynamic data for high
temperature minerals (e.g., silicates) and solution complexes (both
organic and inorganic) which are important for oil shale solid waste
environment studies.

3) There is need to develop a reliable thermodynamic database for
oil shale solid waste geochemical models.

PART II – CRITICAL EVALUATION OF THERMODYNAMIC DATA
ON Sr, Mo, F, AND Se AT 25°C, 0.1 MPa, ZERO IONIC STRENGTH
FOR OIL SHALE SOLID WASTE GEOCHEMICAL MODEL

INTRODUCTION

The most important references to thermodynamic data on various
elements include Garrels and Christ (1965), Technical Notes of the U.S.
National Bureau of Standards (NBS), Wagman et al. (1968, 1969, 1982),
Smith and Martell (1976), Parker et al. (1971), Stull et al. (1971),
Naumov et al. (1971), and Karapet'yants and Karapet'yants (1970).

Often, large differences are found in the free energy of formation
($\Delta G°f$) values reported by the various compilers. Users of these data
are faced with the frustration of trying to select the best value for
their use. In this report, we have attempted to review the available
literature on thermodynamic, electrochemical, and solubility data of
various compounds to obtain the most reliable values.

Selection criteria:

The free energies of formation ($\Delta G°f$) values showing wide scatter
have been eliminated. In cases where the agreement of $\Delta G°f$ values is
poor, the original sources of the compilers were traced and compared
with other available data to obtain the most reliable values. When
solubility data was available, the $\Delta G°f$ value for a species was
calculated using selected $\Delta G°f$ values of the products and reactants
involved in the equilibrium expression.

Methods of calculating standard free energies of formation ($\Delta G°f$):

The standard free energies of formation of elements (in solid
phases, solution complexes, and ion pairs) compiled in this report

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were calculated from calorimetric, electrochemical, or solubility data. In cases where $\Delta G°f$ was derived from calorimetric data, the standard heat of reaction and entropy of reaction, $\Delta H°r$ and $\Delta s°r$, were evaluated. The standard heat of formation ($\Delta H°f$) and standard entropy ($s°$) were calculated from equations:

$$\Delta H°r = \Sigma \, \Delta H°f \text{ (products)} - \Sigma \, \Delta H°f \text{ (reactants)} \qquad (1)$$
$$\Delta s°r = \Sigma \, \Delta s° \text{ (products)} - \Sigma \, \Delta s° \text{ (reactants)} \qquad (2)$$

The Gibbs free energy of reaction ($\Delta G°r$) was calculated from the equations:

$$\Delta G°r = \Delta H°r - T\Delta s°r \qquad (3)$$
$$\Delta G°r = \Sigma \, \Delta G°f \text{ (products)} - \Sigma \, \Delta G°f \text{ (reactants)} \qquad (4)$$

where $\Delta G°f$ is the standard free energy of formation at $298.15°k$ ($25°C$). When electrochemical data were available, $\Delta G°r$ was calculated from the equation:

$$\Delta G°r = -nFE° \qquad (5)$$

where

$\quad$ n $\;=\;$ Number of moles of electrons participating in the reaction

$\quad$ F $\;=\;$ Faraday constant (96.487 kJ volt^{-1} or 23.061 kcal volt^{-1})

$\quad$ E° $=$ Standard cell potential

When $\Delta G°f$ values were available, $\Delta G°r$ was calculated using equation (4). Once $\Delta G°r$ was known, the equilibrium constant ($k°$) was calculated from the equation:

$$\Delta G°r = -RT \, lnk° \qquad (6)$$

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where

$k°$ = Activity equilibrium constant

R = Universal gas constant (0.00831 kJ/mole or 0.001987 kcal/mole)

T = Absolute temperature

At standard conditions (25°C and 1 atm) equation (6) becomes

$$\log k° = -\frac{\Delta G°r}{1.364} \qquad (7)$$

($\Delta G°f$ in kcal/mole), or

$$\log k° = -\frac{\Delta G°r}{5.707} \qquad (8)$$

($\Delta G°f$ in kJ/mole). Substituting

$$\Delta G°r = \Sigma \ \Delta G°f \ (products) - \Sigma \ \Delta G°f \ (reactants)$$

into equations (7) and (8) gives

$$\log k° = -\frac{1}{1.364} [\Delta G°f \ (products) - \Sigma \ \Delta G°f \ (reactants)] \qquad (9)$$

($\Delta G°f$ in kcal/mole), or

$$\log k° = -\frac{1}{5.707} [\Sigma \ \Delta G°f \ (products) - \Sigma \ \Delta G°f \ (reactants)] \qquad (10)$$

($\Delta G°f$ in kJ/mole).

Discussion of selected values:

The auxiliary data (free energy of formation, $\Delta G°f$) for various anionic species, taken from Sadiq and Lindsay (1979), are listed in Table 3. These data were used to calculate equilibrium constants.

Table 3. Free Energy of Formation ($\Delta G°f$) of Anionic Species Selected from Sadiq and Lindsay (1979) to Calculate Equilibrium Constants.

No.	Species	$\Delta G°f$ (kJ/mole)	(kcal/mole)
1.	Br^-	-104.05	-24.87
2.	$CO_2(g)$	-394.38	-94.26
3.	CO_3^{2-}	-527.94	-126.18
4.	HCO_3^-	-586.89	-140.27
5.	$H_2CO_3^°$	-623.20	-148.95
6.	Cl^-	-131.25	-31.37
7.	C	0.00	0.00
8.	F^-	-284.22	-67.93
9.	H^+	0.00	0.00
10.	OH^-	-157.29	-37.59
11.	H_2O	-237.17	-56.69
12.	I^-	-51.80	-12.38

Table 3. (cont.)

No.	Species	$\Delta G°f$ (kJ/mole)	(kcal/mole)
13.	NO_2^-	-37.74	-9.02
14.	NO_3^-	-111.46	-26.64
15.	PO_4^{3-}	-1025.83	-245.18
16.	HPO_4^{2-}	-1096.34	-262.03
17.	$H_2PO_4^-$	-1137.42	-271.85
18.	$H_3PO_4°$	-1149.68	-274.78
19.	SO_4^{2-}	-744.54	-177.95
20.	SiO_4^{4-}	-1045.96	-249.99
21.	$HSiO_4^{3-}$	-1120.72	-267.86
22.	$H_2SiO_4^{2-}$	-1177.00	-281.31
23.	$H_3SiO_4^-$	-1252.77	-299.42
24.	$H_4SiO_4°$	-1308.17	-312.66

## STRONTIUM

Sr^{2+}

Recommended standard free energy of formation ($\Delta G°f$) of Sr^{2+} ion are summarized below:

Investigator	ΔG°f (kJ/mole)	(kcal/mole)
Wagman et al. (1982)	−559.47	−133.72
Busenberg et al. (1984)	−563.83	−134.76
Robie et al. (1978)	−559.43	−133.70
Parker et al. (1971)	−559.44	−133.71
Naumov et al. (1971)	−571.44	−136.58

Wagman et al. (1982) reported $\Delta G°f$ = −559.47 kJ/mole (−133.72 kcal/mole) from $\Delta H°f$ = −545.80 kJ/mole (−130.45 kcal/mole) and s° = −32.6 J/mole (−7.80 cal/mole). Parker et al. (1971) listed similar value (−559.44 kJ/mole) for Sr^{2+}. Robie et al. (1978) reported $\Delta G°f$ = −559.43 kJ/mole (−133.70 kcal/mole) from Parker et al. (1971). Naumov et al. (1971) recommended $\Delta G°f$ = −571.44 kJ/mole (−136.58 kcal/mole) from pk = 6.78 for the reaction:

$$SrCO_3(c) + CO_2(g) + H_2O = Sr^{2+} + HCO_3^-$$
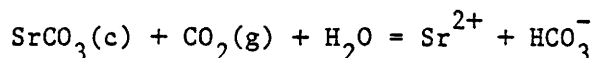
Busenberg et al. (1984) recommended $\Delta G°f$ = −563.83 kJ/mole (−134.76 kcal/mole). Authors reported this value from Khodakovsky et al. (1981).

Khodakovsky et al. (1981) calculated $\Delta G°f$ of Sr^{2+} from $\Delta H°f$ = −551.45 ± 0.59 kJ/mole (−131.80 kcal/mole) and s° = −33.1 ± 2.9 J/mole (7.91 cal/mole) based on their vapor pressure measurements of $Sr(NO_3)_2 \cdot 4H_2O$. The listed $\Delta G°f$ value for Sr^{2+} by Busenberg et al. (1984) is reasonably in agreement with Wagman et al. (1981), Robie et al. (1978), and Parker et al. (1971). Therefore, we adopted $\Delta G°f$ = −563.83 kJ/mole (−134.76 kcal/mole) for Sr^{2+} after Busenberg et al. (1984).

$SrSO_4(c)$

Robie et al. (1978) listed $\Delta G°f = -1340.97$ kJ/mole (-320.50 kcal/mole) from Kelley (1937), Kelley and King (1961), and Parker et al. (1971). Wagman et al. (1982) recommended $\Delta G°f = -1340.89$ kJ/mole (-320.48 kcal/mole) from $\Delta H°f = -1453.10$ kJ/mole (-347.30 kcal/mole) and $s° = 116.98$ J/mole (27.96 cal/mole). Karapet'yants and Karapet'yants (1970) reported $\Delta G°f = -1334.44$ kJ/mole (-318.94 kcal/mole) from $\Delta H°f = -529.70$ kJ/mole (-126.60 kcal/mole).

Helgoson et al. (1978) reported $\Delta G°f = -1340.68$ kJ/mole (-320.43 kcal/mole) for $SrSo_4(c)$ from $\Delta G°f = \Delta H°f - T\Delta s°$. Authors adopted $\Delta H°f = -1453.10$ kJ/mole (-347.30 kcal/mole) and $s° = 117.15$ J/mole (-1353.35 cal/mole) from Wagman et al. (1968, 1969). Naumov et al. (1971) listed $\Delta G°f = -1353.35$ kJ/mole (-323.46 kcal/mole) from $\Delta H°f$ values for the reaction:
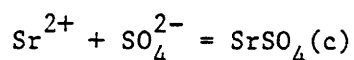
$$Sr^{2+} + SO_4^{2-} = SrSO_4(c)$$

Recently, Reardon and Armstrong (1987) made reliable solubility measurements of $SrSO_4(c)$ and reported pk = 6.63 for the following reaction: $SrSO_4(c) \longrightarrow Sr^{2+} + SO_4^{2-}$. We adopted the above reaction and calculated $\Delta G°f = -1346.16$ kJ/mole (-321.74 kcal/mole) for for $SrSO_4(c)$ using selected $\Delta G°f$ values for Sr^{2+} and SO_4^{2-}.

$SrO(c)$

The standard free energy of formation of $SrO(c)$ ranges from -559.82 kJ/mole (-133.80 kcal/mole) to -574.13 kJ/mole (-137.22 kcal/mole). Recommended $\Delta G°f$ values for $SrO(c)$ by various investigators are summarized below:

| Investigator	$\Delta G°f$ (kJ/mole)	(kcal/mole)
Garrels and Christ (1968)	-559.82	-133.80
Robie et al. (1978)	-560.32	-133.92
Wagman et al. (1982)	-561.87	-134.29
Pankratz (1982)	-560.57	-133.98
Busenberg et al. (1984)	-559.95	-133.83
Karapet'yants and Karapet'yants (1970)	-573.00	-137.07
Naumov et al. (1971)	-574.13	-137.22

Reported $\Delta G°f$ values for $SrO(c)$ agree very well except Karapet'yants and Karapet'yants (1970) and Naumov et al. (1971). Recently Busenberg et al. (1984) critically evaluated $\Delta G°f$ for $SrO(c)$ and recommended -559.95 kJ/mole (-133.83 kcal/mole) from $\Delta H°f$ = -590.57 kJ/mole (-141.15 kcal/mole) and $s°$ = 55.44 J/mole (13.25 kcal/mole).

In this report we selected $\Delta G°f$ = -559.95 kJ/mole (-133.83 kcal/mole) of Busenberg et al. (1984).

$Sr(NO_3)_2(c)$

Robie et al. (1978) reported $\Delta G°f$ = -779.06 kJ/mole (-186.20 kcal/mole). Wagman et al. (1982) listed $\Delta G°f$ = -780.02 kJ/mole (-186.43 kcal/mole) from $\Delta H°f$ = -978.22 kJ/mole (-233.80 kcal/mole) and $s°$ = -194.55 J/mole (-46.50 cal/mole). Naumov et al. (1971) recommended $\Delta G°f$ = -790.40 kJ/mole (-188.91 kcal/mole) from $\Delta H°f$ = 17.53 kJ/mole (4.19 kcal/mole) for the reaction:

$$Sr(NO_3)(c) = Sr^{2+} + 2NO_3^{2-}$$
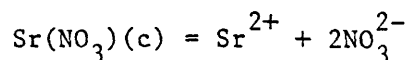
Busenberg et al. (1984) calculated $\Delta G°f$ = -783.28 kJ/mole (-187.21 kcal/mole) from $\Delta H°f$ = -982.36 kJ/mole (-234.79 kcal/mole) and $s°$ = 194.60 J/mole (46.51 cal/mole). Karapet'yants and Karapet'yants (1971) reported $\Delta G°f$ = -778.22 kJ/mole (-186.00 kcal/mole) from approximate calculations of $\Delta H°f$ and $s°$. We adopted $\Delta G°f$ = -783.28 kJ/mole (-187.21 kcal/mole) for $Sr(NO_3)_2(c)$ after Busenberg et al. (1984).

$SrBr_2(c)$

Robie et al. (1978) reported $\Delta G°f$ = -695.89 kJ/mole (-166.32 kcal/mole) from $\Delta H°f$ and $s°$ calculations. Wagman et al. (1982) listed $\Delta G°f$ = -697.10 kJ/mole (-166.61 kcal/mole) from $\Delta H°f$ = -717.60 kJ/mole (-171.51 kcal/mole) and $s°$ = 135.10 J/mole (32.29 cal/mole). Karapet'yants and Karapet'yants (1970) recommended $\Delta G°f$ = -695.80 kJ/mole (-166.30 kcal/mole) from approximate calculations of $\Delta H°f$ and $s°$ values. Pankratz (1984) listed $\Delta G°f$ = -699.77 kJ/mole (-167.25 kcal/mole) from $\Delta H°f$ = -717.97 kJ/mole (-171.60 kcal/mole) and $s°$ = 143.42 J/mole (34.28 cal/mole).

The standard free energy of formation ($\Delta G°f$) for $SrBr_2(c)$ reported by Pankratz (1984) agree well with the values reported by Robie et al. (1978) and Wagman et al. (1982). Therefore, we selected $\Delta G°f$ = -699.77 kJ/mole (-167.25 kcal/mole) of Pankratz (1984).

$SrHPO_4(c)$

Garrels and Christ (1965) reported $\Delta G°f$ = -1672.34 kJ/mole (-399.70 kcal/mole) from $\Delta H°f$ = -1804.56 kJ/mole (-431.30 kcal/mole) and $s°$ = 130.54 J/mole (31.2 cal/mole) from Latimer (1952). However, Latimer (1952) calculated $\Delta G°f$ value for $SrHPO_4(c)$ compound from estimated $s°$ values. Wagman et al. (1982) listed $\Delta G°f$ = -1688.60 kJ/mole (-403.58

kcal/mole) from $\Delta H°f$ = -1821.67 kJ/mole (-435.39 kcal/mole) and s° =
120.96 J/mole (28.91 cal/mole).

Karapet'yants and Karapet'yants (1970) reported $\Delta G°f$ = -1681.13
kJ/mole (-408.80 kcal/mole) from approximate $\Delta H°f$ and s° values. In
this report we adopted $\Delta G°f$ = -1688.60 kJ/mole (-403.58 kcal/mole)
after Wagman et al. (1982).

$SrF_2(c)$

Garrels and Christ (1965) reported $\Delta G°f$ = -1162.31 kJ/mole (-277.80
kcal/mole) from Latimer (1952). However, Latimer (1952) calculated this
value from $\Delta H°f$ = -1214.61 kJ/mole (-290.30 kcal/mole) and estimated s°
of 89.53 J/mole (21.40 cal/mole). Karapet'yants and Karapet'yants
(1970) reported $\Delta G°f$ = -1162.31 kJ/mole (-277.80 kcal/mole) for $SrF_2(c)$.

Pankratz (1984) reported $\Delta G°f$ = -1164.74 kJ/mole (-278.38
kcal/mole) from $\Delta H°f$ = -1216.28 kJ/mole (-290.70 kcal/mole) and s° =
-82.13 J/mole (-19.63 cal/mole) from Parker et al. (1971). Naumov et
al. (1971) reported $\Delta G°f$ = -1180.56 kJ/mole (-282.16 kcal/mole) from pk
= 8.61 for the reaction:

$$SrF_2(c) = Sr^{2+} + 2F^-$$
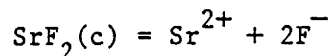
Wagman et al. (1982) recommended $\Delta G°f$ = -1164.57 kJ/mole (-278.34
kcal/mole) from $\Delta H°f$ = -1216.28 kJ/mole (-290.70 kcal/mole) and s° =
82.13 J/mole (19.63 cal/mole). No other information is available to
evaluate $\Delta G°f$ for this compound. In this report we selected $\Delta G°f$ =
-1180.56 kJ/mole (-282.16 kcal/mole) of Naumov et al. (1971).

$SrCrO_4(c)$

Latimer (1952) reported $\Delta G°f$ = -1319.21 kJ/mole (-315.30 kcal/mole)
for $SrCrO_4(c)$. No other information is available. Naumov et al. (1971)

listed $\Delta G°f$ = -1318.37 kJ/mole (-315.10 kcal/mole) from pk = 4.65 ± 0.1

for the reaction:

$$SrCrO_4(c) = Sr^{2+} + CrO_4^{2-}$$
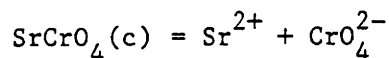
Reported $\Delta G°f$ values for $SrCrO_4(c)$ agree well. Therefore, we adopted

$\Delta G°f$ = -1318.37 kJ/mole (-315.10 kcal/mole) after Naumov et al. (1971).

$SrSeO_3(c)$

Naumov et al. (1971) reported $\Delta G°f$ = -969.43 kJ/mole (-231.70
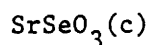
kcal/mole) from pk = 6.10 for the reaction:

$$SrSeO_3(c) = Sr^{2+} + SeO_3^{2-}$$
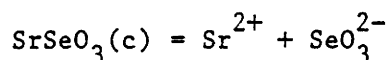
Karapet'yants and Karapet'yants (1970) listed $\Delta G°f$ = -965.83 kJ/mole

(-230.84 kcal/mole) from approximate $\Delta H°f$ and s° values. No further

information is available. Therefore, we selected $\Delta G°f$ = -969.43

kJ/mole (-231.70 kcal/mole) after Naumov et al. (1971).

$Sr_2TiO_4(c)$
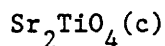
Naumov et al. (1970) listed $\Delta G°f$ = -2196.01 kJ/mole (-524.86

kcal/mole) from $\Delta H°f$ = -158.36 kJ/mole (-37.85 kcal/mole) for the

reaction:

$$2SrO(c) + TiO_2 \text{ (rutile)} = Sr_2TiO_4(c)$$
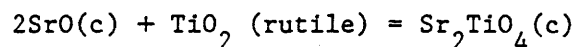
Parker et al. (1971) reported $\Delta G°f$ = -2178.60 kJ/mole (-520.70

kcal/mole) from $\Delta H°f$ = -2287.40 kJ/mole (-546.70 kcal/mole) and s° =

159.00 J/mole (38.00 cal/mole). Wagman et al. (1982) $\Delta G°f$ = -2172.30

kJ/mole (-519.19 kcal/mole) from $\Delta H°f$ = -2287.40 kJ/mole (-546.70

kcal/mole) and s° = 159.00 J/mole (38.00 cal/mole). Therefore, we

selected $\Delta G°f$ = -2196.01 kJ/mole (-524.86 kcal/mole) after Naumov et
et al. (1971).

SrOH$^+$

Recommended $\Delta G°f$ values for SrOH$^+$ species are listed below:

Investigator	$\Delta G°f$ (kJ/mole)	(kcal/mole)
Parker et al. (1971)	-721.32	-172.40
Wagman et al. (1982)	-721.32	-172.40
Naumov et al. (1971)	-733.46	-175.30

Parker et al. (1971) recommended $\Delta G°f$ = -721.32 kJ/mole (-172.40
kcal/mole). No further information is available to evaluate this value.
Wagman et al. (1982) also reported similar (-721.32 kJ/mole) value for
SrOH$^+$ species. The source was not documented.

Naumov et al. (1971) listed $\Delta G°f$ = -733.46 kJ/mole (-175.30
kcal/mole) from pK = 0.82 and s° = -4.81 J/mole (-1.15 cal/mole) for the
reaction:

$$SrOH^+ = Sr^{2+} + OH^-$$
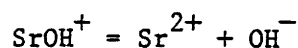
We selected $\Delta G°f$ = -733.46 kJ/mole (-175.30 kcal/mole) for SrOH$^+$ after
Naumov et al. (1970).

SrSO$_4^°$

Wagman et al. (1982) recommended $\Delta G°f$ = -1304.03 kJ/mole (-311.67
kcal/mole) from $\Delta H°f$ and s° values. Sposito and Mattigod (1980)
estimated equilibrium constant for the following equation:

$$Sr^{2+} + SO_4^{2-} \longrightarrow SrSO_4^{\circ} = 10^{2.20}$$
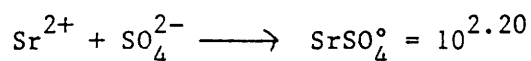
Smith and Martell (1978) reported equilibrium constant of $10^{2.55}$ for the same reaction:

$$Sr^{2+} + SO_4^{2-} \longrightarrow SrSO_4^{\circ}$$
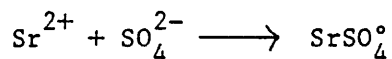
No other information is available to evaluate $\Delta G°f$ of $SrSO_4^{\circ}$. Therefore, we selected Smith and Martell (1978) equilibrium constant for the above reaction and calculated $\Delta G°f = -1320.89$ kJ/mole (-315.70 kcal/mole) for $SrSO_4^{\circ}$ species.

$SrCO_3$ (Strontianite)

The reported $\Delta G°f$ values range from -1137.64 to -1152.31 kJ/mole (-271.90 to -275.40 kcal/mole). Naumov et al. (1971) listed $\Delta G°f = -1152.31$ kJ/mole (-275.40 kcal/mole) for $SrCO_3(c)$. This value was calculated from $\Delta H°f = -982.02$ kJ/mole (-234.71 kcal/mole) for the reaction:

$$SrO(c) + CO_2(g) = SrCO_3(c)$$
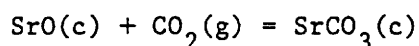
Khodakovsky et al. (1981) reported $\Delta G°f = -114.72$ kJ/mole (-273.60 kcal/mole), based on their vapor pressure measurements of $Sr(NO_3)_2 \cdot 4H_2O(c)$ and $\Delta H°f$ and $s°$ values. Wagman et al. (1982) listed $\Delta G°f = -1140.10$ kJ/mole (-272.49 kcal/mole). Karapet'yants and Karapet'yants (1970) listed $\Delta G°f = -1138.13$ kJ/mole (-272.02 kcal/mole) from approximate calculations of $\Delta H°f$ and $s°$ values. Robie et al. (1978) reported $\Delta G°f = -1137.63$ kJ/mole (-271.90 kcal/mole).

The reported $\Delta G°f$ values for $SrCO_3(c)$ in literature differ significantly. Therefore, further investigation was done to obtain a reliable value for $SrCO_3(c)$. The equilibrium constant ($logk°$) for the following reaction:

$$SrCO_3(c) \longrightarrow Sr^{2+} + CO_3^{2-}$$
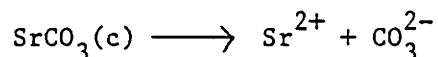
reported by the various investigators and geochemical models are listed below:

Investigator/Geochemical Model	$logk°$
Naumov et al. (1971)	-9.28
Busenberg et al. (1984)	-9.27
WATEQ-2, Ball et al. (1980)	-9.25
PHREEQE, Parkhurst et al. (1980)	-9.25
Smith and Martell (1976)	-9.03
GEOCHEM, Sposito and Mattigod (1980)	-9.00

Naumov et al. (1971) reported a value of -9.28 from products of activities of substances involved in the reaction. However, further information was not available to evaluate this value. Equilibrium constants reported by WATEQ-2, PHREEQE, and Busenberg et al. (1984) agree fairly well, except Smith and Martell (1976) and GEOCHEM.

Recently, Busenberg et al. (1984) made reliable solubility measurements for $SrCO_3$ (Strontianite) in $CO_2 - H_2O$ system between 2 and 91°C. Authors also made corrections for temperature, ionic strength, and solution complexes. Therefore, we selected $logk°$ of -9.271 after Busenberg et al. (1984). The $\Delta G°f$ value for $SrCO_3(c)$ was then

calculated to be −1144.63 kJ/mole (−273.33 kcal/mole) with selected $\Delta G°f$ values of Sr^{2+} and CO_3^{2-}.

$SrSiO_3(c)$

Naumov et al. (1971) listed $\Delta G°f$ = −1561.64 kJ/mole (−373.24 kcal/mole) from $\Delta H°f$ = −546.85 kJ/mole (−130.70 kcal/mole) for the reaction:

$$SrO(c) + SiO_2 \ (\ - \ Quartz) \longrightarrow SrSiO_3(c)$$
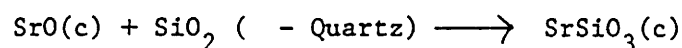
Karapet'yants and Karapet'yants (1971) reported $\Delta G°f$ = −1467.75 kJ/mole (−350.80 kcal/mole). Where as Wagman et al. (1981) listed $\Delta G°f$ = −1549.70 kJ/mole (−370.39 kcal/mole). The source of information was not documented. Therefore, at present we adopted $\Delta G°f$ = −1561.64 kJ/mole (−373.24 kcal/mole) after Naumov et al. (1971).

$Sr_2SiO_4(c)$

Wagman et al. (1982) listed $\Delta G°f$ = −2191.10 kJ/mole (−523.68 kcal/mole). Naumov et al. (1971) reported $\Delta G°f$ = −2215.09 kJ/mole (−529.42 kcal/mole) from $\Delta H°f$ = −876.00 kJ/mole (−209.37 kcal/mole) for the reaction:

$$2SrO + SiO_2 \ (\ - \ Quartz) = Sr_2SiO_4(c)$$
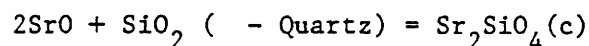
Garrels and Christ (1968) and Karapet'yants and Karapet'yants (1970) listed $\Delta G°f$ = −2074.00 kJ/mole (−495.70 kcal/mole) from Latimer (1952). No further information is available for this compound. We tentatively adopted $\Delta G°f$ = −2191.10 kJ/mole (−523.68 kcal/mole) after Wagman et al. (1982).
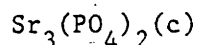
$Sr_3(PO_4)_2(c)$

Garrels and Christ (1965) reported $\Delta G°f$ = -3899.90 kJ/mole (-932.10 kcal/mole) for this compound. Authors listed this value from Latimer (1956). No further information is available on $\Delta G°f$ of $Sr_3(PO_4)_2(c)$ in the literature. We adopted the value reported by Garrels and Christ (1968).
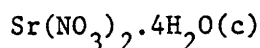
$Sr(NO_3)_2 \cdot 4H_2O(c)$

Busenberg et al. (1984) critically evaluated $\Delta G°f$ of $Sr(NO_3)_2 \cdot 4H_2O(c)$ and recommended -1734.19 kJ/mole (-414.48 kcal/mole). Karapet'yants and Karapet'yants (1970) listed $\Delta G°f$ = -1725.48 kJ/mole (-412.40 kcal/mole) from $\Delta H°f$ and $s°$ calculations. We adopted $\Delta G°f$ = -1734.19 kJ/mole (-414.48 kcal/mole) after Busenberg et al. (1984) for this compound.

$SrCl_2(c)$
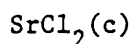
Garrels and Christ (1956) listed $\Delta G°f$ = -781.15 kJ/mole (-186.70 kcal/mole) from Rossini et al. (1952). Latimer (1952) reported $\Delta G°f$ = -781.15 kJ/mole (-186.70 kcal/mole) value calculated from $\Delta H°f$ = -828.43 kJ/mole (-198.00 kcal/mole) and $s°$ = 117.15 J/mole (28.00 cal/mole). Wagman et al. (1982) listed $\Delta G°f$ = -781.10 J/mole (-186.69 kcal/mole). Pankratz (1984) reported $\Delta G°f$ = -781.02 kJ/mole (-186.67 kcal/mole) from $\Delta H°f$ and $s°$ values. Busenberg et al. (1984) recommended $\Delta G°f$ = -785.00 kJ/mole (-187.62 kcal/mole). This value calculated from $\Delta H°f$ = -833.85 kJ/mole (-199.30 kcal/mole) and $s°$ = 114.85 J/mole (27.50 cal/mole). $\Delta G°f$ value reported by Busenberg et al. (1984) agree very well with the other values. Therefore, we adopted Busenberg et al. (1984) recommended value -785.00 kJ/mole (-187.62 kcal/mole) for this compound.

$SrCl_2 \cdot H_2O(c)$
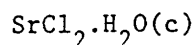
Wagman et al. (1982) reported $\Delta G°f = -1036.30$ kJ/mole (-247.68 kcal/mole). Karapet'yants and Karapet'yants (1971) reported $\Delta G°f = -1038.47$ kJ/mole (-248.20 kcal/mole) from approximate calculations of $\Delta H°f$ and s° values. This value is questionable. At present, we adopted $\Delta G°f = -1036.30$ kJ/mole (-247.68 kcal/mole) reported by Wagman et al. (1982) for this compound.

$SrBr_2 \cdot H_2O(c)$
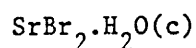
Wagman et al. (1982) reported $\Delta G°f = -954.30$ kJ/mole (-228.08 kcal/mole). No further information is available. We adopted $\Delta G°f = -954.30$ kJ/mole (-228.08 kcal/mole) after Wagman et al. (1982).

$Sr_3(ASO_4)_2(c)$
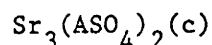
Latimer (1952) reported $\Delta G°f = -3222.10$ kJ/mole (-770.10 kcal/mole) from $\Delta H°f = -3350.13$ kJ/mole (-800.70 kcal/mole) and s° = 312.12 J/mole (-74.60 cal/mole) values. However, s° value was estimated. Recently, Wagman et al. (1982) recommended $\Delta G°f = -3080.10$ kJ/mole (-736.16 kcal/mole) from $\Delta H°f$ and s° values. Therefore, we adopted the Wagman et al. (1982) value.

$SrSeO_4(c)$
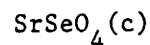
Naumov et al. (1971) reported $\Delta G°f = -1039.14$ kJ/mole (-248.36 kcal/mole) from $\Delta H°f = 2.42$ kJ/mole (0.58 kcal/mole) and from pk = 4.60 for the reaction:

$$SrSeO_4(c) = Sr^{2+} + SeO_4^{2-}$$
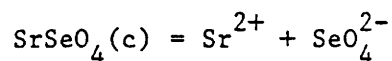
Karapet'yants and Karapet'yants (1970) listed $\Delta G°f = -1023.87$ kJ/mole

(-244.71 kcal/mole) from $\Delta H°f$ and $s°$ values. Since Naumov et al. (1971) reported $\Delta G°f$ from pk values, we adopted their value.

$SrMoO_4(c)$

Naumov et al. (1971) listed $\Delta G°f$ = -1454.36 kJ/mole (-347.60 kcal/mole) from $\Delta H°f$ = 19.24 kJ/mole (-4.60 kcal/mole) and pk = 7.89 for the reaction:

$$SrMoO_4(c) = Sr^{2+} + MoO_4^{2-}$$
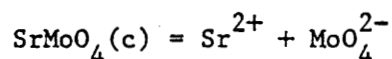
Karapet'yants and Karapet'yants (1970) reported -1448.50 kJ/mole (-346.20 kcal/mole) from $\Delta H°f$ and $s°$ values. No further information is available. Therefore, we adopted $\Delta G°f$ = -1454.36 kJ/mole (-347.60 kcal/mole) for $SrMoO_4(c)$ after Naumov et al. (1971).

$Sr(OH)_2(c)$

Garrels and Christ (1965) reported $\Delta G°f$ = -869.43 kJ/mole (-207.80 kcal/mole) from Latimer (1952). Latimer (1952) calculated this value from $\Delta H°f$ = -959.39 kJ/mole (-229.30 kcal/mole) and $s°$ value of 87.86 J/mole (-21.00 kcal/mole). Karapet'yants and Karapet'yants (1970) reported $\Delta G°f$ = 870.27 kJ/mole (-208.00 kcal/mole). Both $\Delta G°f$ values for $Sr(OH)_2(c)$ agree very well. Therefore, we adopted $\Delta G°f$ = -870.27 kJ/mole (-208.00 kcal/mole) for this compound after Karapet'yants and Karapet'yants (1970).

$SrI_2(c)$

Karapet'yants and Karapet'yants (1970) reported $\Delta G°f$ = -562.33 kJ/mole (-134.40 kcal/mole) from approximate $\Delta H°f$ and $s°$ values. Pankratz (1984) recommended $\Delta G°f$ = -558.71 kJ/mole (-133.53 kcal/mole)

from $\Delta H°f$ = -561.69 kJ/mole (-134.24 kcal/mole) and $s°$ = 159.12 J/mole (-38.03 cal/mole). We adopted $\Delta G°f$ = -558.71 kJ/mole (-133.53 kcal/mole) after Pankratz (1984) for this compound.

$SrTiO_3(c)$

Naumov et al. (1971) reported $\Delta G°f$ = -1600.38 kJ/mole (-382.50 kcal/mole). The enthalpy of formation is determined from average of $\Delta H°f$ (298.18) = -1684.48 ± 4.184 kJ/mole (-402.60 kcal/mole). The $\Delta H°f$ = 99.16 ± 0.83 J/mole (-23.70 cal/mole) for the reaction:

$$SrCO_3(c) + TiO_2 \text{ (rutile)} = SrTiO_3(c) + CO_2(g)$$
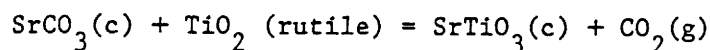
Similar $\Delta H°f$ = -1684.64 ± 4.184 kJ/mole (-402.64 kcal/mole) was calculated from $\Delta H°f$ = -135.770 ± 1.04 kJ/mole (-32.45 kcal/mole) from the reaction:

$$SrO(c) + TiO_2 \text{ (rutile)} = SrTiO_3(c)$$
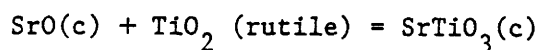
Parker et al. (1971) reported $\Delta G°f$ = -1588.41 kJ/mole (-379.64 kcal/mole) from $\Delta H°f$ = -1672.38 kJ/mole (-399.70 kcal/mole) and $s°$ = 108.78 J/mole (25.00 kcal/mole). Wagman et al. (1982) reported $\Delta G°f$ = -1588.36 kJ/mole (-379.62 kcal/mole) from $\Delta H°f$ = -1672.38 kJ/mole (-399.70 kcal/mole) and $s°$ = 108.87 J/mole (26.02 cal/mole). We selected $\Delta G°f$ = -1600.38 kJ/mole (-382.50 kcal/mole) after Naumov et al. (1971).

$SrZrO_3(c)$

Naumov et al. (1971) reported $\Delta G°f$ = -2548.89 kJ/mole (-609.20 kcal/mole) from $\Delta H°f$ = -2904.20 kJ/mole (-694.12 kcal/mole) for the reaction:

$$SrCO_3(c) + ZrO_2(c) = SrZrO_3(c) + CO_2(g)$$
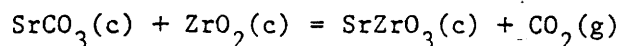
Parker et al. (1971) listed $\Delta G^\circ f$ = -1682.80 kJ/mole (-402.20 kcal/mole) from $\Delta H^\circ f$ = -1767.32 kJ/mole (-422.40 kcal/mole) and s° = 115.06 J/mole (27.50 cal/mole). Wagman et al. (1982) reported $\Delta G^\circ f$ = -1682.80 kJ/mole (-402.20 kcal/mole) from $\Delta H^\circ f$ = -1767.30 kJ/mole and s° = 115.10 J/mole (27.51 cal/mole). We adopted $\Delta G^\circ f$ = -1682.79 kJ/mole (-402.20 kcal/mole) after Wagman et al. (1982).

$SrHCO_3^+$
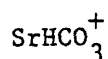
Busenberg et al. (1984) recommended $\Delta G^\circ f$ = -1157.50 kJ/mole (-276.65 kcal/mole) from $\Delta H^\circ f$ = -1215.53 kJ/mole (-290.52 kcal/mole) and s° = 174.39 J/mole (41.68 cal/mole). No other information is available. Therefore, we adopted $\Delta G^\circ f$ = -1157.50 kJ/mole (-276.65 kcal/mole after Busenberg et al. (1984).

$SrCO_3^\circ$

Wagman et al. (1982) reported $\Delta G^\circ f$ = -1087.30 kJ/mole (-259.87 kcal/mole) from $\Delta H^\circ f$ = -1222.94 kJ/mole (-292.29 kcal/mole) and s° = -87.50 J/mole (-21.39 cal/mole). Parker et al. (1971) reported $\Delta G^\circ f$ = -1087.33 kJ/mole (-259.88 kcal/mole) from $\Delta H^\circ f$ = -1222.94 kJ/mole (-292.29 kcal/mole) and s° = 89.53 J/mole (-21.40 cal/mole). Busenberg et al. (1984) reported $\Delta G^\circ f$ = -1175.50 kJ/mole (-280.95 kcal/mole) from $\Delta H^\circ f$ = -1226.12 kJ/mole (-293.05 kcal/mole) and s° = -81.46 J/mole (-19.47 cal/mole). Since reported $\Delta G^\circ f$ values for $SrCO_3$ agree very well, we selected $\Delta G^\circ f$ = -1175.50 kJ/mole (-280.95 kcal/mole) for $SrCO_3$ species after Busenberg et al. (1984).

$Sr(NO_3)_2^\circ$
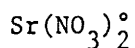
Wagman et al. (1982) reported $\Delta G°f$ = -781.99 kJ/mole (-186.90 kcal/mole) from $\Delta H°f$ = -960.52 kJ/mole (-229.57 kcal/mole) and $s°$ = 260.20 J/mole (-62.19 cal/mole). No other information is available. Therefore, we adopted $\Delta G°f$ = -781.99 kJ/mole (-186.90 kcal/mole) after Wagman et al. (1982).

$SrCl_2^\circ$

Wagman et al. (1982) listed $\Delta G°f$ = -821.90 kJ/mole (-196.44 kcal/mole) from $\Delta H°f$ = -880.10 kJ/mole (-210.35 kcal/mole) and $s°$ = 80.29 J/mole (-19.19 cal/mole). We adopted $\Delta G°f$ = -821.90 kJ/mole (-196.44 kcal/mole) after Wagman et al. (1982).

SrI_2°

Only Wagman et al. (1982) reported $\Delta G°f$ = -662.62 kJ/mole (-158.37 kcal/mole). No other information is available. Therefore, we adopted $\Delta G°f$ value from Wagman et al. (1982) for this species.

$SrBr_2^\circ$

Parker et al. (1971) reported $\Delta G°f$ = -767.38 kJ/mole (-183.41 kcal/mole) from $\Delta H°f$ = -788.89 kJ/mole (-188.55 kcal/mole) and $s°$ = 132.21 J/mole (-31.60 cal/mole). No other information is available. Therefore, we adopted $\Delta G°f$ = -763.38 kJ/mole (-183.41 kcal/mole) after Parker et al. (1971) for this species.

FLUORINE

F^-

Wagman et al. (1982) reported $\Delta G°f$ = -278.79 kJ/mole (-66.63 kcal/mole) from $\Delta H°f$ = -332.63 kJ/mole (-79.50 kcal/mole) and $s°$ = -13.8

J/mole (−3.29 cal/mole). Sadiq and Lindsay (1979) used $\Delta H°f = -335.34$ kJ/mole (−80.15 kcal/mole) of Johnson et al. (1973) and $s° = -13.18$ J/mole (−3.15 cal/mole) of CODATA (1976) to calculate $\Delta G°f = -284.22$ kJ/mole (−67.93 kcal/mole) for F^- species.

Robie et al. (1978) recommended $\Delta G°f = -281.70$ kJ/mole (−67.33 kcal/mole) from $\Delta H°f = -335.350$ kJ/mole (−80.15 kcal/mole) which is similar to Sadiq and Lindsay (1979) selection to calculate $\Delta G°f$ for F^- species. Recently, Elrashidi and Lindsay (1984) critically evaluated standard free energies of formation of F species and reported $\Delta G°f = -284.22$ kJ/mole (−67.93 kcal/mole). In this report we selected $\Delta G°f = -284.22$ kJ/mole (−67.93 kcal/mole) after Sadiq and Lindsay (1979).

HF°

Naumov et al. (1971) used pk = 3.180 and 3.173 for the reaction:

$$HF° \longrightarrow F^- + H^+$$
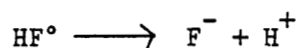
after Ellis (1963), and Broene and Devries (1947) to calculate the mean $\Delta G°f = -298.11$ kJ/mole (−71.25 kcal/mole). Wagman et al. (1982) recommended $\Delta G°f = -296.82$ kJ/mole (−70.94 kcal/mole) from $\Delta H°f = -320.08$ kJ/mole (−76.50 kcal/mole) and $s° = 88.7$ J/mole (21.20 cal/mole).

We adopted $\Delta G°f = -296.82$ kJ/mole (−70.94 kcal/mole) after Wagman et al. (1982).

HF_2^-

Naumov et al. (1971) calculated $\Delta G°f = -581.50$ kJ/mole (−138.98 kcal/mole) from pk = 0.59 for the reaction:

$$HF_2^- \longrightarrow HF° + F^-$$
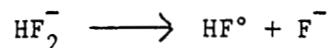
after Broene and Devries (1947). Authors also calculated s° = 67.78 J/mole (16.2 cal/mole) from S°r = 7.99 J/mole (1.91 cal/mole) for the equation:

$$LiHF_2(c) \longrightarrow Li^+ + HF_2^-$$
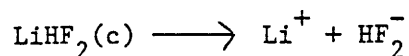
after Cox and Harrop (1965).

Wagman et al. (1982) listed $\Delta G°f$ = -578.08 kJ/mole (-138.16 kcal/mole) from $\Delta H°f$ = -649.94 kJ/mole (-155.34 kcal/mole) and s° = 92.5 J/mole (22.10 cal/mole).

In this report, we selected $\Delta G°f$ = -578.08 kJ/mole (-138.16 kcal/mole) after Wagman et al. (1982) for HF^- species.

AlF_2^+

Sadiq and Lindsay (1979) reported $\Delta G°f$ = -1131.27 kJ/mole (-270.38 kcal/mole) from Baumann (1969) measurements on pk = 5.62 ± 0.04 for reaction:

$$AlF_2^+ \longrightarrow AlF^{2+} + F^-$$
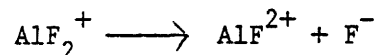
Smith and Martell (1976) listed pk = 12.60 for the reaction:

$$AlF_2^+ \longrightarrow Al^{3+} + 2F^-$$
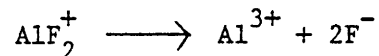
Wagman et al. (1982) reported $\Delta G°f$ = -1113.00 kJ/mole (-266.01 kcal/mole) which agree with the value reported by Sadiq and Lindsay (1979).

We selected $\Delta G°f$ = -1131.27 kJ/mole (-270.38 kcal/mole) after Sadiq and Lindsay (1979) for our purpose.

AlF^{2+}

Naumov et al. (1971) reported $\Delta G°f = -811.82$ kJ/mole (-194.03 kcal/mole). Authors based their calculation on pk = 6.98 for the reaction:

$$AlF^{2+} \longrightarrow Al^{3+} + F^-$$
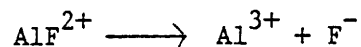
adopted from the solubility measurements of Baumann (1969). Where as Brosset (1941), Paul (1955), and Smith and Martell (1976) reported pk = 7.0 for the above reaction. Sadiq and Lindsay (1979) selected pk = 6.98 for the reaction:

$$AlF_2^{2+} \longrightarrow Al^{3+} + 2F^-$$
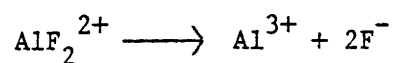
and calculated $\Delta G°f$ to be -814.96 kJ/mole (-194.78 kcal/mole). Wagman et al. (1982) reported $\Delta G°f = -803.00$ kJ/mole (-191.92 kcal/mole).

We selected $\Delta G°f = -814.96$ kJ/mole (-194.78 kcal/mole) after Sadiq and Lindsay (1979).

$AlF_3°$

Naumov et al. (1971) listed $\Delta G°f = -1427.03$ kJ/mole (-341.07 kcal/mole). Smith and Martell (1976) recommended pk = 16.7 for the reaction:

$$AlF_3° \longrightarrow Al^{3+} + 3F^-$$
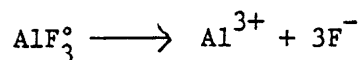
which determined $\Delta G°f = -1438.88$ kJ/mole (-343.90 kcal/mole) for $AlF_3°$ species. Baumann (1969) reported pk = 4.05 for the reaction:

$$AlF_3° \longrightarrow AlF_2^+ + F^-$$
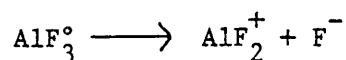
This pk calculated $\Delta G°f$ = -1438.58 kJ/mole (-343.83 kcal/mole). Sadiq and Lindsay (1979) reported $\Delta G°f$ = -1438.58 kJ/mole (-343.83 kcal/mole) based on the solubility measurements of Baumann (1969). Wagman et al. (1982) reported $\Delta G°f$ = -1414.00 kJ/mole (-337.95 kcal/mole) from $\Delta H°f$ = -1519.00 kJ/mole (-363.05 kcal/mole) and s° = -25.00 J/mole (-5.97 cal/mole).

In this report, we selected $\Delta G°f$ = -1438.58 kJ/mole (-343.83 kcal/mole) after Sadiq and Lindsay (1979).

AlF_4^-

Naumov et al. (1971) $\Delta G°f$ = -1720.63 kJ/mole (-411.24 kcal/mole) from pk = -2.39 for the reaction:

$$AlF_4^- \longrightarrow AlF_3^° + F^-$$
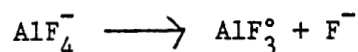
Smith and Martell (1976) recommended pk = 19.1 for the reaction:

$$AlF_4^- \longrightarrow Al^{3+} + 4F^-$$
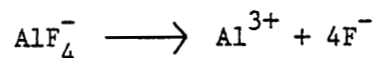
Sadiq and Lindsay (1979) calculated $\Delta G°f$ = -1736.40 kJ/mole (-415.01 kcal/mole) from pk = -2.39 recommended by Naumov et al. (1971). Therefore, we selected $\Delta G°f$ = -1736.40 kJ/mole (-415.01 kcal/mole) for this species.

FeF^{2+}

Wagman et al. (1982) reported $\Delta G°f$ = -322.60 kJ/mole (-77.10 kcal/mole) from $\Delta H°f$ = -371.10 kJ/mole (-88.70 kJ/mole) and s° = -163.00 kJ/mole (-38.96 kJ/mole). Naumov et al. (1971) listed $\Delta G°f$ = -332.33 kJ/mole (-79.43 kcal/mole). Authors based their calculations on pk = 6.04 for the reaction:

$$FeF^{2+} \longrightarrow Fe^{3+} + F^-$$
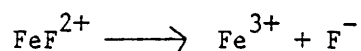
given by Davies (1938a and 1938b). Where as Ashland (1967) and Smith and Martell (1976) recommended pk = 6.03 and 6.00, respectively for the above reaction. Sadiq and Lindsay (1979) selected pk = 6.00 and calculated $\Delta G°f$ = -335.30 kJ/mole (-80.14 kcal/mole) for FeF^{2+} species.

In this report, we selected $\Delta G°f$ = -335.30 kJ/mole (-80.14 kcal/mole) after Sadiq and Lindsay (1979).

$FeF_2°$

Wagman et al. (1982) reported $\Delta G°f$ = -636.48 kJ/mole (-152.12 kcal/mole) from $\Delta H°f$ = -754.40 kJ/mole (-180.30 kcal/mole) and s° = -165.30 J/mole (-39.50 cal/mole). No other information was available. Therefore, we selected $\Delta G°f$ = -636.48 kJ/mole (-152.12 kcal/mole) after Wagman et al. (1982).

FeF_2^+

Wagman et al. (1982) reported $\Delta G°f$ = -628.40 kJ/mole (-150.19 kcal/mole) from $\Delta H°f$ = -696.20 kJ/mole (-166.40 kcal/mole) and s° = -63.00 J/mole (-15.05 cal/mole). Elrashidi and Lindsay (1984) recommended $\Delta G°f$ = -645.55 kJ/mole (-154.29 kcal/mole) from $\Delta H°f$ = -696.21 kJ/mole (-166.40 kcal/mole) and s° = -62.76 J/mole (-15.00 cal/mole).

Sadiq and Lindsay (1979) listed $\Delta G°f$ = -637.76 kJ/mole (-152.43 kcal/mole) from pk = 9.2 for the reaction:

$$FeF_2^+ \longrightarrow Fe^{3+} + 2F^-$$
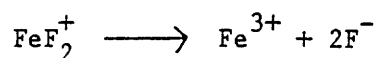
after Smith and Martell (1976). We selected $\Delta G°f$ = -637.76 kJ/mole (-152.43 kcal/mole) after Sadiq and Lindsay (1984).

FeF_3°

Sadiq and Lindsay (1979) reported $\Delta G^\circ f$ = -936.25 kJ/mole (-233.77 kcal/mole) from pk = 11.7 for the reaction:

$$FeF_3^\circ \longrightarrow Fe^{3+} + 3F^-$$
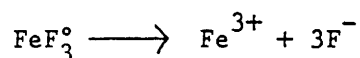
after Smith and Martell (1976). No other information was available. Therefore, we adopted $\Delta G^\circ f$ = -936.25 kJ/mole (-223.77 kcal/mole) after Sadiq and Lindsay (1979).

PbF^+

Naumov et al. (1971) listed $\Delta G^\circ f$ = -311.70 kJ/mole (-74.50 kcal/mole). Wagman et al. (1982) reported $\Delta G^\circ f$ = -310.37 kJ/mole (-74.18 kcal/mole). No other information was available. The value reported by Naumov et al. (1971) was based on pk = 1.26 for the reaction:

$$PbF^+ \longrightarrow Pb^{2+} + F^-$$
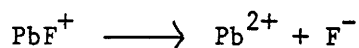
determined at ionic strength (u) = 2.0. Sadiq and Lindsay (1979) reported $\Delta G^\circ f$ = -317.40 kJ/mole (-75.86 kcal/mole) from pk = 1.65 at u=0.

We selected $\Delta G^\circ f$ = -317.40 kJ/mole (-75.86 kcal/mole) for PbF^+ species after Sadiq and Lindsay (1979).

PbF_2°

Sadiq and Lindsay (1979) calculated $\Delta G^\circ f$ = -606.09 kJ/mole (-164.86 kcal/mole) for PbF_2° species after the solubility measurements of Talipov and Kutumova (1956). Naumov et al. (1971) calculated $\Delta G^\circ f$ = -597.47 kJ/mole (-142.80 kcal/mole) from pk = 2.27 for the equation:

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$$PbF_2^\circ \longrightarrow Pb^{2+} + 2F^-$$
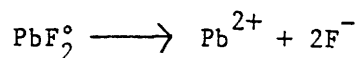
Wagman et al. (1982) reported $\Delta G^\circ f = -596.60$ kJ/mole (-142.60 kcal/mole) but their source was not known. In this report, we selected $\Delta G^\circ f = -606.09$ kJ/mole (-144.86 kcal/mole) after Sadiq and Lindsay (1979).

PbF_3^-

Sadiq and Lindsay (1979) recommended $\Delta G^\circ f = -896.84$ kJ/mole (-214.35 kcal/mole) for PbF_3^- species from pk = 3.42 reported by Talipov and Kutumova (1956). Naumov et al. (1971) reported $\Delta G^\circ f = -884.08$ kJ/mole (-211.30 kcal/mole) but their source was not known. Therefore, we adopted $\Delta G^\circ f = -896.84$ kJ/mole (-216.35 kcal/mole) after Sadiq and Lindsay (1979).

PbF_4^{2-}

Sadiq and Lindsay (1979) recommended $\Delta G^\circ f = -1179.26$ kJ/mole (-281.85 kcal/mole) from pk = 3.1 reported by Talipov and Kutumova (1956) for the reaction:

$$PbF_4^{2-} \longrightarrow Pb^{2+} + 4F^-$$
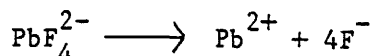
No other information was available. Therefore, we selected $\Delta G^\circ f = -1179.26$ kJ/mole (-281.85 kcal/mole) after Sadiq and Lindsay (1979).

SiF_4°

Wagman et al. (1982) reported $\Delta G^\circ f = -1607.40$ kJ/mole (-384.18 kcal/mole) for SiF_4°. They did not list $\Delta H^\circ f$ or s° for SiF_4°. Naumov et al. (1971) calculated $\Delta G^\circ f = -1611.67$ kJ/mole (-385.20 kcal/mole) from pk = 6.19 for reaction:

$$SiF_6^{2-} \longrightarrow SiF_4^{\circ} + 2F^-$$
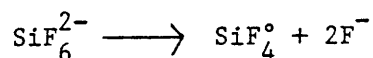
after Russian investigators. No further information was available to evaluate Naumov et al. (1971) pk value. Therefore, we accepted $\Delta G^{\circ}f$ = -1607.40 kJ/mole (-384.18 kcal/mole) for SiF_4° after Wagman et al. (1982).

SiF_6^{2-}

The standard free energy of formation listed for SiF_6^{2-} ranges from -2138.02 kJ/mole (-511.00 kcal/mole) to -2207.06 kJ/mole (-527.50 kcal/mole). Wagman et al. reported $\Delta G^{\circ}f$ = -2199.40 kJ/mole (-525.67 kcal/mole) from $\Delta H^{\circ}f$ = -2389.10 kJ/mole (-571.00 kcal/mole) and s° = 122.20 J/mole (29.20 cal/mole). Naumov et al. (1971) calculated $\Delta G^{\circ}f$ = -2207.31 kJ/mole (-527.56 kcal/mole) from pk = 26.38 for the reaction:

$$SiF_6^{2-} + 2H_2O \longrightarrow SiO_2(c) + 4H^+ + 6F^-$$
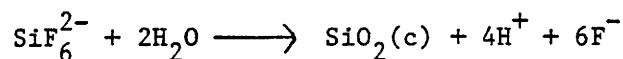
They also calculated $\Delta H^{\circ}f$ = -2395.60 kJ/mole (-572.56 kcal/mole) and s° = 125.10 kJ/mole (29.9 cal/mole) after Stephenson et al. (1964).

Karapet'yants and Karapet'yants (1970) reported $\Delta G^{\circ}f$ = -2138.24 kJ/mole (-511.00 kcal/mole) using thermodynamic data determined by Latimer (1952).

In this report we selected $\Delta G^{\circ}f$ = -2199.40 kJ/mole (-525.67 kcal/mole) for SiF_6^{2-} species after Wagman et al. (1982).

ZnF^+

Wagman et al. (1982) reported $\Delta G^{\circ}f$ = -433.00 kJ/mole (-103.49 kcal/mole) but no $\Delta H^{\circ}f$ or s° values were listed. Naumov et al. (1971)

calculated $\Delta G°f$ = -434.38 kJ/mole (-103.82 kcal/mole) from pk = 1.26 for the equation:

$$ZnF^+ \longrightarrow Zn^{2+} + F^-$$

after Smith and Martell (1976). But Smith and Martell (1976) reported pk = 1.15 for the same reaction. Elrashidi and Lindsay (1984) reported $\Delta G°f$ = -437.98 kJ/mole (-104.68 kcal/mole) from pk = 1.15 for the above reaction after Smith and Martell (1976).

In this report, we selected $\Delta G°f$ = -437.98 kJ/mole (-104.68 kcal/mole) after Elrashidi and Lindsay (1984) for ZnF^+ species.

$ZnF_2°$

Wagman et al. (1982) reported $\Delta G°f$ = -704.64 kJ/mole (-168.41 kcal/mole) from $\Delta H°f$ = -819.14 kJ/mole (-195.78 kcal/mole) and $s°$ = -139.7 J/mole (-33.39 cal/mole). No further information was available for this species. We selected $\Delta G°f$ = -704.64 kJ/mole (-168.41 kcal/mole) after Wagman et al. (1982).

$NaF°$

Wagman et al. (1982) reported $\Delta G°f$ = -540.68 kJ/mole (129.22 kcal/mole) from $\Delta H°f$ = -572.75 kJ/mole (-136.90 kcal/mole) and $s°$ = 45.2 J/mole (10.80 cal/mole). We adopted $\Delta G°f$ = -540.68 kJ/mole (-129.22 kcal/mole) for $NaF°$ after Wagman et al. (1982).

$KF°$

Wagman et al. (1982) calculated $\Delta G°f$ = -562.07 kJ/mole (-134.34 kcal/mole) from $\Delta H°f$ = -585.01 kJ/mole (-139.82 kcal/mole) and $s°$ = 88.7 J/mole (21.20 cal/mole). No other information was available. We

selected $\Delta G°f$ = -562.07 kJ/mole (-134.34 kcal/mole) after Wagman et al. (1982).

CuF^+

Wagman et al. (1982) reported $\Delta G°f$ = -220.50 kJ/mole (-52.70 kcal/mole) from $\Delta H°f$ = -261.10 kJ/mole (-62.40 kcal/mole) and $s°$ = -67.00 J/mole (-16.01 kcal/mole). Naumov et al. (1971) calculated $\Delta G°f$ = -221.75 kJ/mole (-53.00 kcal/mole), $\Delta H°f$ = -261.50 kJ/mole (-62.50 kcal/mole), and $s°$ = 64.01 J/mole (15.30 cal/mole) for CuF^+. They based their calculations on pk = 1.23 and Sr = -46.02 J/mole (-11.00 cal/mole) for the reaction:

$$CuF^+ \longrightarrow Cu^{2+} + F^-$$
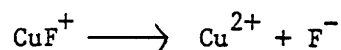
after Sillen and Martell (1964).

Smith and Martell (1976) reported pk = 1.2 for the same reaction. Elrashidi and Lindsay (1984) adopted pk = 1.2 for the above reaction after Smith and Martell (1976) and calculated $\Delta G°f$ = -225.51 kJ/mole (-53.90 kcal/mole) for CuF^+ species.

In this report, we selected $\Delta G°f$ = -225.51 kJ/mole (-53.90 kcal/mole) after Elrashidi and Lindsay (1984).

$CdF_2°$

Wagman et al. (1982) reported $\Delta G°f$ = -635.18 kJ/mole (-151.81 kcal/mole) from $\Delta H°f$ = -741.15 kJ/mole (-177.14 kcal/mole) and $s°$ = -100.80 J/mole (-24.10 cal/mole). Elrashidi and Lindsay recommended $\Delta G°f$ = -619.57 kJ/mole (-148.08 kcal/mole). They used $\Delta H°f$ = -770.23 kJ/mole (-172.14 kcal/mole) and $s°$ = -100.83 J/mole (-24.10 cal/mole)

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after Wagman et al. (1968) to calculate $\Delta G°f = -619.57$ kJ/mole (-148.08 kcal/mole) for $CdF_2°$.

We adopted $\Delta G°f = -635.18$ kJ/mole (-151.81 kcal/mole) after Wagman et al. (1982).

HgF^+

Wagman et al. (1982) reported $\Delta G°f = -123.40$ kJ/mole (-29.50 kcal/mole) from $\Delta H°f = -158.20$ kJ/mole (-37.81 kcal/mole) and $s° = -4.00$ J/mole (-0.95 cal/mole). Paul (1955) reported $\Delta G°f = -128.40$ kJ/mole (-30.69 kcal/mole) from pk = 1.56 for the reaction:

$$HgF^+ \longrightarrow Hg^{2+} + F^-$$
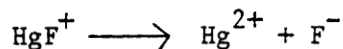
Hepler and Olofason (1975) calculated $\Delta G°f = -128.40$ kJ/mole (-30.69 kcal/mole) from pk = 1.58 for the above reaction. Smith and Martell (1976) recommended $\Delta G°f = -128.64$ kJ/mole (-30.74 kcal/mole) from pk = 1.60 for the same reaction. Elrashidi and Lindsay (1984) calculated $\Delta G°f = -128.66$ kJ/mole (-30.75 kcal/mole) from pk = 1.60 for the above reaction.

In this report, we selected $\Delta G°f = -128.66$ kJ/mole (-30.75 kcal/mole) after Elrashidi and Lindsay (1984).

MnF^+

Wagman et al. (1982) reported $\Delta G°f = -511.70$ kJ/mole (-122.30 kcal/mole) for MnF^+ species. They did not recommend $\Delta H°f$ or $s°$ values for this species. We accepted the only available value $\Delta G°f = -511.70$ kJ/mole (-122.30 kcal/mole).

CaF^+

Smith and Martell (1976) reported pk = 1.10 for the reaction:

$$CaF^+ \longrightarrow Ca^{2+} + F^-$$
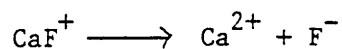
No other information was available. We calculated $\Delta G°f = -844.00$ kJ/mole (-201.72 kcal/mole) using selected $\Delta G°f$ values for Ca^{2+} and F^-.

MgF^+

    Smith and Martell (1976) reported pk = 1.80 for the reaction:

$$MgF^+ \longrightarrow Mg^{2+} + F^-$$
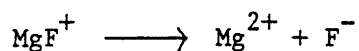
We calculated $\Delta G°f = -750.60$ kJ/mole (-179.40 kcal/mole) for MgF^+ species using selected $\Delta G°f$ values for Mg^{2+} and F^-.

SrF^+

    Sposito and Mattigod (1980) reported logk° = -0.60 for the reaction:

$$SrF^+ \longrightarrow Sr^{2+} + F^-$$
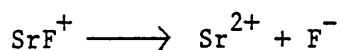
No other information was available. We calculated $\Delta G°f = -851.44$ kJ/mole (-203.50 kcal/mole) for SrF^+ species using equation (8) and selected $\Delta G°f$ values for Sr^{2+} and F^-.

$CaF_2^°$

    Wagman et al. (1982) reported $\Delta G°f = -111.15$ kJ/mole (-265.57 kcal/mole) from $\Delta H°f = -1208.09$ kJ/mole (-288.74 kcal/mole) and s° = -80.8 J/mole (-19.31 cal/mole). We adopted these values for $CaF_2^°$ species and selected $\Delta G°f = -1111.15$ kJ/mole (-265.57 kcal/mole) after Wagman et al. (1982).

GaF^{2+}

Wagman et al. (1982) calculated $\Delta G°f$ = -464.90 kJ/mole (-111.11 kcal/mole) from $\Delta H°f$ = -536.80 kJ/mole (-128.30 kcal/mole) and $s°$ = -226.00 J/mole (-54.01 cal/mole). We adopted $\Delta G°f$ = -464.90 kJ/mole (-111.11 kcal/mole) for GaF^{2+} species.

GaF_2^+

Wagman et al. (1982) reported $\Delta G°f$ = -764.80 kJ/mole (-182.80 kcal/mole) for GaF_2^+ species from $\Delta H°f$ = -863.20 kJ/mole (-206.30 kcal/mole) and $s°$ = -146.00 J/mole (-34.90 cal/mole). We selected $\Delta G°f$ = -764.80 kJ/mole (-182.80 kcal/mole) after Wagman et al. (1982).

$TlF°$

Wagman et al. (1982) reported $\Delta G°f$ = -311.19 kJ/mole (74.37 kcal/mole) from $\Delta H°f$ = -327.27 kJ/mole (-78.22 kcal/mole) and $s°$ = 111.70 J/mole (+26.70 cal/mole). We selected $\Delta G°f$ = -311.19 kJ/mole (-74.37 kcal/mole) for $TlF°$ species.

$AgF°$

Wagman et al. (1982) calculated $\Delta G°f$ = -201.69 kJ/mole (-48.20 kcal/mole) from $\Delta H°f$ = -227.07 kJ/mole (-54.27 kcal/mole) and $s°$ = 59.00 J/mole (14.10 cal/mole). We adopted $\Delta G°f$ = -201.69 kJ/mole (-48.20 kcal/mole) for $AgF°$ species after Wagman et al. (1982).

$NiF_2°$

Wagman et al. (1982) calculated $\Delta G°f$ = -603.30 kJ/mole (-144.20 kcal/mole) from $\Delta H°f$ = -719.20 kJ/mole (-171.90 kcal/mole) and $s°$ = -156.5 J/mole (-37.40 cal/mole). We selected $\Delta G°f$ = -603.30 kJ/mole (-144.20 kcal/mole) for $NiF_2°$ species after Wagman et al. (1982).

BaF_2°

Wagman et al. (1982) reported $\Delta G^{\circ}f = -1118.35$ kJ/mole (-267.30 kcal/mole) from $\Delta H^{\circ}f = -1202.90$ kJ/mole (-287.50 kcal/mole) and $s^{\circ} = -18.00$ J/mole (-4.30 cal/mole). We selected $\Delta G^{\circ}f = -1118.35$ kJ/mole (-267.30 kcal/mole) for BaF_2° species after Wagman et al. (1982).

$AlF_3(c)$
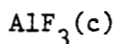
Naumov et al. (1971) reported $\Delta H^{\circ}f = -1510.42$ kJ/mole (-361.00 kcal/mole) after Rudzites et al. (1967) and $s^{\circ} = 66.48$ J/mole (15.89 cal/mole) after King (1957). Wagman et al. (1982) calculated $\Delta G^{\circ}f = -1425.00$ kJ/mole (-340.58 kcal/mole) from $\Delta H^{\circ}f = -1504.10$ kJ/mole (-359.50 kcal/mole) and $s^{\circ} = -66.44$ J/mole (15.90 cal/mole). Stull et al. (1971) and CODATA (1978) listed $\Delta H^{\circ}f = -1510.42$ kJ/mole (-361.00 kcal/mole) and $s^{\circ} = 66.48$ J/mole (15.89 cal/mole) for $AlF_3(c)$ compound.

Elrashidi and Lindsay (1984) calculated $\Delta G^{\circ}f = -1444.06$ kJ/mole (-345.14 kcal/mole) from $\Delta H^{\circ}f = -1510.42$ kJ/mole (-361.00 kcal/mole) and $s^{\circ} = 66.48$ J/mole (15.89 cal/mole) after CODATA (1978). In this report, we selected $\Delta G^{\circ}f = -1444.06$ kJ/mole (-345.14 kcal/mole) after Elrashidi and Lindsay (1984).

$CdF_2(c)$
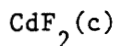
Wagman et al. (1982) reported $\Delta G^{\circ}f = -647.70$ kJ/mole (-154.80 kcal/mole) from $\Delta H^{\circ}f = -700.40$ kJ/mole (-167.40 kcal/mole) and $s^{\circ} = -77.40$ J/mole (18.50 cal/mole). Karapet'yants and Karapet'yants (1970) calculated $\Delta G^{\circ}f = -649.35$ kJ/mole (-155.20 kcal/mole) from $\Delta H^{\circ}f = -700.36$ kJ/mole (-167.39 kcal/mole) and $s^{\circ} = 83.26$ J/mole (19.90 cal/mole).

Naumov et al. (1971) reported $\Delta G°f$ = -651.07 kJ/mole (-155.61 kcal/mole) from $\Delta H°f$ = -700.36 kJ/mole (-167.39 kcal/mole) and s° = 89.12 J/mole (21.30 cal/mole). In general, the reported $\Delta G°f$ values for CdF_2(c) were reasonably close. We selected $\Delta G°f$ = -647.70 kJ/mole (-154.80 kcal/mole) after Wagman et al. (1982) for CdF_2(c).
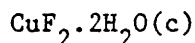
$CuF_2 \cdot 2H_2O$(c)

Wagman et al. (1982) reported $\Delta G°f$ = -981.40 kJ/mole (-234.56 kcal/mole). But no values for $\Delta H°f$ or s° were recommended. We selected available $\Delta G°f$ = -981.40 kJ/mole (-234.56 kcal/mole) for $CuF_2 \cdot 2H_2O$(c) after Wagman et al. (1982).

FeF_3(c)
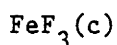
Stull et al. (1970) calculated $\Delta G°f$ = -972.33 kJ/mole (-232.40 kcal/mole) from $\Delta H°f$ and s° values. Elrashidi and Lindsay (1984) reported $\Delta G°f$ = -979.71 kJ/mole (-234.16 kcal/mole) from $\Delta H°f$ = -1041.82 kJ/mole (-249.00 kcal/mole) and s° = 98.32 J/mole (23.50 cal/mole). We selected $\Delta G°f$ = -979.71 kJ/mole (-234.16 kcal/mole) for FeF_3(c) after Elrashidi and Lindsay (1984).

Hg_2F_2(c)
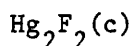
Stull et al. (1971) reported $\Delta G°f$ = -427.47 kJ/mole (-102.17 kcal/mole) from the cell measurements of Koerber and Devries (1952). Sadiq and Lindsay (1979) recommended $\Delta G°f$ = -427.48 kJ/mole (-102.17 kcal/mole) from $\Delta H°f$ = -485.34 kJ/mole (-116.00 kcal/mole) and s° = -160.66 J/mole (38.40 cal/mole). In this report, we selected $\Delta G°f$ = -427.48 kJ/mole (-102.17 kcal/mole) for Hg_2F_2(c) after Sadiq and Lindsay (1979).

KF(c)

Wagman et al. (1982) reported $\Delta G°f$ = -537.75 kJ/mole (-128.52 kcal/mole) from $\Delta H°f$ = -567.27 kJ/mole (-135.58 kcal/mole) and $s°$ = 66.57 J/mole (15.91 cal/mole). Karapet'yants and Karapet'yants (1970) listed $\Delta G°f$ = -537.70 kJ/mole (-128.51 kcal/mole) from $\Delta H°f$ = -567.35 kJ/mole (-135.60 kcal/mole) and $s°$ = 66.60 J/mole (15.92 cal/mole). Naumov et al. (1971) reported $\Delta G°f$ = -538.95 kJ/mole (-128.81 kcal/mole) from $\Delta H°f$ = -568.44 kJ/mole (-135.86 kcal/mole) and $s°$ = 66.57 J/mole (15.91 cal/mole).

We selected $\Delta G°f$ = -537.75 kJ/mole (-128.52 kcal/mole) for KF(c) after Wagman et al. (1982).

MgF_2(c)

Wagman et al. (1982) reported $\Delta G°f$ = -1070.20 kJ/mole (-255.78 kcal/mole) from $\Delta H°f$ = -1123.40 kJ/mole (-268.50 kcal/mole) and $s°$ = 57.24 J/mole (13.68 cal/mole). Naumov et al. (1971) calculated $\Delta G°f$ = -1071.10 kJ/mole (-256.00 kcal/mole) from $\Delta H°f$ = -1124.24 kJ/mole (-268.70 kcal/mole) and $s°$ = 57.23 J/mole (13.68 cal/mole). Stull et al. (1971) reported $\Delta G°f$ = -1071.10 kJ/mole (-256.00 kcal/mole) from similar $\Delta H°f$ and $s°$ values as reported by Naumov et al. (1971).

CODATA (1978) also reported similar $\Delta H°f$ = -1124.24 kJ/mole (-268.70 kcal/mole) and $s°$ = -57.23 kJ/mole (13.68 cal/mole) values for MgF_2(c). We selected $\Delta G°f$ = -1070.20 kJ/mole (-255.78 kcal/mole) after Wagman et al. (1982).

NaF(c)

Robie and Waldbaum (1968) reported $\Delta G°f$ = -543.13 kJ/mole (-129.81 kcal/mole) from $\Delta H°f$ = -573.33 kJ/mole (-137.03 kcal/mole) and $s°$ =

-51.30 J/mole (12.26 cal/mole). Wagman et al. (1982) calculated $\Delta G°f$ = -543.50 kJ/mole (-129.90 kcal/mole) from $\Delta H°f$ = -573.65 kJ/mole (-137.10 kcal/mole) and s° = 51.46 J/mole (12.30 cal/mole). Naumov et al. (1971) calculated $\Delta G°f$ = -546.51 kJ/mole (-130.62 cal/mole) from $\Delta H°f$ = -575.26 kJ/mole (-137.49 kcal/mole) and s° = 51.30 J/mole (12.26 cal/mole).

We adopted $\Delta G°f$ = -543.50 kJ/mole (-129.90 kcal/mole) after Wagman et al. (1982) for NaF(c).

PbF_2(c)

Wagman et al. (1982) reported $\Delta G°f$ = -617.10 kJ/mole (-147.49 kcal/mole) from $\Delta H°f$ = -664.00 kJ/mole (-158.70 kcal/mole) and s° = 110.50 J/mole (26.41 cal/mole). Naumov et al. (1971) calculated $\Delta G°f$ = -627.60 kJ/mole (-150.00 kcal/mole) from $\Delta H°f$ = -678.64 kJ/mole (-162.20 kcal/mole) and s° = 96.23 J/mole (23.00 cal/mole). Karapet'yants and Karapet'yants (1970) calculated $\Delta G°f$ = -715.88 kJ/mole (-148.10 kcal/mole) from $\Delta H°f$ = -662.32 kJ/mole (158.30 kcal/mole) and s° = 112.97 J/mole (27.00 cal/mole).

In this report, we selected $\Delta G°f$ = -617.10 kJ/mole (147.49 kcal/mole) after Wagman et al. (1982) for PbF_2(c).

ZnF_2(c)

Wagman et al. (1982) reported $\Delta G°f$ = -713.30 kJ/mole (-170.48 kcal/mole) from $\Delta H°f$ = -764.40 kJ/mole (-186.70 kcal/mole) and s° = 73.68 J/mole (17.60 cal/mole). Karapet'yants and Karapet'yants (1971) and Naumov et al. (1971) also reported similar $\Delta G°f$ values for ZnF_2(c). We selected $\Delta G°f$ = -713.30 kJ/mole (-170.48 kcal/mole) after Wagman et al. (1982).

$Na_2SiF_6(c)$
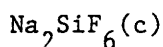
Wagman et al. (1982) reported $\Delta G°f$ = -2754.20 kJ/mole (658.27 kcal/mole) from $\Delta H°f$ = -2909.60 kJ/mole (-695.41 kcal/mole) and $s°$ = 207.10 J/mole (49.50 cal/mole). Karapet'yants and Karapet'yants (1971) listed $\Delta G°f$ = -2553.91 kJ/mole (-610.40 kcal/mole) from $\Delta H°f$ = -2849.72 kJ/mole (-681.10 kcal/mole) and $s°$ = 214.64 J/mole (51.30 cal/mole) after Latimer (1952). Naumov et al. (1972) calculated $\Delta G°f$ = -2757.25 kJ/mole from $\Delta H°f$ = -2917.80 kJ/mole (-697.37 kcal/mole) and $s°$ = 190.80 J/mole (45.60 cal/mole).

We accepted $\Delta G°f$ = -2754.20 kJ/mole (-658.27 cal/mole) for $Na_2SiF_6(c)$ after Wagman et al. (1982).

$Na_3AlF_6(c)$

Naumov et al. (1971) calculated $\Delta G°f$ = -3152.64 kJ/mole (-753.50 kcal/mole) from $\Delta H°f$ = -3322.51 kJ/mole (-794.10 kcal/mole) and $s°$ = 238.49 J/mole (57.00 cal/mole). Robie and Waldbaum (1968) listed $\Delta G°f$ = -3140.90 kJ/mole (-750.69 kcal/mole) from $\Delta H°f$ = -3305.36 kJ/mole (-759.00 kcal/mole) after Stull et al. (1960) and $s°$ = +238.40 J/mole (56.98 cal/mole) after Kelly and King (1961). Wagman et al. (1982) reported $\Delta G°f$ = -3136.60 kJ/mole (-749.67 kcal/mole) from $\Delta H°f$ = -3301.20 kJ/mole (-789.00 kcal/mole) and $s°$ = 238.50 J/mole (57.00 cal/mole).

Karapet'yants and Karapet'yants (1970) listed $\Delta G°f$ = -3015.82 kJ/mole (-720.80 kcal/mole) from $\Delta H°f$ = -3283.60 kJ/mole (-784.80 kcal/mole) after Coughlin (1958) and $s°$ = 238.40 J/mole (56.98 cal/mole). In this report, we adopted $\Delta G°f$ = -3136.60 kJ/mole (-739.67 kcal/mole) for $Na_3AlF_6(c)$ after Wagman et al. (1982).

$NaCa_2Mg_4Al_3Si_6O_{22}F_2(c)$
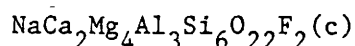
Westerich and Navrotsky (1981) calculated $\Delta G°f = -12117.78$ kJ/mole (-2896.22 kcal/mole) from $\Delta H°f = -12799.48$ kJ/mole (-3059.15 kcal/mole) and $s° = 2287.60$ J/mole (546.75 cal/mole). They used $\Delta H°r = -349.36$ kJ/mole (-83.50 kcal/mole) for the reaction:

$$NaF + 2Cao + 4MgO + 1/3\ AlF_3 + 11\ 1/3\ Al_2O_7 + 6SiO_2 \longrightarrow$$
$$NaCa_2Mg_4Al_3Si_6O_{22}F_2(c)$$
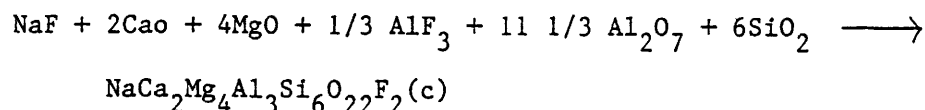
using the volume-corrected algorithm method described by Helgeson et al. (1978), authors determined $s° = 2287.60$ J/mole (546.75 cal/mole) for this mineral. We adopted $\Delta G°f = -12117.78$ kJ/mole (-2896.22 kcal/mole) after Westrich and Navrotsky (1981).

$NaMoF_7(c)$
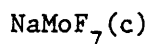
Wagman et al. (1982) listed $\Delta G°f = -2006.10$ kJ/mole (-479.47 kcal/mole) from $\Delta H°f = -2180.30$ kJ/mole (-521.10 kcal/mole) and $s° = 205.00$ J/mole (49.00 cal/mole). No other compiler listed thermodynamic data for this compound.

We adopted the only available $\Delta G°f = -2006.10$ kJ/mole (-479.47 kcal/mole) after Wagman et al. (1982).

K_2SiF_6 (hieratite)
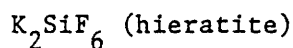
Wagman et al. (1982) listed $\Delta G°f = -2798.60$ kJ/mole (-668.88 kcal/mole) from $\Delta H°f = -2956.00$ kJ/mole (-706.50 kcal/mole) and $s° = 225.90$ J/mole (53.99 cal/mole). Karapet'yants and Karapet'yants (1970) recommended $\Delta G°f = -2723.78$ kJ/mole (-651.00 kcal/mole) and $s° = 228.86$ J/mole (54.70 cal/mole) for this mineral after Latimer (1952). Authors did not list any $\Delta H°f$ values for this mineral.

Naumov et al. (1971) recommended $\Delta G°f$ = -2810.40 kJ/mole (-671.70 kcal/mole), $\Delta H°f$ = -2965.62 kJ/mole (708.80 kcal/mole), and $s°$ = 235.56 J/mole (56.30 cal/mole) from pk = 6.47 for the reaction:

$$K_2SiF_6(c) \longrightarrow 2K^+ + SiF_6^{2-}$$
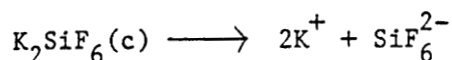
In this report, we selected $\Delta G°f$ = -2798.60 kJ/mole (-668.88 kcal/mole) after Wagman et al. (1982) for K_2SiF_6 (hieratite) mineral.

$KMg_3AlSi_3O_{10}F_2$ (fluorphlogopite)

The standard free energy of formation ($\Delta G°f$) reported by different investigators are listed below:

Investigator	$\Delta G°f$ (kJ/mole)	(kcal/mole)
Wagman et al. (1982)	-6044.00	-1444.55
Naumov et al. (1971)	-6026.21	-1440.30
Robie and Waldbaum (1968)	-6022.95	-1439.52
Sadiq and Lindsay (1979)	-6115.46	-1461.63
Westrich and Navrotsky (1981)	-6019.68	-1438.74

Kelly et al. (1959) reported $\Delta H°f$ = -31.21 kJ/mole for the reaction:

$$3SiO_2(g) + KCl(c) + AlCl_3 \cdot 6H_2O(c) + 3Mg(OH)_2(c) + 2HF(21.462\ H_2O)$$
$$\longrightarrow KMg_3AlSi_3O_{10}F_2(c) + 8H_2O + 4HCl(12.731\ H_2O)$$
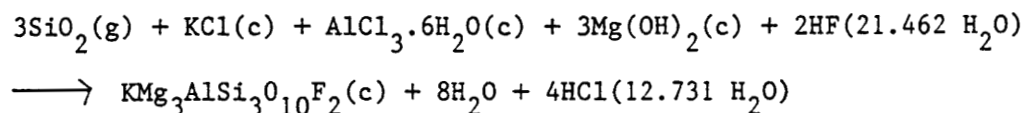
This source was adopted by almost all the compilers using new available data. However, Sadiq and Lindsay (1979) made critical evaluation of $\Delta G°f$ of this mineral. They used $\Delta H°f$ = -6392.90 kJ/mole (-1527.94

kcal/mole) and s° = 336.30 J/mole (80.38 cal/mole) for fluorphlogopite
after Hemingway and Robie (1977) to calculate $\Delta G°f$ value for
flurphlogopite mineral.

In this report, we accepted $\Delta G°f$ = -6115.46 kJ/mole (-1461.63
kcal/mole) for this mineral after Sadiq and Lindsay (1979).

$Ca_5(PO_4)_3F$ (fluorapatite)

The standard free energy of formation ($\Delta G°f$) reported by different
compiling for $Ca_5(Po_4)_3F$ are listed below:

Compiler	$\Delta G°f$	
	(kJ/mole)	(kcal/mole)
Parker et al. (1971)	-6491.47	-1551.50
Naumov et al. (1971)	-6507.37	-1555.30
Sadiq and Lindsay (1979)	-6474.19	-1547.37
Westrich and Navrotsky (1981)	-6501.51	-1553.90

Parker et al. (1971) and Naumov et al. (1971) reported $\Delta G°f$ values for
fluorapatite from $\Delta H°f$ and s° values. Fan et al. (1962) reported pk =
120.86 on the reaction:

$$Ca_{10}F_2(PO_4)_6(c) \longrightarrow 10Ca^{2+} + 2F^- + 6PO_4^{3-}$$
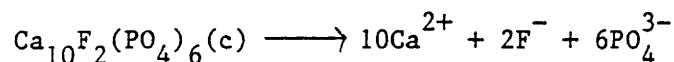
which determined $\Delta G°f$ = -12952.87 kJ/mole (-3095.81 kcal/mole) for
$Ca_{10}F_2(PO_4)_6(c)$ and $\Delta G°f$ = -6476.43 kJ/mole (-1547.90 kcal/mole) for
$Ca_5(PO_4)_3F$.

Chien and Black (1976) recommended pk = 119.20 for the same equation
which determined $\Delta G°f$ = -12948.35 kJ/mole (-3094.73 kcal/mole) for
$Ca_{10}(PO_4)_6F_2(c)$ and $\Delta G°f$ = -6474.17 kJ/mole (-1547.36 kcal/mole for

$Ca_5(PO_4)_3F$. These values are similar to that calculated from Farr et al. (1962) solubility data. Sadiq and Lindsay (1979) accepted solubility data of Chien and Black (1976) and recommended $\Delta G°f$ = -6474.19 kJ/mole (-1547.37 kcal/mole) for $Ca_5(PO_4)_3(c)$.

In this report, we selected $\Delta G°f$ = -6474.19 kJ/mole (-1547.37 kcal/mole) for $Ca_5(Po_4)_3F(c)$ after Sadiq and Lindsay (1979).

$Ca_4Si_2O_7F_2$ (cuspidine)

Naumov et al. (1971) listed $\Delta G°f$ = -4988.58 kJ/mole (-1192.30 kcal/mole) from $\Delta H°f$ = -5240.46 kJ/mole (-1252.50 kcal/mole) and $s°$ = 279.90 J/mole (66.90 cal/mole) for $Ca_4Si_2O_7F_2$ mineral. No other information was available for $Ca_4Si_2O_7F_2$ mineral.

We selected only available $\Delta G°f$ = -4988.58 kJ/mole (-1192.30 kcal/mole) for cuspidine mineral after Naumov et al. (1971).

$(NH_4)_2SiF_6$ (bararite)

Naumov et al. (1971) calculated $\Delta G°f$ = -2372.24 kJ/mole (-566.98 kcal/mole) from $\Delta H°f$ = -2688.43 kJ/mole (-642.55 kcal/mole) and $s°$ = 280.24 J/mole (66.98 cal/mole). No other information was available. We accepted $\Delta G°f$ = -2372.24 kJ/mole (-566.98 kcal/mole) for bararite mineral after Naumov et al. (1971).

$Pb_5(PO_4)_3F$ (fluoropyromorphite)

Nriagu (1973) studied the reaction:

$$Pb_5(PO_4)_3F(c) \longrightarrow F^- + 5Pb^{2+} + 3PO_4^{3-}$$
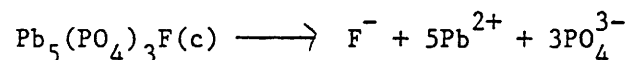
and reported pk = 71.60 for this reaction. Sadiq and Lindsay (1979) adopted this pk value and reported $\Delta G°f$ = -3893.75 kJ/mole (-930.63

kcal/mole) for this mineral. We adopted $\Delta G°f$ = -3893.75 kJ/mole (930.63 kcal/mole) for $Pb_5(PO_4)_3F$ mineral after Sadiq and Lindsay (1979).

CaF_2 (fluorite)

The standard free energy of formation of CaF_2 reported by different investigators are listed below:

Investigator	$\Delta G°f$ (kJ/mole)	(kcal/mole)
Wagman et al. (1982)	-1167.30	-278.99
Helgeson et al. (1978)	-1173.58	-280.49
Stull et al. (1971)	-1173.53	-280.48
Naumov et al. (1971)	-1175.99	-281.07
Karapet'yants and Karapet'yants (1970)	-1163.15	-278.00
Robie and Waldbaum (1968)	-1162.31	-277.80
Sadiq and Lindsay (1979)	-1182.31	-282.58

Naumov et al. (1971) reported $\Delta G°f$ value for CaF_2 (fluorite) from pk = 11.09 for the reaction:

$$CaF_2(c) \longrightarrow Ca^{2+} + 2F^-$$
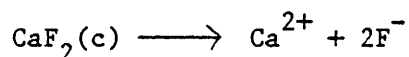
Smith and Martell (1976) reported pk = 10.41 for the same reaction which correponds to $\Delta G°f$ = -1182.31 kJ/mole (-282.58 kcal/mole). Elrashidi and Lindsay (1984) reported $\Delta G°f$ = -1182.31 kJ/mole (-282.5 kcal/mole) from pk = 11.41 for the above reaction after Smith and Martell (1976).

Recently, Street and Elwali (1983) confirmed the solubility data reported by Smith and Martell (1976). Sadiq and Lindsay critically

evaluated available thermodynamic data for $CaF_2(c)$ and reported similar

$\Delta G°f$ = -1182.31 kJ/mole (-282.58 kcal/mole). In this report, we adopted

$\Delta G°f$ = -1182.31 kJ/mole (-282.58 kcal/mole) for CaF_2 (fluorite) after

Elrashidi and Lindsay (1984).

MOLYBDENUM

MoO_4^{2-}

Wagman et al. (1982) reported $\Delta G°f$ = -836.30 kJ/mole (-199.88

kcal/mole) from $\Delta H°f$ = -997.70 kJ/mole (-238.45 kcal/mole) and $s°$ =

27.20 J/mole (6.50 cal/mole). Sadiq and Lindsay (1979) critically

evaluated $\Delta G°f$ values for MoO_4^{2-} and recommended $\Delta G°f$ = -836.13 kJ/mole

(-199.84 kcal/mole) from pk = 12.10 for the reaction:

$$MoO_3(c) + H_2O \longrightarrow 2H^+ + MoO_4^{2-}$$
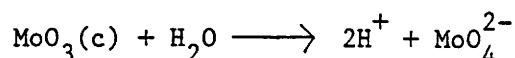
after Smith and Martell (1976). Sadiq and Lindsay (1979) calculated

$\Delta G°f$ value for MoO_4^{2-} is in good agreement with Wagman et al. (1982).

Therefore, we selected $\Delta G°f$ = -836.30 kJ/mole (-199.88 kcal/mole) for

MoO_4 species after Wagman et al. (1982).

MoO_2^{2+}

Naumov et al. (1971) recommended $\Delta G°f$ = -411.28 kJ/mole (-98.30

kcal/mole) from pk = 3.45 for the reaction:

$$MoO_3(c) + 2H^+ \longrightarrow MoO_2^{2+} + H_2O$$
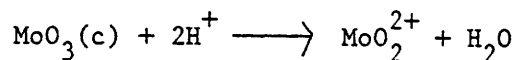
No other information was available. Therefore, we adopted the available

value after Naumov et al. (1971) for MoO_2^{2+} species.

$MoO_2(OH)^+$
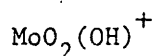
Naumov et al. (1971) reported $\Delta G°f$ = -645.88 kJ/mole (-154.37 kcal/mole). Authors based their calculation on pk = 0.45 for the reaction:

$$MoO_2^{2+} + H_2O \longrightarrow MoO_2(OH)^+ + H^+$$
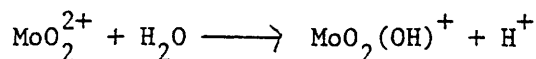
Sadiq and Lindsay (1979) calculated $\Delta G°f$ = -645.75 kJ/mole (-154.34 kcal/mole) from the above pk value. No other information was available. We selected $\Delta G°f$ = -645.75 kJ/mole (-154.34 kcal/mole) for $MoO_2(OH)^+$ species after Sadiq and Lindsay (1979).

$HMoO_4^-$

Naumov et al. (1971) reported $\Delta G°f$ = -866.63 kJ/mole (-207.13 kcal/mole). Garrels and Christ (1965) listed $\Delta G°f$ = -893.70 kJ/mole (-213.60 kcal/mole) from $\Delta H°f$ and s° values. Sadiq and Lindsay (1979) calculated $\Delta G°f$ = -860.31 kJ/mole (-205.62 kcal/mole) from pk = -4.24 for the reaction:
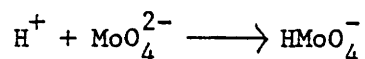
$$H^+ + MoO_4^{2-} \longrightarrow HMoO_4^-$$

after Rohwer and Cruywagen (1963) and Smith and Martell (1976). No other information was available. We selected pk = -4.24 (Smith and Martell, 1976) and calculated $\Delta G°f$ = -860.48 kJ/mole (-205.66 kcal/mole) for $HMoO_4^{2-}$ species.

$H_2MoO_4^°$
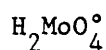
Latimer (1952) reported $\Delta G°f$ = -949.76 kJ/mole (-227.00 kcal/mole) from estimated $\Delta H°f$ = -1072.77 kJ/mole (-256.40 kcal/mole) and s° =

150.62 J/mole (36.00 cal/mole). Naumov et al. (1971) reported $\Delta G°f$ = -877.13 kJ/mole (-209.64 kcal/mole) from $\Delta H°f$ and $s°$ values.

Wagman et al. (1982) listed $\Delta H°f$ = -1007.50 kJ/mole (-240.80 kcal/mole). But the author did not list any $\Delta G°f$ or $s°$ values for this species.

Sadiq and Lindsay (1979) calculated $\Delta G°f$ = -883.15 kJ/mole (-211.08 kcal/mole) from pk = -4.0 for the reaction:

$$HMoO_4^- + H^+ \longrightarrow H_2MoO_4^°$$
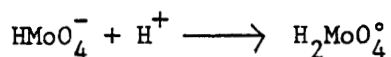
after Rohwer and Cruywagen (1963). No other information was available. We calculated $\Delta G°f$ = -883.28 kJ/mole (-211.11 kcal/mole) using pk = -4.0 for the above equation.

MoO_3(molybdite)

Wagman et al. (1982) listed $\Delta G°f$ = -667.97 kJ/mole (-159.64 kcal/mole) from $\Delta H°f$ = -745.09 kJ/mole (-178.08 kcal/mole) and $s°$ = 77.74 J/mole (18.58 cal/mole). Stull et al. (1971) reported $\Delta G°f$ = -668.10 kJ/mole (-159.68 kcal/mole) from $\Delta H°f$ = -745.17 kJ/mole (-178.10 kcal/mole) and $s°$ = 77.73 J/mole (18.58 cal/mole).

Sadiq and Lindsay (1979) calculated $\Delta G°f$ = -668.01 kJ/mole (-159.66 kcal/mole) from $\Delta H°f$ = -745.08 kJ/mole (-178.08 kcal/mole) after Mah (1957) and Staskiewitcz et al. (1955) and $s°$ = 77.73 J/mole (18.58 cal/mole) after Kelley and King (1961).

Listed $\Delta G°f$ values for MoO_3(molybdite) by different investigators are in agreement. Therefore, we selected $\Delta G°f$ = -667.97 kJ/mole (-159.64 kcal/mole) after Wagman et al. (1982).

$H_2MoO_4(c)$
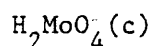
Wagman et al. (1982) reported $\Delta H°f = -1046.00$ kJ/mole (-250.00 kcal/mole). But the authors did not list any $\Delta G°f$ or $s°$ values for this species. Sadiq and Lindsay (1979) calculated $\Delta G°f = -912.44$ kJ/mole (-218.08 kcal/mole) from $\Delta H°f = -1046.00$ kJ/mole (-250.00 kcal/mole) after Graham and Hepler (1956) and $s° = 121.33$ J/mole (29.00 cal/mole) after Dellien et al. (1976).

No other information was available. Therefore, we selected $\Delta G°f = -912.44$ kJ/mole (-218.08 kcal/mole) after Sadiq and Lindsay (1979).

$MoS_2(c)$(molybdenite)
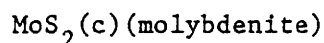
Latimer (1952) reported $\Delta G°f = -225.09$ kJ/mole (-53.80 kcal/mole) from $\Delta H°f = -232.21$ kJ/mole (-55.50 kcal/mole) and $s° = 63.17$ J/mole (15.10 cal/mole). Wagman et al. (1982) listed $\Delta G°f = -225.90$ kJ/mole (-53.99 kcal/mole) from $\Delta H°f = -235.10$ kJ/mole (-56.19 kcal/mole) and $s° = 62.59$ J/mole (14.96 cal/mole). Sadiq and Lindsay (1979) critically evaluated $\Delta H°f$ and $s°$ values for MoS_2(molybdenite) and calculated $\Delta G°f = -266.47$ kJ/mole (-63.69 kcal/mole). The authors adopted $\Delta H°f = -275.30$ kJ/mole (-65.80 kcal/mole) after O'Hare et al. (1970) and $s° = 62.59$ J/mole (14.96 cal/mole) after Westrum and McBride (1955). Recently, Chase et al. (1982) reported $\Delta G°f = -267.14$ kJ/mole (-63.85 kcal/mole) which is similar to Sadiq and Lindsay (1979) selection.

In this report, we selected $\Delta G°f = -266.47$ kJ/mole (-63.69 kcal/mole) for MoO_2 species after Sadiq and Lindsay (1979).

$Ag_2MoO_4(c)$
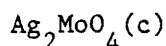
Sadiq and Lindsay (1979) calculated $\Delta G°f = -747.89$ kJ/mole (-178.75 kcal/mole) from pk = 11.55 for the reaction:

$$Ag_2MoO_4(c) \longrightarrow 2Ag^+ + MoO_4^{2-}$$

after Smith and Martell (1976). Similar pk values for the above reaction were reported by Muldrew and Hepler (1956) and Pan (1954).

Latimer (1952) reported $\Delta G°f = -821.73$ kJ/mole (-196.40 kcal/mole). But the author did not report any $\Delta H°f$ or $s°$ values.

The equilibrium constant ($logk°$) for the following reaction:
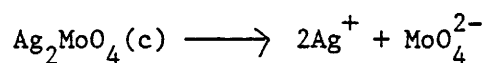
$$Ag_2MoO_4(c) \longrightarrow 2Ag^+ + MoO_4^{2-}$$

reported by various investigators and geochemical models are summarized below:

Investigator/Geochemical Model	logk°
Smith and Martell (1976)	-11.55
Muldrew and Hepler (1956)	-11.55
Pan (1954)	-11.55
Ricci and Linke (1951)	-10.51
Lindsay (1979)	-11.55
WATEQFC (Runnells and Lindberg, 1980)	-11.55
GEOCHEM (Sposito and Mattigod, 1980)	-11.42

Reported logk values are in good agreement except Ricci and Linke (1951). Therefore, we selected pk = 11.55 for the above reaction after Smith and Martell and calculated $\Delta G°f = -748.01$ kJ/mole (-178.78 kcal/mole) for $Ag_2MoO_4(c)$.

$BaMoO_4(c)$

Latimer (1952) reported $\Delta G°f = -1075.28$ kJ/mole (-257.00 kcal/mole) from $\Delta H°f = -1179.88$ kJ/mole (-282.00 kcal/mole) and estimated s° = 153.97 J/mole (36.80 cal/mole). Similar $\Delta G°f$, $\Delta H°f$ and s° values reported by Garrels and Christ (1965).

Wagman et al. (1982) reported $\Delta G°f = -1439.60$ kJ/mole (-344.07 kcal/mole) from $\Delta H°f = -1548.00$ kJ/mole (-369.98 kcal/mole) and s° = 138.00 J/mole (32.98 cal/mole). No other information was available. In this report, we selected $\Delta G°f = -1439.60$ kJ/mole (-344.07 kcal/mole) for $BaMoO_4(c)$ after Wagman et al. (1982).

$CaMoO_4(c)$

Wagman et al. (1982) listed $\Delta G°f = -1434.60$ kJ/mole (-342.87 kcal/mole) from $\Delta H°f = -1541.40$ kJ/mole (-368.40 kcal/mole) and s° = 122.60 J/mole (29.30 cal/mole). Sadiq and Lindsay (1979) reported $\Delta G°f = -1435.90$ kJ/mole (-343.19 kcal/mole) from $\Delta H°f = -1545.99$ kJ/mole (-369.50 kcal/mole) after Barany (1962) and s° = 122.59 J/mole (29.30 cal/mole) after Weller and King (1963).

The equilibrium constant (logk°) for the following reaction:
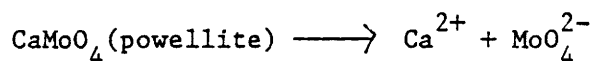
$$CaMoO_4(\text{powellite}) \longrightarrow Ca^{2+} + MoO_4^{2-}$$

reported by various investigators and geochemical models are summarized below:

Investigator/Geochemical Model	logk°
Smith and Martell (1976)	-8.00
Lindsay (1979)	-7.94
GEOCHEM (Sposito and Mattigod, 1980)	-7.41
WATEQFC (Runnells and Lindberg, 1980)	-8.36

The equilibrium constant reported by Lindsay (1979) calculated from selected $\Delta G°f$ values of Sadiq and Lindsay (1979) is in good agreement with Smith and Martell (1979). In this report, we adopted $\log k° = -7.94$ (Lindsay, 1979) for the above reaction and calculated $\Delta G°f = -1435.99$ kJ/mole (-343.21 kcal/mole) for $CaMoO_4(c)$.

$CuMoO_4(c)$

Latimer (1952) listed $\Delta H°f = -948.09$ kJ/mole (-266.60 kcal/mole) and estimated $s° = 141.41$ J/mole (33.80 cal/mole) for $CuMoO_4(c)$.

Naumov et al. (1971) recommended $\Delta G°f = -809.60$ kJ/mole (-193.50 kcal/mole) from $pk = 6.48$ for the reaction:

$$CuMoO_4(c) \longrightarrow Cu^{2+} + MoO_4^{2-}$$
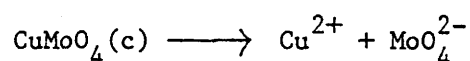
No other information was available for this compound. Therefore, we adopted $\Delta G°f = -809.60$ kJ/mole (-193.50 kcal/mole) for $CuMoO_4(c)$ after Naumov et al. (1971).

$FeMoO_4(c)$

Latimer (1951) reported $\Delta G°f = -982.40$ kJ/mole (-234.80 kcal/mole) from $\Delta H°f = -1077.38$ kJ/mole (-257.50 kcal/mole) and estimated $s° = 139.74$ J/mole (33.40 cal/mole). Garrels and Christ (1965) listed similar $\Delta G°f$, $\Delta H°f$, and $s°$ values from Latimer (1951).

Wagman et al. (1982) recommended $\Delta G°f = -975.00$ kJ/mole (-233.03 kcal/mole) from $\Delta H°f = -1075.00$ kJ/mole (-256.93 kcal/mole) and $s° = 129.30$ J/mole (30.90 cal/mole). Naumov et al. (1971) reported $\Delta G°f = -974.28$ kJ/mole (-232.86 kcal/mole) from $pk = 7.7$ for the reaction:

$$FeMoO_4(c) \longrightarrow Fe^{2+} + MoO_4^{2-}$$
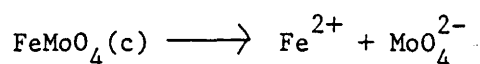
O'Hare et al. (1974) reported pk = 9.11 for the same reaction, which

determined $\Delta G°f$ = -979.38 kJ/mole (-234.07 kcal/mole) for $FeMoO_4$(c).

Sadiq and Lindsay (1979) critically evaluated $\Delta G°f$ for $FeMoO_4$(c)

and reported that calorimetric data of Wagman et al. (1982) and Latimer

(1951) and solubility measurements of O'Hare et al. (1974) had higher

uncertainties. Therefore, authors selected pk = 7.7 for the above

reaction after Naumov et al. (1971) and calculated $\Delta G°f$ = -971.27

kJ/mole (-232.14 kcal/mole) for $FeMoO_4$(c) to be internally consistent to

their selection.

In this report, we selected pk = 7.7 (Naumov et al., 1971) for the

above reaction and calculated $\Delta G°f$ = -971.44 kJ/mole (-232.18

kcal/mole) for $FeMoO_4$(c) to be internally consistent to our selection.

Li_2MoO_4(c)

Wagman et al. (1982) listed $\Delta G^\sigma f$ = -1409.50 kJ/mole (336.87

kcal/mole) from $\Delta H°f$ = -1520.30 kJ/mole (-363.36 kcal/mole) and s° =

126.00 J/mole (-30.11 cal/mole). No other ingredients was available.

We selected the available $\Delta G°f$ value for Li_2MoO_4(c).

$MgMoO_4$(c)

Wagman et al. (1982) recommended $\Delta G°f$ = -1295.68 kJ/mole (-309.67

kcal/mole) from $\Delta H°f$ = -1400.85 kJ/mole (-334.81 kcal/mole) and s° =

118.80 J/mole (28.39 cal/mole). Naumov et al. (1971) reported $\Delta G°f$ =

-1295.78 kJ/mole (-309.70 kcal/mole) from $\Delta H°f$ = -1400.88 kJ/mole

(-334.82 kcal/mole) after Barany (1962) and s° = 118.82 J/mole (28.40

cal/mole) after Weller and King (1963). Dellien et al. (1976) reported

similar values for $MgMoO_4$(c). Sadiq and Lindsay (1979) adopted Naumov

et al. (1971) values.

Reported $\Delta G°f$ values for $MgMoO_4(c)$ are in good agreement. Therefore, we selected $\Delta G°f = -1295.68$ kJ/mole (-309.67 kcal/mole) for $MgMoO_4(c)$ after Wagman et al. (1982).

$MnMoO_4(c)$

Sadiq and Lindsay (1979) recommended $\Delta G°f = -1090.30$ kJ/mole (-260.59 kcal/mole) from $\Delta H°f = -1191.35$ kJ/mole (-284.74 kcal/mole) after Barany (1965) and $s° = 131.79$ J/mole (31.50 cal/mole) after Naumov et al. (1971). Wagman et al. (1982) reported $\Delta H°f = -1191.31$ kJ/mole (-284.73 kcal/mole), which is similar to Baramy (1965). But the authors did not list $\Delta G°f$ or $s°$ values for $MnMoO_4(c)$.

Naumov et al. (1971) reported $\Delta G°f = -1090.39$ kJ/mole (-260.61 kcal/mole) from $\Delta H°r$ for the reaction:

$$MnO(c) + MoO_3(c) \longrightarrow MnMoO_4(c)$$
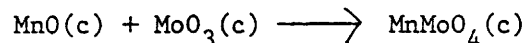
In this report, we selected $\Delta G°f = -1090.39$ kJ/mole (-260.61 kcal/mole) for $MnMoO_4(c)$ compound after Naumov et al. (1971).

$Na_2MoO_4(c)$

Wagman et al. (1982) reported $\Delta G°f = -1354.34$ kJ/mole (-323.69 kcal/mole) from $\Delta H°f = -1468.12$ kJ/mole (-350.89 kcal/mole) and $s° = 159.70$ J/mole (38.17 cal/mole). WATEQFC (Runnells and Lindberg, 1980) reported $logk° = 1.18$ for the reaction:

$$Na_2MoO_4(c) \longrightarrow 2Na^+ + MoO_4^{2-}$$
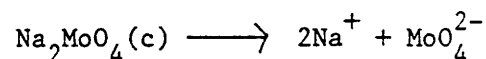
This equilibrium constant yield $\Delta G°f = -1353.31$ kJ/mole (-323.45 kcal/mole) which is in good agreement with $\Delta G°f$ value reported by Wagman

et al. (1982). Therefore, we selected $\Delta G°f = -1354.34$ kJ/mole (-323.69 kcal/mole) for Na_2MoO_4(c) after Wagman et al. (1982).
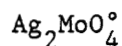
$Ag_2MoO_4°$

Wagman et al. (1982) listed $\Delta G°f = -681.90$ kJ/mole (-162.97 kcal/mole) from $\Delta H°f = -786.60$ kJ/mole (-188.00 kcal/mole) and $s° = 172.80$ J/mole (41.30 cal/mole). No other information was available. We adopted only available $\Delta G°f$ value for $Ag_2MoO_4°$.
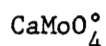
$CaMoO_4°$

Wagman et al. (1982) recommended $\Delta G°f = -1389.90$ kJ/mole (-332.19 kcal/mole) from $\Delta H°f = -154.50$ kJ/mole (-368.18 kcal/mole) and $s° = 25.90$ J/mole (6.19 cal/mole). We adopted the only available $\Delta G°f$ value for $CaMoO_4°$.
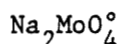
$Na_2MoO_4°$

Wagman et al. (1982) recommended $\Delta G°f = -1360.20$ kJ/mole (-325.09 kcal/mole) from $\Delta H°f = -1478.20$ kJ/mole (-353.30 kcal/mole) and $s° = 145.20$ J/mole (34.70 cal/mole). No other information was available. We selected the only available $\Delta G°f$ value for $Na_2MoO_4°$.
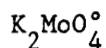
$K_2MoO_4°$

Wagman et al. (1982) listed $\Delta G°f = -1402.80$ kJ/mole (-335.27 kcal/mole) from $\Delta H°f = -1502.50$ kJ/mole (-359.10 kcal/mole) and $s° = 232.20$ J/mole (55.49 cal/mole). No other information was available. We adopted the available $\Delta G°f$ value for $K_2MoO_4°$.

$PbMoO_4$(c)
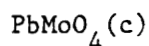
Wagman et al. (1982) reported $\Delta G°f = -951.40$ kJ/mole (-227.39 kcal/mole) from $\Delta H°f = -1051.90$ kJ/mole (-251.41 kcal/mole) and $s° =$

166.10 J/mole (39.70 cal/mole). Latimer (1952) listed pk = 5.39 for the reaction:

$$PbMoO_4(c) \longrightarrow Pb^{2+} + MoO_4^{2-}$$
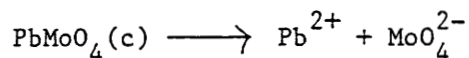
Smith and Martell (1976) reported pk = 13.0 for the same reaction from Muldrow and Hepler (1958). But the authors considered this pk value to be questionable because of the difficulties associated with measuring of solubility of $PbMoO_4(c)$. GEOCHEM (Runnells and Lindberg, 1980) and WATEQFC (Sposito and Mattigod, 1980) reported pk = 13.0 and 15.07, respectively.

Sadiq and Lindsay (1979) calculated $\Delta G°f$ = -952.36 kJ/mole (-227.62 kcal/mole) from $\Delta H°f$ = -1052.94 kJ/mole (-251.66 kcal/mole) after Dillien et al. (1976) and s° = 166.10 J/mole (39.70 cal/mole) after Weller and Kelley (1964). These values are similar to values reported by Wagman et al. (1982).

In this report, we selected $\Delta G°f$ = -952.36 kJ/mole (-227.62 kcal/mole) after Sadiq and Lindsay (1979).

$ZnMoO_4(c)$
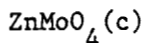
Naumov et al. (1971) recommended $\Delta G°f$ = -1010.85 kJ/mole (-241.60 kcal/mole) from pk = 4.49 for the reaction:

$$ZnMoO_4(c) \longrightarrow Zn^{2+} + MoO_4^{2-}$$
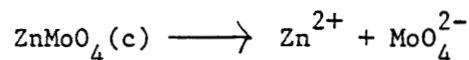
No other information was available. Therefore, we selected pk = 4.49 for the above reaction after Naumov et al. (1971) and calculated $\Delta G°f$ = -1009.09 kJ/mole (-241.18 kcal/mole) for $ZnMoO_4(c)$ to be internally consistent to our selection.

SELENIUM

Se^{2-}

Wagman et al. (1982) reported $\Delta G^\circ f$ = -129.30 kJ/mole (-30.90 kcal/mole). Authors did not list $\Delta H^\circ f$ and s° values for this species. Naumov et al. (1971) listed $\Delta G^\circ f$ = -129.30 kJ/mole (-30.90 kcal/mole) from $\Delta H^\circ f$ = 64.01 kJ/mole (15.30 kcal/mole) and s° = -46.02 J/mole (-11.00 cal/mole). Karapet'yants and Karapet'yants (1970) reported $\Delta G^\circ f$ = -129.30 kJ/mole (-30.90 kcal/mole) from $\Delta H^\circ f$ = 74.05 kJ/mole (17.70 kcal/mole) and s° = 173.63 J/mole (41.50 cal/mole). The reported $\Delta H^\circ f$ and s° values differ significantly for Se^{2-} species. However, $\Delta G^\circ f$ values agree very well. Therefore, we selected $\Delta G^\circ f$ = -129.30 kJ/mole (-30.90 kcal/mole) for Se^{2-} after Wagman et al. (1982).

SeO_3^{2-}

Naumov et al. (1971) listed $\Delta G^\circ f$ = -363.80 kJ/mole (-86.95 kcal/mole) from $\Delta H^\circ f$ = -509.19 kJ/mole (-121.70 kcal/mole) and s° = -7.12 J/mole (-1.7 cal/mole). Garrels and Christ (1965) listed $\Delta G^\circ f$ = -373.76 kJ/mole (-89.33 cal/mole) from $\Delta H^\circ f$ = -512.08 kJ/mole (-122.39 kcal/mole) and s° = 16.31 J/mole (3.9 cal/mole). Wagman et al. (1982) reported $\Delta H^\circ f$ = -369.78 kJ/mole (-88.38 kcal/mole) from $\Delta H^\circ f$ = -509.19 kJ/mole (-121.70 kcal/mole) and s° = 12.97 J/mole (3.10 cal/mole). Karapet'yants and Karapet'yants (1970) reported only $\Delta H^\circ f$ = -518.39 kJ/mole (-123.90 kcal/mole) and s° = 16.31 J/mole (3.9 cal/mole) values for SeO_3^{2-} species. Even though the $\Delta H^\circ f$ and s° values did not agree well, the $\Delta G^\circ f$ values agree very well. We selected $\Delta G^\circ f$ = -369.78 kJ/mole (-88.38 kcal/mole) for SeO_3^{2-} species after Wagman et al. (1982).

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SeO_4^{2-}

Wagman et al. (1982) reported $\Delta G°f = -441.28$ kJ/mole (-105.47 kcal/mole) from $\Delta H°f = 599.15$ kJ/mole (-143.20 kcal/mole) and $s° = 53.97$ J/mole (12.90 cal/mole). Naumov et al. (1971) listed $\Delta G°f = -441.41$ kJ/mole (-105.50 kcal/mole) from $\Delta H°f = -599.15$ kJ/mole (-143.20 kcal/mole) and $s° = 53.97$ J/mole (12.90 cal/mole). No other information is available for SeO_4^{2-} species. Therefore, we selected $\Delta G°f = -441.28$ kJ/mole (-105.47 kcal/mole) after Wagman et al. (1982).

HSe^-

Wagman et al. (1982) listed $\Delta G°f = 43.93$ kJ/mole (10.50 kcal/mole) from $\Delta H°f = 15.90$ kJ/mole (3.80 kcal/mole) and $s° = 79.50$ J/mole (19.00 cal/mole). Naumov et al. (1971) reported similar $\Delta G°f$, $\Delta H°f$, and $s°$ values. We selected $\Delta G°f = 43.93$ kJ/mole (10.50 kcal/mole) after Wagman et al. (1982).

$H_2Se°$

Wagman et al. (1982) reported $\Delta G°f = 22.17$ kJ/mole (5.30 kcal/mole) from $\Delta H°f = 19.24$ kJ/mole (4.6 kcal/mole) and $s° = 163.60$ J/mole (39.10 cal/mole). Similar $\Delta G°f$, $\Delta H°f$, and $s°$ values were listed by Naumov et al. (1971). In this report, we selected $\Delta G°f = 22.17$ kJ/mole (5.30 kcal/mole) for $H_2Se°$ after Wagman et al. (1982).

$HSeO_4^-$

Wagman et al. (1982) reported $\Delta G°f = -452.16$ kJ/mole (-108.07 kcal/mole) from $\Delta H°f = -581.58$ kJ/mole (-139.00 kcal/mole). Naumov et al. (1971) listed $\Delta G°f = -450.87$ kJ/mole (-107.76 kcal/mole) from $\Delta H°f = -576.14$ kJ/mole (-137.70 kcal/mole) and $s° = 162.76$ J/mole (38.90

cal/mole). Reported $\Delta G°f$ values for $HSeO_4^-$ are in good agreement. We selected $\Delta G°f$ = -452.16 kJ/mole (-108.07 kcal/mole) after Wagman et al. (1982).
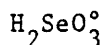
$H_2SeO_3^°$

Wagman et al. (1982) reported $\Delta G°f$ = -426.14 kJ/mole (-101.85 kcal/mole) from $\Delta H°f$ = -507.48 kJ/mole (-121.29 kcal/mole) and s° = 207.95 J/mole (49.70 cal/mole). Similar $\Delta G°f$, $\Delta H°f$, s° values for $H_2SeO_3^°$ species were reported by Naumov et al. (1971). We selected $\Delta G°f$ = -426.14 kJ/mole (-101.85 kcal/mole) after Wagman et al. (1981).
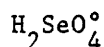
$H_2SeO_4^°$

Garrels and Christ (1965) listed $\Delta G°f$ = -441.08 kJ/mole (-105.42 kcal/mole) from $\Delta H°f$ = -607.94 kJ/mole (-145.30 kcal/mole) and s° = 23.85 J/mole (5.70 cal/mole). No other information is available for $H_2SeO_4^°$ species. Therefore, we selected available $\Delta G°f$ of -441.08 kJ/mole (-105.42 kcal/mole) after Garrels and Christ (1965).

$BaSeO_3$
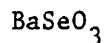
Wagman et al. (1982) reported $\Delta G°f$ = -968.18 kJ/mole (-231.40 kcal/mole) from $\Delta H°f$ = -1040.56 kJ/mole (-248.70 kcal/mole) and s° = 167.36 J/mole (40.00 cal/mole). Karapet'yants and Karapet'yants (1970) listed $\Delta G°f$ = -971.95 kJ/mole (-232.30 kcal/mole) from $\Delta H°f$ = -1043.11 kJ/mole (-249.31 kcal/mole) and s° = 177.82 J/mole (42.50 cal/mole). Reported $\Delta G°f$ values for $BaSeO_3$ agree fairly well. Therefore, we selected $\Delta G°f$ = -968.18 kJ/mole (-231.40 kcal/mole) after Wagman et al. (1982).

CaSe

Wagman et al. (1982) reported $\Delta G°f = -363.17$ kJ/mole (-86.80 kcal/mole) from $\Delta H°f = -368.20$ kJ/mole (-88.00 kcal/mole) and $s° = 66.95$ J/mole (16.00 cal/mole). Karapet'yants and Karapet'yants (1970) reported $\Delta G°f = 75.32$ kJ/mole (18.00 kcal/mole). The agreement between $\Delta G°f$ values for CaSe was very poor. In this report, we selected $\Delta G°f = 363.17$ kJ/mole (86.80 kcal/mole) after Wagman et al. (1982). Because the $\Delta G°f$ value reported by Karapet'yants and Karapet'yants (1970) was derived from approximate calculations.

$CaSe_3 \cdot 2H_2O$

Naumov et al. (1971) reported $\Delta G°f = -1423.40$ kJ/mole (-340.20 kcal/mole) from $\Delta H°f = -1609.60$ kJ/mole (-384.70 kcal/mole) $s° = 233.05$ J/mole (55.70 cal/mole). Wagman et al. (1982) listed only $\Delta G°f$ value of -1428.84 kJ/mole (-341.50 kcal/mole). Similar $\Delta G°f$ value for $CaSe_3 \cdot 2H_2O$ was reported by Karapet'yants and Karapet'yants (1970). We selected Wagman et al. (1982) $\Delta G°f$ value for $CaSe_3 \cdot 2H_2O$.

$CaSeO_4$

No source gives a value of $\Delta G°f$ for $CaSeO_4$. However, Smith and Martell (1976) reported equilibrium constant of $10^{3.09}$ for the following reaction:

$$CaSeO_4 \rightleftharpoons Ca^{2+} + SeO_4^{2-}$$
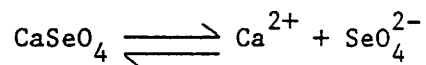
Using $\Delta G°f = -554.46$ kJ/mole (-132.52 kcal/mole) for Ca^{2+} from Lindsay (1979) and $\Delta G°f = -441.28$ kJ/mole (-105.47 kcal/mole) for SeO_4^{2-} from Wagman et al. (1982), we calculated $\Delta G°f = -1013.50$ kJ/mole (-242.23 kcal/mole) for $CaSeO_4$ compound from the above reaction.

$CaSeO_4 \cdot 2H_2O$
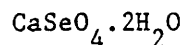
Wagman et al. (1982) reported $\Delta G°f = -1486.80$ kJ/mole (-355.35 kcal/mole) from $\Delta H°f = -1706.66$ kJ/mole (-407.90 kcal/mole) and $s° = 221.75$ J/mole (53.00 cal/mole). Karapet'yants and Karapet'yants (1970) listed $\Delta G°f = -1402.40$ kJ/mole (-335.18 kcal/mole) from $\Delta H°f = -1727.03$ kJ/mole (-412.77 kcal/mole) and $s° = 131.80$ J/mole (31.50 cal/mole). Naumov et al. (1971) reported $\Delta G°f = -1486.16$ kJ/mole (-335.20 kcal/mole) from $\Delta H°f = -1717.33$ kJ/mole (-410.45 kcal/mole) and $s° = 184.94$ J/mole (44.20 cal/mole). Listed $\Delta G°f$ values for $CaSeO_4 \cdot 2H_2O$ agree very well. Therefore, we adopted $\Delta G°f = 1486.80$ kJ/mole (-355.35 kcal/mole) for $CaSeO_4 \cdot 7H_2O$ after Wagman et al. (1982).

CuSe

Smith and Martell (1976) reported equilibrium constant of $10^{-48.10}$ for the following reaction:

$$CuSe \rightleftharpoons Cu^{2+} + Se^{2-}$$
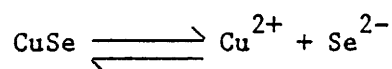
Using $\Delta G°f = 65.57$ kJ/mole (15.67 kcal/mole) for Cu^{2+} from Lindsay (1979) and $\Delta G°f = 129.30$ kJ/mole (30.90 kcal/mole) for Se^{2-} from Wagman et al. (1982), we calculated $\Delta G°f = -79.50$ kJ/mole (-19.00 kcal/mole) for CuSe compound from the above reaction.

Cu_2Se

Smith and Martell (1976) listed equilibrium constant of $10^{-60.80}$ for the following reaction:

$$Cu_2Se \rightleftharpoons 2Cu^+ + Se^{2-}$$
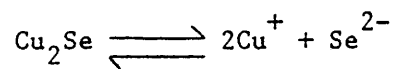
No other information is available for this compound. Therefore, we calculated $\Delta G°f$ = -116.44 kJ/mole (-27.83 kcal/mole) for Cu_2Se using = 50.63 kJ/mole (12.10 kcal/mole) for Cu^+ (Lindsay, 1979) and $\Delta G°f$ = 129.30 kJ/mole (30.90 kcal/mole) for Se^{2-} (Wagman et al. 1982) from reaction.
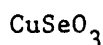
$CuSeO_3$

Wagman et al. (1982) reported $\Delta G°f$ = -348.07 kJ/mole (-83.19 kcal/mole). No other information is available for this compound. Therefore, we selected available $\Delta G°f$ = -348.07 kJ/mole (-83.19 kcal/mole) for $CuSeO_3$ after Wagman et al. (1982).

$CuSeO_3 \cdot 2H_2O$
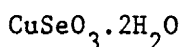
Karapet'yants and Karapet'yants (1970) reported $\Delta G°f$ = -827.60 kJ/mole (-197.80 kcal/mole) from $\Delta H°f$ = -1003.32 kJ/mole (-239.80 kcal/mole) and $s°$ = 258.57 J/mole (61.80 cal/mole). Naumov et al. (1971) listed $\Delta G°f$ = -817.39 kJ/mole (-195.36 kcal/mole) from $\Delta H°f$ = -983.66 kJ/mole (-235.10 kcal/mole) and $s°$ = 292.46 J/mole (69.90 cal/mole).

Smith and Martell (1976) reported a equilibrium constant of $10^{-7.78}$ for the following reaction at 20°C:

$$CuSeO_3 \cdot 2H_2O \rightleftharpoons Cu^{2+} + SeO_3^{2-} + 2H_2O$$
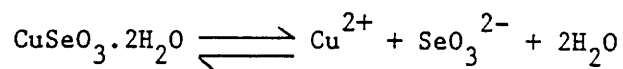
using $\Delta G°f$ = 65.56 kJ/mole (15.67 kcal/mole) for Cu^{2+} (Lindsay, 1979) and $\Delta G°f$ = 369.78 kJ/mole (-88.38 kcal/mole) for SeO_3^{2-} (Wagman et al., 1982) from the above reaction, we estimated $\Delta G°f$ = -823.00 kJ/mole (-196.70 kcal/mole) for $CuSeO_3 \cdot 2H_2O$ compound. This estimated value for $CuSeO_3 \cdot 2H_2O$ agrees well with Karapet'yants and Karapet'yants (1970).

Therefore, we adopted $\Delta G°f = -827.60$ kJ/mole (-197.80 kcal/mole) for $CuSeO_3 \cdot 2H_2O$ after Karapet'yants and Karapet'yants (1970).

FeSe

Garrels and Christ (1965) reported $\Delta G°f = -58.16$ kJ/mole (-13.90 kcal/mole) from $\Delta H°f = -69.03$ kJ/mole (-16.50 kcal/mole). However, authors did not list $s°$ values. Karapet'yants and Karapet'yants (1970) reported a range of $\Delta G°f$ values from -58.16 kJ/mole (-13.90 kcal/mole) to -74.06 kJ/mole (-17.70 kcal/mole). Smith and Martell (1976) reported a equilibrium constant of $10^{-26.00}$ for the following reaction:

$$FeSe \rightleftharpoons Fe^{2+} Se^{2-}$$
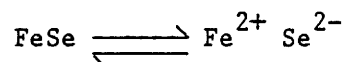
using $\Delta G°f = -91.21$ kJ/mole (-21.80 kcal/mole) for Fe^{2+} (Lindsay, 1979) and $\Delta G°f = -129.28$ kJ/mole (-30.90 kcal/mole) for Se^{2-} (Wagman et al., 1982). We calculated $\Delta G°f = -110.29$ kJ/mole (-26.36 kcal/mole) for FeSe from the above reaction.

$Fe_2(SeO_3)_3$

Garrels and Christ (1965) reported equilibrium constant of $10^{-33.00}$ for the following reaction:

$$Fe_2(SeO_3)_3 \rightleftharpoons 2Fe^{3+} + 3SeO_3^{2-}$$
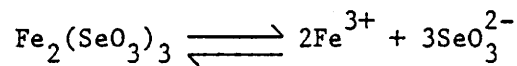
No other information is available for this compound.

Therefore, we calculated $\Delta G°f = -1331.56$ kJ/mole (-318.25 kcal/mole) for $Fe_2(SeO_3)_3$ from the above reaction using $\Delta G°f = -16.82$ kJ/mole (-4.02 kcal/mole) for Fe^{3+} (Lindsay, 1979) and $\Delta G°f = -369.78$ kJ/mole (-88.38 kcal/mole) for SeO_3^{2-} (Wagman et al., 1982).
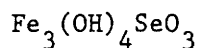
$Fe_3(OH)_4SeO_3$

Garrels and Christ (1965) reported equilibrium constant of $10^{62.70}$ for the following reaction:

$$Fe_2(OH)_4SeO_3 \xrightleftharpoons{} 2Fe^{3+} + 4OH^- + SeO_3^{2-}$$
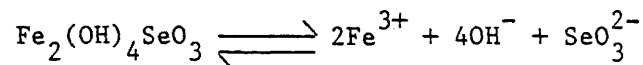
No other information is available for this compound. Therefore, we calculated $\Delta G°f = -1390.56$ kJ/mole (-332.35 kcal/mole) for $Fe_3(OH)_4$ SeO_3 from the above reaction, using $\Delta G°f = -16.82$ kJ/mole (-4.02 kcal/mole) for Fe^{3+}, $\Delta G°f = -157.30$ kJ/mole (-37.594 kcal/mole) for OH^- (Lindsay, 1979), and $\Delta G°f = -369.78$ kJ/mole (-88.38 kcal/mole) for SeO_3^{2-} (Wagman et al., 1982).

MnSe

Wagman et al. (1982) reported $\Delta G°f = -111.71$ kJ/mole (-26.70 kcal/mole) from $\Delta H°f = -106.70$ kJ/mole (-25.50 kcal/mole) and $s° = 90.79$ J/mole (21.70 cal/mole). Naumov et al. (1971) listed $\Delta G°f = -153.55$ kJ/mole (-36.70 kcal/mole) from $\Delta H°f = 148.53$ kJ/mole (-35.50 kcal/mole) and $s° = 90.79$ J/mole (21.70 cal/mole) Karapet'yants and Karapet'yants (1970) reported $\Delta G°f = -122.30$ kJ/mole (-29.25 kcal/mole) from $\Delta H°f = -157.73$ kJ/mole (-37.70 kcal/mole). However, authors did not list $s°$ values. Smith and Martel (1976) reported equilibrium constant of $10^{-11.50}$ for the following reaction:

$$MnSe \xrightleftharpoons{} Mn^{2+} + Se^{2-}$$
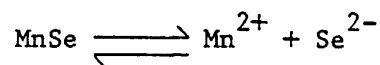
Since reported $\Delta G°f$ values for MnSe agree poorly, we calculated $\Delta G°f = -166.94$ kJ/mole (-39.90 kcal/mole) from the above reaction using $\Delta G°f = -230.58$ kJ/mole (-55.11 kcal/mole) for Mn^{2+} (Lindsay, 1979) and $\Delta G°f = -129.30$ kJ/mole (-30.90 kcal/mole) for Se^{2-} (Wagman et al., 1982).

PbSe

Garrels and Christ (1965) reported $\Delta G°f$ = -64.43 kJ/mole (-15.40 kcal/mole) from $\Delta H°f$ = -75.31 kJ/mole (-18.00 kcal/mole) and $s°$ = 112. J/mole (26.90 cal/mole). Karapet'yants and Karapet'yants (1970) reported a range of $\Delta G°f$ values from -64.43 kJ/mole (-15.40 kcal/mole) to -73.64 kJ/mole (-17.60 kcal/mole). These authors calculated $\Delta G°f$ values from $\Delta H°f$ = -75.31 kJ/mole (-18.00 kcal/mole) and $s°$ = 96.23 J/mole (23.00 cal/mole) and also from $s°$ = 112.55 J/mole (26.90 cal/mole). Smith and Martell (1976) reported equilibrium constant of $10^{-42.10}$ for the following reactions:

$$PbSe \rightleftharpoons Pb^{2+} + Se^{2-}$$
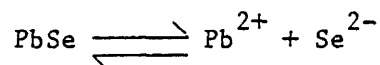
Since reported $\Delta G°f$ values for PbSe compound agree poorly, we calculated $\Delta G°f$ = -131.88 kJ/mole (-31.52 kcal/mole) from above reaction using $\Delta G°f$ = -24.68 kJ/mole (-5.90 kcal/mole) for Pb^{2+} (Lindsay, 1979) and $\Delta G°f$ = -129.30 kJ/mole (-30.90 kcal/mole) for Se^{2-} (Wagman et al. 1982).

$PbSeO_3$

Karapet'yants and Karapet'yants (1970) reported $\Delta G°f$ = -463.80 kJ/mole (-110.85 kcal/mole) from $\Delta H°f$ = -533.04 kJ/mole (-127.40 kcal/mole) and $s°$ = 181.87 J/mole (43.47 cal/mole). Since no other information is available, we adopted the Karapet'yants and Karapet'yants value for $PbSeO_3$.

$PbSeO_4$

Wagman et al. (1982) reported $\Delta G°f$ = -504.88 kJ/mole (-120.67 kcal/mole) from $\Delta H°f$ = 609.20 kJ/mole (-145.60 kcal/mole) and $s°$ = 167.78 J/mole (40.10 cal/mole). Karapet'yants and Karapet'yants (1970)

listed $\Delta G°f = 497.90$ kJ/mole (-119.00 kcal/mole) from $\Delta H°f = 622.16$ kJ/mole (-148.70 kcal/mole) and $s° = 103.35$ J/mole (24.7 cal/mole). Naumov et al. (1971) reported $\Delta G°f = -504.84$ kJ/mole (-120.88 kcal/mole) from $\Delta H°f = 615.05$ kJ/mole (-147.00 kcal/mole) and $s° = 142.25$ J/mole (34.00 cal/mole). Reported $\Delta G°f$ values for $PbSeO_4$ agree fairly well. Therefore, we selected $\Delta G°f = -504.88$ kJ/mole (-120.67 kcal/mole) after Wagman et al. (1982).

ZnSe

Garrels and Christ (1965) reported $\Delta G°f = 145.18$ kJ/mole (-34.70 kcal/mole) from $\Delta H°f = -142.25$ kJ/mole (-34.00 kcal/mole) and $s° = 93.30$ J/mole (23.30 cal/mole). Wagman et al. (1982) reported $\Delta G°f = -163.00$ kJ/mole (-38.96 kcal/mole) from $\Delta H°f = -163.00$ kJ/mole (-38.96 kcal/mole) and $s° = 83.68$ J/mole (20.00 cal/mole). Karapet'yants and Karapet'yants (1970) listed $\Delta G°f = -145.18$ kJ/mole (-34.70 kcal/mole) from $\Delta H°f = -129.70$ kJ/mole (-31.00 kcal/mole) and $s° = 61.08$ J/mole (14.60 cal/mole). Smith and Martell (1976) reported equilibrium constant of $10^{-29.40}$ for the following reaction:

$$ZnSe \xrightleftharpoons{} Zn^{2+} + Se^{2-}$$
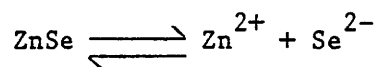
Since reported $\Delta G°f$ values for ZnSe compound agree poorly, we calculated $\Delta G°f = -185.72$ kJ/mole (-44.39 kcal/mole) from the above reaction using $\Delta G°f = -147.22$ kJ/mole (-35.18 kcal/mole) for Zn^{2+} (Lindsay, 1979) and $\Delta G°f = -129.20$ kJ/mole (-30.90 kcal/mole) for Se^{2-} (Wagman et al., 1982).

$ZnSe_3 \cdot H_2O$

Wagman et al. (1982) reported $\Delta G°f = -729.80$ kJ/mole (-174.43 kcal/mole) from $\Delta H°f = -930.90$ kJ/mole (-222.490 kcal/mole) and $s° =$

163.00 J/mole (38.96 cal/mole). No other information is available for this compound. Therefore, we adopted available $WG°f$ value after Wagman et al. (1982).
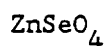
$ZnSeO_4$

Smith and Martell (1976) reported equilibrium constant of $10^{2.19}$ for the following reaction:

$$Zn^{2+} + SeO_4^{2-} \rule[0.5ex]{3em}{0.4pt} ZnSeO_4$$
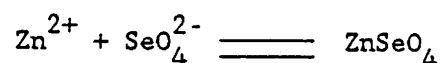
No other information is available for this compound. Therefore, we calculated $WG°f = -601.12$ kJ/mole (-143.67 kcal/mole) for $ZnSeO_4$ from the above reaction using $WG°f = -147.22$ kJ/mole (-35.19 kcal/mole) for Zn^{2+} (Lindsay, 1979) and $WG°f = -441.28$ kJ/mole (-105.47 kcal/mole) for SeO_4^{2-} (Wagman et al. 1982).

Table 4. Summary of Collected $\Delta G°f$ (kJ/mole) values for Strontium Species. Values in Parenthesis are kcal/mole.

No.	Species	Source*									
		1	2	3	4	5	6	7	8	9	10
1.	Sr^{2+}	−559.47 (−133.72)	−559.44 (−133.71)	---	−571.44 (−136.58)	---	---	−563.83 (−134.76	−559.43 (−133.70)	---	---
2.	$SrSO_4(c)$	−1340.89 (−320.48)	---	−1334.44 (−318.94)	−1353.35 (−323.46)	---	---	---	−1340.97 (−320.50)	---	−1340.68 (−320.43)
3.	$SrO(c)$	−561.87 (−134.29)	---	−573.00 (−137.07)	−574.13 (−137.22)	−559.82 (−133.80)	---	−559.95 (−133.83)	−560.32 (−133.92)	−560.57 (−133.98)	---
4.	$Sr(NO_3)_2(c)$	−780.02 (−186.43)	---	−778.22 (−186.00)	−790.40 (−188.91)	---	---	−783.28 (−187.21)	−779.06 (−186.20)	---	---
5.	$SrBr_2(c)$	−697.10 (−166.61)	---	−695.80 (−166.30)	---	---	---	---	−695.89 (−166.32)	−699.77 (−167.25)	---
6.	$SrHPO_4(c)$	−1688.60 (−403.58)	---	−1681.31 (−401.80)	---	−1672.34 (−399.70)	---	---	---	---	---
7.	$SrF_2(c)$	−1164.57 (−278.34)	---	−1162.31 (−277.80)	−1180.56 (−282.16)	−1162.31 (−277.80)	---	---	---	−1164.74 (−278.38)	---
8.	$SrCrO_4(c)$	---	---	---	−1318.37 (−315.10)	---	−1319.21 (−315.30)	---	---	---	---
9.	$SrSeO_3(c)$	---	---	−965.83 (−230.84)	−969.43 (−231.70)	---	---	---	---	---	---
10.	$Sr_2TiO_4(c)$	−2172.30 (−519.19)	−2178.60 (−520.70)	---	−2196.01 (−524.86)	---	---	---	---	---	---
11.	$SrOH^+$	−721.32 (−172.40)	−721.32 (−172.40)	---	−733.45 (−175.30)	---	---	---	---	---	---

Table 4. Summary of Collected $\Delta G°f$ (kJ/mole) values for Strontium Species. Values in Parenthesis are kcal/mole. (cont.)

No.	Species	Source*									
		1	2	3	4	5	6	7	8	9	10
12.	$SrSO_4°$	-1304.03 (-311.67)	---	---	---	---	---	---	---	---	---
13.	$SrCO_3$(c)	-1140.10 (-272.49)	---	-1138.13 (-272.02)	-1152.31 (-275.40)	---	---	---	-1137.63 (-271.90)	---	---
14.	$SrSiO_3$(c)	-1549.70 (-370.39)	---	-1467.75 (-350.80)	-1561.64 (-373.24)	---	---	---	---	---	---
15.	Sr_2SiO_4(c)	-2191.10 (-523.68)	---	-2074.00 (-495.70)	-2215.09 (-529.68)	-2074.00 (-495.70)	---	---	---	---	---
16.	$Sr_3(PO_4)_2$(c)	---	---	---	---	-3899.90 (-932.10)	---	---	---	---	---
17.	$Sr(NO_3).4H_2O$(c)	---	---	-1725.48 (-412.40)	---	---	---	-1734.19 (-414.48)	---	---	---
18.	$SrCl_2$(c)	-781.10 (-186.69)	---	---	---	-781.15 (-186.70)	-781.15 (-186.70)	-785.00 (-187.62)	---	-781.02 (-186.67)	---
19.	$SrCl_2.H_2O$(c)	-1036.30 (-247.68)	---	-1038.47 (-248.20)	---	---	---	---	---	---	---
20.	$SrBr_2.H_2O$(c)	-954.30 (-228.08)	---	---	---	---	---	---	---	---	---
21.	$Sr_3(ASO_4)_2$(c)	-3080.10 (-736.16)	---	---	---	---	-3222.10 (-770.10)	---	---	---	---
22.	$SrSeO_4$(c)	---	---	-1023.87 (-244.71)	-1039.14 (-248.36)	---	---	---	---	---	---

Table 4. Summary of Collected $\Delta G°f$ (kJ/mole) values for Strontium
Species. Values in Parenthesis are kcal/mole. (cont.)

No.	Species	Source* 1	2	3	4	5	6	7	8	9	10
23.	$SrMoO_4(c)$	---	---	-1448.50 (-346.20)	-1454.36 (-347.60)	---	---	---	---	---	---
24.	$Sr(OH)_2(c)$	---	---	-870.27 (-208.00)	-869.43 (-207.80)	---	---	---	---	---	---
25.	$SrI_2(c)$	---	---	-562.33 (-134.40)	---	---	---	---	---	-558.71 (-133.53)	---
26.	$SrTiO_3(c)$	-1588.36 (-379.62)	-1588.41 (-379.64)	---	-1600.38 (-382.50)	---	---	---	---	---	---
27.	$SrZrO_3(c)$	-1682.80 (-402.20)	-1682.80 (-402.20)	---	-2548.89 (-609.20)	---	---	---	---	---	---
28.	$SrHCO_3^+$	---	---	---	---	---	---	-1157.50 (-276.65)	---	---	---
29.	$SrCO_3°$	-1087.30 (-259.87)	-1087.33 (-259.88)	---	---	---	---	-1175.50 (-280.95)	---	---	---
30.	$Sr(NO_3)_2°$	-781.99 (-186.90)	---	---	---	---	---	---	---	---	---
31.	$SrCl_2°$	-821.90 (-196.44)	---	---	---	---	---	---	---	---	---
32.	$SrI_2°$	-662.62 (-158.37)	---	---	---	---	---	---	---	---	---
33.	$SrBr_2°$	---	-767.38 (-183.41)	---	---	---	---	---	---	---	---

Table 4. Summary of collected ΔG°f (kJ/mole) values for Strontium
          Species. Values in parenthesis are kcal/mole. (cont.)

Source*

1. Wagman et al. (1982)
2. Parker et al. (1971)
3. Karapet'yants and Karapet'yants (1970)
4. Naumov et al. (1971)
5. Garrels and Christ (1968)
6. Latimer (1952)
7. Busenberg et al. (1984)
8. Robie et al. (1978)
9. Pankratz (1984)
10. Helgeson et al. (1978)

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Table 5. Summary of Selected $\Delta G°f$ of Strontium Species.

No.	Species	$\Delta G°f$ (kJ/mole)	(kcal/mole)	Source	Remarks
1.	Sr^{2+}	-563.83	-134.76	Busenberg et al. (1984)	pk
2.	$SrSO_4(c)$	-1346.16	-321.74	Reardon and Armstrong (1987)	pk
3.	$SrO(c)$	-559.95	-133.83	Busenberg et al. (1984)	pk
4.	$Sr(NO_3)(c)$	-783.28	-187.21	Busenberg et al. (1984)	pk
5.	$SrBr_2(c)$	-699.77	-167.25	Pankratz (1984)	$\Delta H°f$ and $s°$
6.	$SrHPO_4(c)$	-1688.60	-403.58	Wagman et al. (1982)	$\Delta H°f$ and $s°$
7.	$SrF_2(c)$	-1180.56	-282.16	Naumov et al. (1971)	$\Delta H°f$ and $s°$
8.	$SrCrO_4(c)$	-1318.37	-315.10	Naumov et al. (1971)	$\Delta H°f$ and $s°$
9.	$SrSeO_3(c)$	-969.43	-231.70	Naumov et al. (1971)	$\Delta H°f$ and $s°$
10.	$Sr_2TiO_4(c)$	-2196.01	-524.86	Naumov et al. (1971)	$\Delta H°f$ and $s°$
11.	$SrOH^+$	-733.46	-175.30	Naumov et al. (1971)	$\Delta H°f$ and $s°$
12.	$SrSO_4°$	-1320.89	-315.70	Smith and Martell (1978)	pk
13.	$SrCO_3(c)$	-1144.63	-273.33	Busenberg et al. (1984)	pk
14.	$SrSiO_3(c)$	-1561.64	-373.24	Naumov et al. (1971)	$\Delta H°f$ and $s°$
15.	$Sr_2SiO_4(c)$	-2191.10	-523.68	Wagman et al. (1982)	$\Delta H°f$ and $s°$
16.	$Sr_3(PO_4)_2(c)$	-3899.90	-932.10	Garrels and Christ (1968)	$\Delta H°f$ and $s°$
17.	$Sr(NO_3)_2 \cdot 4H_2O(c)$	-1734.19	-414.48	Busenberg et al. (1984)	pk

Table 5. Summary of Selected ΔG°f of Strontium Species.

No.	Species	ΔG°f (kJ/mole)	(kcal/mole)	Source	Remarks
18.	$SrCl_2(c)$	-785.00	-187.62	Busenberg et al. (1984)	pk
19.	$SrCl_2 \cdot H_2O(c)$	-1036.30	-247.68	Wagman et al. (1982)	ΔH°f and s°
20.	$SrBr_2 \cdot H_2O(c)$	-954.30	-228.08	Wagman et al. (1982)	ΔH°f and s°
21.	$Sr_3(ASO_4)_2(c)$	-3080.10	-736.16	Wagman et al. (1982)	ΔH°f and s°
22.	$SrSeO_4(c)$	-1039.14	-248.36	Naumov et al. (1971)	pk
23.	$SrMoO_4(c)$	-1454.36	-347.60	Naumov et al. (1971)	pk
24.	$Sr(OH)_2(c)$	-870.27	-208.00	Karapet'yants and Karapet'yants (1970)	ΔH°f and s°
25.	$SrI_2(c)$	-558.71	-133.53	Pankratz (1984)	ΔH°f and s°
26.	$SrTiO_3(c)$	-1600.38	-382.50	Naumov et al. (1971)	ΔH°f and s°
27.	$SrZrO_3(c)$	-1682.77	-402.20	Wagman et al. (1982)	ΔH°f and s°
28.	$SrHCO_3^+$	-1157.50	-276.65	Busenberg et al. (1984)	pk
29.	$SrCO_3^\circ$	-1175.50	-280.95	Busenberg et al. (1984)	pk
30.	$Sr(NO_3)_2^\circ$	-781.99	-186.90	Wagman et al. (1982)	ΔH°f and s°
31.	$SrCl_2^\circ$	-821.90	-196.44	Wagman et al. (1982)	ΔH°f and s°
32.	SrI_2°	-662.62	-158.37	Wagman et al. (1982)	ΔH°f and s°
33.	$SrBr_2^\circ$	-767.38	-183.41	Parker et al. (1971)	ΔH°f and s°

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Table 6. Equilibrium Reactions of Strontium.

No.	Reaction			logk°
	I. Solid Phases			
1.	$SrO(c) + 2H^+$	$\longrightarrow$	$Sr^{2+} + H_2O$	42.23
2.	$Sr(OH)_2(c) + 2H^+$	$\longrightarrow$	$Sr^{2+} + 2H_2O$	29.42
3.	$SrSiO_3(c) + 2H^+ + H_2O$	$\longrightarrow$	$Sr^{2+} + H_4SiO_4^\circ$	12.82
4.	$Sr_2SiO_4(c) + 4H^+$	$\longrightarrow$	$2Sr^{2+} + H_4SiO_4^\circ$	42.88
5.	$SrCO_3(c)$	$\longrightarrow$	$Sr^{2+} + CO_3^{2-}$	-9.27
6.	$SrSO_4(c)$	$\longrightarrow$	$Sr^{2+} + SO_4^{2-}$	-6.63
7.	$Sr(NO_3)_2(c)$	$\longrightarrow$	$Sr^{2+} + 2NO_3^-$	0.61
8.	$SrBr_2(c)$	$\longrightarrow$	$Sr^{2+} + 2Br^-$	12.64
9.	$SrHPO_4(c) + H^+$	$\longrightarrow$	$Sr^{2+} + H_2PO_4^-$	2.22
10.	$Sr_3(PO_4)_2(c) + 4H^+$	$\longrightarrow$	$3Sr^{2+} + 2H_2PO_4^-$	11.64
11.	$Sr(NO_3)_2 \cdot 4H_2O(c)$	$\longrightarrow$	$Sr^{2+} + 2NO_3^- + 4H_2O$	0.22
12.	$SrF_2(c)$	$\longrightarrow$	$Sr^{2+} + 2F^-$	-8.46
13.	$SrCl_2(c)$	$\longrightarrow$	$Sr^{2+} + 2Cl^-$	7.24
14.	$SrCl_2 \cdot H_2O(c)$	$\longrightarrow$	$Sr^{2+} + 2Cl^- + H_2O$	4.77
15.	$SrBr_2 \cdot H_2O(c)$	$\longrightarrow$	$Sr^{2+} + 2Br^- + H_2O$	9.60
16.	$Sr_3(ASO_4)_2(c) + 2H^+$	$\longrightarrow$	$3Sr^{2+} + 2HASO_4^{2-}$	5.46
17.	$SrCrO_4(c)$	$\longrightarrow$	$Sr^{2+} + CrO_4^{2-}T$	-4.70
18.	$SrSeO_3(c)$	$\longrightarrow$	$Sr^{2+} + SeO_3^{2-}T$	-6.27
19.	$SrSeO_4(c)$	$\longrightarrow$	$Sr^{2+} + SeO_4^{2-}$	-5.96
20.	$SrMoO_4(c)$	$\longrightarrow$	$Sr^{2+} + MoO_4^{2-}$	-9.53
21.	$SrI_2(c)$	$\longrightarrow$	$Sr^{2+} + 2I^-$	19.14
22.	$Sr^{2+} + H_2O$	$\longrightarrow$	$SrOH^+ + H^+$	-11.83
23.	$Sr^{2+} + CO_2(g) + H_2O$	$\longrightarrow$	$SrHCO_3^+ + H^+$	-6.64

Table 6. Equilibrium Reactions of Strontium. (cont.)

No.	Reaction			$\log k°$

II. Solution Phases

No.	Reaction	$\log k°$
24.	$Sr^{2+} + CO_2(g) + H_2O \longrightarrow SrCO_3° + 2H^+$	-18.15
25.	$Sr^{2+} + SO_4^{2-} \longrightarrow SrSO_4°$	2.55
26.	$Sr^{2+} + 2NO_3^- \longrightarrow Sr(NO_3)_2°$	-0.84
27.	$Sr^{2+} + 2Cl^- \longrightarrow SrCl_2°$	-0.78
28.	$Sr^{2+} + 2I^- \longrightarrow SrI_2°$	-0.84
29.	$Sr^{2+} + 2Br^- \longrightarrow SrBr_2°$	-0.80

$T\Delta G°f$ values for CrO_4^{2-}, SeO_3^{2-}, and SeO_4^{2-}, were selected from Wagman et al. (1982).

Table 7. Summary of Collected Standard Free Energies of Formation ($\Delta G°f$, kJ/mole) of F Species. Values in the Parenthesis are kcal/mole.

No.	Species	Source 1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1.	F^-	-278.79 (-66.63)	-284.22 (-67.93)	-----	-281.70 (-67.33)	-284.22 (-67.93)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
2.	$HF°$	-296.82 (-70.94)	-----	-----	-----	-----	-298.11 (-71.25)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
3.	HF_2^-	-578.08 (-138.16)	-----	-----	-----	-----	-581.50 (-138.98)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
4.	AlF_2^+	-1113.00 (-266.01)	-1131.27 (-270.38)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
5.	AlF^{2+}	-803.00 (-191.92)	-814.96 (-194.78)	-----	-----	-----	-811.82 (-194.03)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
6.	$AlF_3°$	-1414.00 (-337.95)	-1438.58 (-343.08)	-----	-----	-----	-1427.03 (-341.07)	-----	-----	-----	-----	-----	-1438.88 (-343.90)	-----	-----	-----	-----
7.	AlF_4^-	-----	-1736.40 (-415.01)	-----	-----	-----	-1720.63 (-411.24)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
8.	FeF^{2+}	-322.60 (-77.10)	-335.00 (-80.14)	-----	-----	-----	-332.33 (-79.43)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
9.	$FeF_2°$	-636.48 (-152.12)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
10.	FeF_2^+	-628.40 (-150.19)	-637.76 (-152.43)	-----	-----	-645.55 (-154.29)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
11.	$FeF_3°$	-----	-936.25 (-223.77)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
12.	PbF^+	-310.37 (-74.18)	-317.40 (-75.86)	-----	-----	-----	-311.70 (-74.50)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
13.	$PbF_2°$	-596.60 (-142.60)	-606.09 (-144.86)	-----	-----	-----	-597.47 (-142.80)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
14.	PbF_3^-	-----	-896.84 (-214.35)	-----	-----	-----	-884.08 (-211.80)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
15.	PbF_4^{2-}	-----	-1179.26 (-281.85)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
16.	$SiF_4°$	-1607.40 (-384.18)	-----	-----	-----	-----	-1611.67 (-385.20)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
17.	SiF_6^{2-}	-2207.06 (-525.67)	-----	-----	-----	-----	-2207.31 (-527.56)	-2138.24 (-511.00)	-----	-----	-----	-----	-----	-----	-----	-----	-----

Table 7. Summary of Collected Standard Free Energy of Formation ($\Delta G°f$, kJ/mole) of F Species. Values in the Parenthesis are kcal/mole. (cont.)

No.	Species	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
									Source*								
18.	ZnF^+	-433.00 (-103.49)	-----	-----	-437.98 (-104.68)	-434.38 (-103.82)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
19.	$ZnF_2°$	-704.64 (-168.41)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
20.	$NaF°$	-540.68 (-129.22)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
21.	$KF°$	-562.06 (-134.34)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
22.	CuF^+	-220.50 (-52.70)	-----	-----	-----	-225.50 (-53.90)	-221.75 (53.00)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
23.	$CdF_2°$	-635.18 (-151.81)	-----	-----	-----	-619.57 (-148.08)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
24.	HgF^+	-123.40 (-29.50)	-----	-----	-----	-128.66 (-30.75)	-----	-----	-----	-----	-----	-----	-128.64 (-30.74)	-128.40 (-30.69)	-128.40 (-30.69)	-----	-----
25.	MnF^+	-511.70 (-122.30)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
26.	GF^+	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-844.00 (-201.72)	-----	-----	-----	-----
27.	MgF^+	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-750.60 (-179.40)	-----	-----	-----	-----
28.	SrF^+	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-851.44 (-203.50)	-----
29.	$CaF_2°$	-1111.15 (-265.57)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
30.	GaF^{2+}	-464.90 (-111.11)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
31.	CaF_2^+	-764.80 (-182.80)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
32.	$TlF°$	-311.19 (-74.37)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
33.	$AgF°$	-201.69 (-48.20)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
34.	$NiF_2°$	-603.30 (-144.20)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Table 7. Summary of Collected Standard Free Energy of Formation (ΔG°f, kJ/mole) of F Species. Values in the Parenthesis are kcal/mole. (cont.)

No.	Species	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
35.	BaF_2^*	-1118.35 (-267.30)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
36.	$AlF_3(c)$	-1425.00 (-340.58)	-----	-----	-----	-1444.06 (-354.14)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
37.	$CdF_2(c)$	-647.70 (-154.80)	-----	-----	-----	-----	-651.07 (-155.61)	-649.35 (-155.20)	-----	-----	-----	-----	-----	-----	-----	-----	-----
38.	$CuF_2 \cdot 2H_2O$	-981.40 (-234.56)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
39.	$FeF_3(c)$	-----	-----	-----	-----	-979.71 (-234.16)	-----	-----	-972.33 (-232.40)	-----	-----	-----	-----	-----	-----	-----	-----
40.	$Hg_2F_2(c)$	-----	-427.48 (-102.17)	-----	-----	-----	-----	-----	-427.47 (-102.17)	-----	-----	-----	-----	-----	-----	-----	-----
41.	$KF(c)$	-537.75 (-128.52)	-----	-----	-----	-----	-538.95 (-128.81)	-537.70 (-128.51)	-----	-----	-----	-----	-----	-----	-----	-----	-----
42.	$MgF_2(c)$	-1070.20 (-255.78)	-----	-----	-----	-----	-1071.10 (-256.00)	-----	-1071.10 (-256.00)	-----	-----	-----	-----	-----	-----	-----	-----
43.	$NaF(c)$	-543.50 (-129.90)	-----	-----	-----	-----	-546.51 (-137.49)	-----	-----	-----	-543.13 (-129.81)	-----	-----	-----	-----	-----	-----
44.	$PbF_2(c)$	-617.10 (-147.49)	-----	-----	-----	-----	-627.60 (-150.00)	-715.88 (-148.10)	-----	-----	-----	-----	-----	-----	-----	-----	-----
45.	$ZnF_2(c)$	-713.30 (-170.48)	-----	-----	-----	-----	-713.30 (-170.48)	-713.30 (-170.48)	-----	-----	-----	-----	-----	-----	-----	-----	-----
46.	$Na_2SiF_6(c)$	-2754.20 (-658.27)	-----	-----	-----	-----	-2757.25 (-2917.80)	-2553.91 (-610.40)	-----	-----	-----	-----	-----	-----	-----	-----	-----
47.	$Na_3AlF_6(c)$	-3136.60 (-749.67)	-----	-----	-----	-----	-3152.64 (-753.50)	-3015.82 (-720.80)	-----	-----	-3140.90 (-750.69)	-----	-----	-----	-----	-----	-----
48.	$NaCa_2Mg_4Al_5Si_6O_{22}F_2$	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-12117.78 (-2896.22)	-----	-----	-----	-----	-----
49.	$NaMoF_7(c)$	-2006.10 (-479.47)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
50.	K_2SiF_6	-2798.60 (-668.88)	-----	-----	-----	-----	-2810.40 (-671.70)	-2723.78 (-651.00)	-----	-----	-----	-----	-----	-----	-----	-----	-----
51.	$KMg_3AlSi_3O_{10}F_2$	-6044.00 (-1444.55)	-6115.46 (-1461.63)	-----	-----	-----	-6026.21 (-1440.30)	-----	-----	-----	-6022.95 (-1439.52)	-6091.68 (-1438.74)	-----	-----	-----	-----	-----

Table 7. Summary of Collected Standard Free Energy of Formation ($\Delta G°f$, kJ/mole) of F Species. Values in the Parenthesis are kcal/mole. (cont.)

No.	Species	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
										Source*							
52.	$Ca_5(Po_4)_3F$	-----	-6474.19 (-1547.37)	-----	-----	-----	-6507.37 (-1555.30)	-----	-----	-6491.47 (-1551.50)	-----	-6501.51 (-1553.90)	-----	-----	-----	-----	-----
53.	$Ca_4Si_2O_7F_2$	-----	-----	-----	-----	-----	-4988.58 (-1192.30)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
54.	$(NH_4)_2SiF_6$	-----	-----	-----	-----	-----	-2372.24 (-566.98)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
55.	$Pb_5(Po_4)_3F$	-----	-3893.75 (-930.63)	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
56.	CaF_2	-1167.30 (-278.99)	-1162.31 (-282.58)	-----	-----	-1182.31 (-282.58)	-1175.99 (-281.07)	-1163.15 (-278.00)	-1173.53 (-280.48)	-----	-1162.31 (-277.80)	-----	-----	-----	-----	-----	-1173.58 (-280.49)

Source*
1. Wagman et al. (1982)
2. Sadiq and Lindsay (1979)
3. CODATA (1976)
4. Robie et al. (1978)
5. Elrashidi and Lindsay (1984)
6. Naumov et al. (1971)
7. Karapet'yants and Karapet'yants (1970)
8. Stull et al. (1971)
9. Parker et al. (1971)
10. Robie and Waldbaum (1968)
11. Westrich and Navrotsky (1981)
12. Smith and Martell (1976)
13. Helplera and Olofason (1975)
14. Paul (1955)
15. Sposito and Mattigod (1980)
16. Helgeson et al. (1978)

Table 8. Selected Standard Free Energies of Formation ($\Delta G°f$) of F Species.

No.	Species	$\Delta G°f$ (kJ/mole)	(kcal/mole)	Source	Remarks
1.	F^-	−284.22	−67.93	Sadiq and Lindsay (1979)	$\Delta H°f$, $s°$
2.	$HF°$	−296.82	−70.94	Wagman et al. (1982)	$\Delta H°f$, $s°$
3.	HF_2^-	−578.08	−138.16	Wagman et al. (1982)	$\Delta H°f$, $s°$
4.	AlF_2^+	−1131.27	−270.38	Sadiq and Lindsay (1979)	pk
5.	AlF^{2+}	−814.96	−194.78	Sadiq and Lindsay (1979)	pk
6.	$AlF_3°$	−1438.58	−343.83	Sadiq and Lindsay (1979)	pk
7.	AlF_4^-	−1736.40	−415.01	Sadiq and Lindsay (1979)	pk
8.	FeF^{2+}	−335.30	−80.14	Sadiq and Lindsay (1979)	pk
9.	$FeF_2°$	−636.48	−152.12	Wagman et al. (1982)	$\Delta H°f$, $s°$
10.	FeF_2^+	−637.76	−152.43	Sadiq and Lindsay (1979)	pk
11.	$FeF_3°$	−936.25	−223.77	Sadiq and Lindsay (1979)	pk
12.	PbF^+	−317.40	−75.86	Sadiq and Lindsay (1979)	pk
13.	$PbF_2°$	−606.09	−144.86	Sadiq and Lindsay (1979)	$K°$
14.	PbF_3^-	−896.84	−216.35	Sadiq and Lindsay (1979)	pk
15.	PbF_4^{2-}	−1179.26	−281.85	Sadiq and Lindsay (1979)	pk
16.	$SiF_4°$	−1607.40	−384.18	Wagman et al. (1982)	$\Delta H°f$, $s°$

Table 8. Selected Standard Free Energies of Formation ($\Delta G°f$) of F Species. (cont.)

No.	Species	$\Delta G°f$ (kJ/mole)	(kcal/mole)	Source	Remarks
17.	SiF_6^{2-}	-2199.40	-525.67	Wagman et al. (1982)	$\Delta H°f$, $s°$
18.	ZnF^+	-437.98	-104.68	Elrashidi and Lindsay (1979)	pk
19.	$ZnF_2^°$	-704.64	-168.41	Wagman et al. (1982)	$\Delta H°f$, $s°$
20.	$NaF°$	-540.68	-129.22	Wagman et al. (1982)	$\Delta H°f$, $s°$
21.	$KF°$	-562.06	-134.34	Wagman et al. (1982)	$\Delta H°f$, $s°$
22.	CuF^+	-225.52	-53.90	Elrashidi and Lindsay (1984)	pk
23.	$CdF_2^°$	-635.18	-151.81	Wagman et al. (1982)	$\Delta H°f$, $s°$
24.	HgF^+	-128.66	-30.75	Elrashidi and Lindsay (1979)	pk
25.	MnF^+	-511.70	-122.30	Wagman et al. (1982)	$\Delta H°f$, $s°$
26.	CaF^+	-844.00	-201.72	Smith and Martell (1976)	pk
27.	MgF^+	-750.60	-179.40	Smith and Martell (1976)	pk
28.	SrF^+	-851.44	-203.50	Sposito and Mattigod (1980)	pk
29.	$CaF_2^°$	-1111.15	-265.57	Wagman et al. (1982)	$\Delta H°f$, $s°$
30.	GaF^{2+}	-464.90	-111.11	Wagman et al. (1982)	$\Delta H°f$, $s°$
31.	GaF_2^+	-764.80	-182.80	Wagman et al. (1982)	$\Delta H°f$, $s°$
32.	$TlF°$	-311.19	-74.37	Wagman et al. (1982)	$\Delta H°f$, $s°$
33.	$AgF°$	-201.69	-48.20	Wagman et al. (1982)	$\Delta H°f$, $s°$

Table 8. Selected Standard Free Energies of Formation ($\Delta G°f$) of F Species. (cont.)

No.	Species	$\Delta G°f$ (kJ/mole)	(kcal/mole)	Source	Remarks
34.	NiF_2°	−603.30	−144.20	Wagman et al. (1982)	$\Delta H°f$, $s°$
35.	BaF_2°	−1118.35	−267.30	Wagman et al. (1982)	$\Delta H°f$, $s°$
36.	$AlF_3(c)$	−1444.06	−345.14	Elrashidi and Lindsay (1984)	$\Delta H°f$, $s°$
37.	$CdF_2(c)$	−647.70	−154.80	Wagman et al. (1982)	$\Delta H°f$, $s°$
38.	$CuF_2 \cdot 2H_2O$	−981.40	−234.56	Wagman et al. (1982)	$\Delta H°f$, $s°$
39.	$Hg_2F_2(c)$	−427.48	−102.17	Sadiq and Lindsay (1979)	$\Delta H°f$, $s°$
40.	$FeF_3(c)$	−979.71	−234.16	Elrashidi and Lindsay (1986)	$\Delta H°f$, $s°$
41.	$KF(c)$	−537.75	−128.52	Wagman et al. (1982)	$\Delta H°f$, $s°$
42.	$MgF_2(c)$	−1070.20	−255.78	Wagman et al. (1982)	$\Delta H°f$, $s°$
43.	$NaF(c)$	−543.50	−129.90	Wagman et al. (1982)	$\Delta H°f$, $s°$
44.	$PbF_2(c)$	−617.10	−147.49	Wagman et al. (1982)	$\Delta H°f$, $s°$
45.	$ZnF_2(c)$	−713.30	−170.48	Wagman et al. (1982)	$\Delta H°f$, $s°$
46.	$Na_2SiF_6(c)$	−2754.20	−658.27	Wagman et al. (1982)	$\Delta H°f$, $s°$
47.	$Na_3AlF_6(c)$	−3136.60	−749.67	Wagman et al. (1982)	$\Delta H°f$, $s°$
48.	$NaCa_2Mg_4Al_3Si_6O_{22}F_2$	−12117.78	−2896.22	Westrich and Navrotsky (1981)	$\Delta H°f$, $s°$
49.	$NaMoF_7(c)$	−2006.10	−479.47	Wagman et al. (1982)	$\Delta H°f$, $s°$

Table 8. Selected Standard Free Energies of Formation ($\Delta G°f$) of F Species. (cont.)

No.	Species	$\Delta G°f$ (kJ/mole)	(kcal/mole)	Source	Remarks
50.	$K_2SiF_6(c)$ (hieratite)	-2798.60	-668.88	Wagman et al. (1982)	$\Delta H°f$, $s°$
51.	$KMg_3AlSi_3O_{10}F_2$ (Fluorphlogopite)	-6115.46	-1461.63	Sadiq and Lindsay (1979)	$\Delta H°f$, $s°$
52.	$Ca_5(PO_4)_3F$ (Fluorapatite)	-6474.19	-1547.37	Sadiq and Lindsay (1979)	pk
53.	$Ca_4Si_2O_7F_2$ (Cuspidine)	-4988.58	-1192.30	Naumov et al. (1971)	$\Delta H°f$, $s°$
54.	$(NH_4)_2SiF_6$ (Bararite)	-2372.24	-566.98	Naumov et al. (1971)	$\Delta H°f$, $s°$
55.	$Pb_5(PO_4)_3F$ (Fluoropyrorphite)	-3893.75	-930.63	Sadiq and Lindsay (1979)	pk
56.	CaF_2 (Fluorite)	-1182.31	-282.58	Elrashidi and Lindsay (1984)	pk

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Table 9. Equilibrium Reactions of Fluoride.

No.	Reaction	logk°
	I. Solid Phases	
1.	$AlF_3(c) \longrightarrow Al^{3+} + 3F^-$	-17.61
2.	$CaF_2 \text{ (fluorite)} \longrightarrow Ca^{2+} + 2F^-$	-10.42
3.	$CdF_2(c) \longrightarrow Cd^{2+} + 2F^-$	-0.24
4.	$CuF_2 \cdot 2H_2O(c) \longrightarrow Cu^{2+} + 2F^- + 2H_2O$	-0.73
5.	$FeF_3(c) \longrightarrow Fe^{3+} + 3F^-$	-19.31
6.	$Hg_2F_2(c) \longrightarrow Hg_2^{2+} + 2F^-$	-2.22
7.	$KF(c) \longrightarrow K^+ + F^-$	5.07
8.	$MgF_2 \text{ (sellaite)} \longrightarrow Mg^{2+} + 2F^-$	-8.01
9.	$MgF_2 \text{ (villiaumite)} \longrightarrow Mg^{2+} + 2F^-$	0.45
10.	$PbF_2(c) \longrightarrow Pb^{2+} + 2F^-$	-4.21
11.	$ZnF_2(c) \longrightarrow Zn^{2+} + 2F^-$	0.40
12.	$Na_2SiF_6 + 4H_2O \longrightarrow 2Na^+ + H_4SiO_4^\circ + 6F^- + 4H^+$ (malladrite)	-27.88
13.	$Na_3AlF_6 \text{ (cryolite)} \longrightarrow 3Na^+ + Al^{3+} + 6F^-$	-27.14
14.	$NaCa_2Mg_4Al_3Si_6O_{22}F_2 \longrightarrow Na^+ + 2Ca^{2+} + 4Mg^{2+} + 3Al$ $+ 2H_2O + 20H^+ \quad + 6H_4SiO_4^\circ + 2F^-$	84.39
15.	$NaMoF_7(c) + 4H_2O \longrightarrow Na^+ + H_2MoO_4^\circ + 7F^- + 6H^+$	31.48
16.	$K_2SiF_6 \text{ (hieratite)} \longrightarrow 2K^+ + H_4SiO_4^\circ + 6F^- + 4H^+$ $+ 4H_2O$	-29.61
17.	$KMg_3AlSi_3O_{10}F_2 + 2H_2O \longrightarrow K^+ + 3Mg^{2+} + Al^{3+} + 3H_4SiO_4^\circ$ $+ 8H^+ \quad + 2F^-$	7.85
18.	$Ca_5(PO_4)_3F + 6H^+ \longrightarrow 5Ca^{2+} + 3H_2PO_4^- + F^-$	-0.95
19.	$Ca_4Si_2O_7F_2 + H_2O + 6H^+ \longrightarrow 4Ca^{2+} + 2H_4SiO_4^\circ + 2F^-$	30.99

Table 9. Equilibrium Reactions of Fluoride. (cont).

No.	Reaction			$\log k°$
20.	$(NH_4)_2SiF_6 + 4H_2O$		$2NH_4^+ + H_4SiO_4° + 6F^- + 4H^-$	-26.03
21.	$Pb_5(PO_4)_3F + 6H^+$		$5Pb^{2+} + 3H_2PO_4^- + F^-$	-12.98

II. Solution Complexes

No.	Reaction			$\log k°$
22.	$HF°$	⇌	$F^- + H^+$	-2.21
23.	HF_2^-	⇌	$2F^- + H^+$	-1.70
24.	AlF^{2+}	⇌	$Al^{3+} + F^-$	-6.98
25.	AlF_2^+	⇌	$Al^{3+} + 2F^-$	-12.60
26.	$AlF_3°$	⇌	$Al^{3+} + 3F^-$	-16.65
27.	AlF_4^-	⇌	$Al^{3+} + 4F^-$	-19.03
28.	$FeF_3°$	⇌	$Fe^{3+} + 3F^-$	-11.70
29.	FeF_2^+	⇌	$Fe^{3+} + 2F^-$	-9.20
30.	FeF^{2+}	⇌	$Fe^{3+} + F^-$	-6.00
31.	$FeF_2°$	⇌	$Fe^{2+} + 2F^-$	-0.03
32.	$PbF_2°$	⇌	$Pb^{2+} + 2F^-$	-2.27
33.	PbF^+	⇌	$Pb^{2+} + F^-$	-1.49
34.	PbF_3^-	⇌	$Pb^{2+} + 3F^-$	-3.42
35.	PbF_4^{2-}	⇌	$Pb^{2+} + 4F^-$	-3.10
36.	$SiF_4° + 4H_2O$	⇌	$H_4SiO_4° + 4F^- + 4H^+$	-19.48
37.	$SiF_6^{2-} + 4H_2O$	⇌	$H_4SiO_4° + 6F^- + 4H^+$	-23.61
38.	$ZnF_2°$	⇌	$Zn^{2+} + 2F^-$	1.93
39.	ZnF^+	⇌	$Zn^{2+} + F^-$	-0.27
40.	$NaF°$	⇌	$Na^+ + F^-$	0.95
41.	$KF°$	⇌	$K^+ + F^-$	0.81
42.	CuF^+	⇌	$Cu^{2+} + F^-$	-0.32

Table 9. Equilibrium Reactions of Fluoride. (cont.)

No.	Reaction		$\log k°$
43.	$CdF_2°$	$\longrightarrow$ $Cu^{2+} + 2F^-$	1.95
44.	HgF^+	$\longrightarrow$ $Hg^{2+} + F^-$	-1.56
45.	MnF^+	$\longrightarrow$ $Mn^{2+} + F^-$	0.54
46.	CaF^+	$\longrightarrow$ $Ca^{2+} + F^-$	-1.10
47.	MgF^+	$\longrightarrow$ $Mg^{2+} + F^-$	-1.80
48.	SrF^+	$\longrightarrow$ $Sr^{2+} + F^-$	-0.60
49.	GaF^{2+}	$\longrightarrow$ $Ga^{3+} + F^-$ TT	-3.79
50.	GaF_2^+	$\longrightarrow$ $Ga^{3+} + 2F^-$ TT	-6.55
51.	$TlF°$	$\longrightarrow$ $Tl^+ + F^-$ TT	0.95
52.	$AgF°$	$\longrightarrow$ $Ag^+ + F^-$ TT	0.96
53.	$NiF_2°$	$\longrightarrow$ $Ni^{2+} + 2F^-$ TT	1.87
54.	$BaF_2°$	$\longrightarrow$ $Ba^{2+} + 2F^-$ TT	1.89

TT Ga^{3+}, Tl^+, Ag^+, Ni^{2+}, and Ba^{2+} $\Delta G°f$ values were taken from Wagman et al. (1982)

Table 10. Summary of Collected $\Delta G°f$ (kJ/mole) Values for Molybdenum Species.
Values in the parenthesis are kcal/mole.

No.	Species	Source* 1	2	3	4	5	6	7
1.	MoO_4^{2-}	-836.30 (-199.88)	-836.13 (-199.84)	-----	-----	-----	-----	-----
2.	MoO_2^{2+}	-----	-----	-411.28 (-98.30)	-----	-----	-----	-----
3.	$MoO_2(OH)^+$	-----	-645.75 (-154.34)	-645.88 (-154.37)	-----	-----	-----	-----
4.	$HMoO_4^-$	-----	-860.31 (-205.62)	-866.63 (-207.13)	-----	-----	-893.70 (-213.60)	-----
5.	$H_2MoO_4°$	-----	-883.15 (-211.08)	-877.13 (-209.04)	-949.76 (-227.00)	-----	-----	-----
6.	MoO_3 (molybdite)	-667.97 (-159.64)	-668.01 (-159.66)	-----	-----	-668.10 (-159.64)	-----	-----
7.	$H_2MoO_4(c)$	-----	-912.44 (-218.08)	-----	-----	-----	-----	-----
8.	$MoS_2(c)$ (molybdenite)	-225.90 (-53.99)	-266.47 (-63.69)	-----	-255.09 (-53.80)	-----	-----	-267.14 (-63.85)
9.	$Ag_2MoO_4(c)$	-----	-747.89 (-178.75)	-----	-821.73 (-196.40)	-----	-----	-----
10.	$BaMoO_4(c)$	-1439.60 (-346.07)	-----	-----	-1075.28 (-257.00)	-----	-----	-----
11.	$CaMoO_4(c)$	-1434.60 (-342.87)	-1435.90 (-343.19)	-----	-----	-----	-----	-----
12.	$CuMoO_4(c$	-----	-----	-809.60 (-193.50)	-----	-----	-----	-----

Table 10. Summary of Collected $\Delta G°f$ (kJ/mole) Values for Molybdenum Species.
Values in the parenthesis are kcal/mole. (cont.)

No.	Species	Source*						
		1	2	3	4	5	6	7
13.	$FeMoO_4(c)$	-975.00 (-233.03)	-971.27 (-232.14)	-974.28 (-232.86)	-982.40 (-234.80)	-----	-----	-----
14.	$Li_2MoO_4(c)$	-1409.50 (-336.87)	-----	-----	-----	-----	-----	-----
15.	$MgMoO_4(c)$	-1295.68 (-309.67)	-----	-1295.78 (-309.70)	-----	-----	-----	-----
16.	$MnMoO_4(c)$	-----	-1090.30 (-260.59)	-1090.39 (-260.61)	-----	-----	-----	-----
17.	$Na_2MoO_4(c)$	-1354.34 (-323.69)	-----	-----	-----	-----	-----	-----
18.	$Ag_2MoO_4°$	-681.90 (-162.97)	-----	-----	-----	-----	-----	-----
19.	$CaMoO_4°$	-1389.90 (-332.19)	-----	-----	-----	-----	-----	-----
20.	$Na_2MoO_4°$	-1360.20 (-325.09)	-----	-----	-----	-----	-----	-----
21.	$K_2MoO_4°$	-1402.80 (-335.27)	-----	-----	-----	-----	-----	-----
22.	$PbMoO_4(c)$	-951.40 (-227.39)	-952.36 (-227.62)	-----	-----	-----	-----	-----
23.	$ZnMoO_4(c)$	-----	-----	-1010.35 (-241.60)	-----	-----	-----	-----

Table 10. Summary of Collected ΔG°f (kJ/mole) Values for Molybdenum Species.
Values in the parenthesis are kcal/mole. (cont.)

*Source

1. Wagman et al. (1982)

2. Sadiq and Lindsay (1979)

3. Naumov et al. (1971)

4. Latimer (1952)

5. Stull et al. (1971)

6. Garrels and Christ (1965)

7. Chase et al. (1982)

Table 11. Selected $\Delta G°f$ Values for Molybdenum Species.

No.	Species	$\Delta G°f$ (kJ/mole)	(kcal/mole)	Source	Remarks
1.	MoO_4^{2-}	-836.30	-199.88	Wagman et al. (1982)	$\Delta H°f$ and $s°$
2.	MoO_2^{2+}	-411.28	-98.30	Naumov et al. (1971)	pk
3.	$MoO_2(OH)^+$	-645.75	-154.34	Sadiq and Lindsay (1979)	pk
4.	$HMoO_4^-$	-860.48	-205.66	Smith and Martell (1976)	pk
5.	$H_2MoO_4^°$	-883.28	-211.11	Rohwer and Cruywagen (1963)	pk
6.	$MoO_3(c)$ (molybdite)	-667.97	-159.64	Wagman et al. (1982)	$\Delta H°f$ and $s°$
7.	$H_2MoO_4(c)$	-912.44	-218.08	Sadiq and Lindsay (1979)	$\Delta H°f$ and $s°$
8.	$MoS_2(c)$ (molybdenite)	-266.47	-63.69	Sadiq and Lindsay (1979)	$\Delta H°f$ and $s°$
9.	$Ag_2MoO_4(c)$	-748.01	-178.78	Smith and Martell (1976)	pk
10.	$BaMoO_4(c)$	-1439.60	-344.07	Wagman et al. (1982)	$\Delta H°f$ and $s°$
11.	$CaMoO_4(c)$	-1435.99	-343.21	Lindsay (1979)	pk
12.	$CuMoO_4(c)$	-809.60	-193.50	Naumov et al. (1971)	pk
13.	$FeMoO_4(c)$	-971.44	-232.18	Naumov et al. (1971)	pk
14.	$Li_2MoO_4(c)$	-1409.50	-336.87	Wagman et al. (1982)	$\Delta H°f$ and $s°$
15.	$MgMoO_4(c)$	-1295.68	-309.67	Wagman et al. (1982)	$\Delta H°f$ and $s°$
16.	$MnMoO_4(c)$	-1090.39	-260.01	Naumov et al. (1971)	$\Delta H°r$
17.	$Na_2MoO_4(c)$	-1354.34	-323.69	Wagman et al. (1982)	$\Delta H°f$ and $s°$

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Table 11. Selected $\Delta G°f$ Values for Molybdenum Species. (cont.)

No.	Species	$\Delta G°f$ (kJ/mole)	(kcal/mole)	Source	Remarks
18.	$Ag_2MoO_4^\circ$	-681.90	-162.97	Wagman et al. (1982)	$\Delta H°f$ and $s°$
19.	$CaMoO_4^\circ$	-1389.90	-332.19	Wagman et al. (1982)	$\Delta H°f$ and $s°$
20.	$Na_2MoO_4^\circ$	-1360.20	-325.09	Wagman et al. (1982)	$\Delta H°f$ and $s°$
21.	$K_2MoO_4^\circ$	-1402.80	-335.27	Wagman et al. (1982)	$\Delta H°f$ and $s°$
22.	$PbMoO_4(c)$	-952.36	-227.62	Sadiq and Lindsay (1979)	$\Delta H°f$ and $s°$
23.	$ZnMoO_4(c)$	-1009.09	-241.18	Naumov et al. (1971)	pk

Table 12. Equilibrium Reactions of Molybdenum.

No.	Reaction		logk°
	I. SOLID PHASES		
1.	$H_2MoO_4(c)$	$\rightleftharpoons$ $2H^+ + MoO_4^{2-}$	-13.34
2.	$MoO_3(molybdite) + H_2O$	$\rightleftharpoons$ $MoO_4^{2-} + 2H^+$	-12.05
3.	$Ag_2MoO_4(c)$	$\rightleftharpoons$ $2Ag^+ + MoO_4^{2-}$	-11.54
4.	$BaMoO_4(c)$	$\rightleftharpoons$ $Ba^{2+} + MoO_4^{2-}$ T	-7.45
5.	$CaMoO_4(c)$	$\rightleftharpoons$ $Ca^{2+} + MoO_4^{2-}$	-7.94
6.	$CuMoO_4(c)$	$\rightleftharpoons$ $Cu^{2+} + MoO_4^{2-}$	-6.81
7.	$FeMoO_4(c)$	$\rightleftharpoons$ $Fe^{2+} + MoO_4^{2-}$	-7.70
8.	$Li_2MoO_4(c)$	$\rightleftharpoons$ $2Li^+ + MoO_4^{2-}$ T	2.35
9.	$MgMoO_4(c)$	$\rightleftharpoons$ $Mg^{2+} + MoO_4^{2-}$	-0.57
10.	$MnMoO_4(c)$	$\rightleftharpoons$ $Mn^{2+} + MoO_4^{2-}$	-4.12
11.	$Na_2MoO_4(c)$	$\rightleftharpoons$ $2Na^+ + MoO_4^{2-}$	1.00
12.	$PbMoO_4(c)$	$\rightleftharpoons$ $Pb^{2+} + MoO_4^{2-}$	-16.01
13.	$ZnMoO_4(c)$	$\rightleftharpoons$ $Zn^{2+} + MoO_4^{2-}$	-4.48
14.	$MoS_2(molybdenite) + 4H_2O$	$\rightleftharpoons$ $MoO_4^{2-} + 2S^{2-} + 2e^- + 8H^+$	-96.43
	II. SOLUTION PHASES		
15.	$H_2MoO_4^\circ$	$\rightleftharpoons$ $H^+ + HMoO_4^-$	-3.99
16.	$HMoO_4^-$	$\rightleftharpoons$ $H^+ + MoO_4^{2-}$	-4.23
17.	$H_2MoO_4^\circ$	$\rightleftharpoons$ $2H^+ + MoO_4^{2-}$	-8.23
18.	$MoO_2(OH)^+ + H_2O$	$\rightleftharpoons$ $MoO_4^{2-} + 3H^+$	-8.17
19.	$MoO_2^{2+} + 2H_2O$	$\rightleftharpoons$ $MoO_4^{2-} + 4H^+$	-8.64
20.	$Ag_2MoO_4^\circ$	$\rightleftharpoons$ $2Ag^+ + MoO_4^{2-}$	0.05
21.	$CaMoO_4^\circ$	$\rightleftharpoons$ $Ca^{2+} + MoO_4^{2-}$	0.14

Table 12. Equilibrium Reactions of Molybdenum. (cont.)

No.	Reaction		logk°
22. $Na_2MoO_4^o$	$\rightleftharpoons$	$2Na^+ + MoO_4^{2-}$	-0.02
23. $K_2MoO_4^o$	$\rightleftharpoons$	$2K^+ + MoO_4^{2-}$	-0.27

$T\Delta G°f$ values for Ba^{2+} and Li^+ were taken from Wagman et al. (1982).

Table 13. Summary of Collected Standard Free Energies of Formation ($\Delta G°f$, kJ/mole) of Se Species. Values in the Parenthesis are kcal/mole.

Species	Source*					
	1	2	3	4	5	6
1. Se^{2-}	-129.30 (-30.90)	-129.30 (-30.90)	-129.30 (-30.90)	-	-	-
2. SeO_3^{2-}	-369.78 (-88.38)	-363.80 (-86.95)	-	-	-	-373.76 (-89.33)
3. SeO_4^{2-}	-441.28 (-105.47)	-441.41 (-105.50)	-	-	-	-
4. HSe^-	43.93 (10.53)	43.93 (10.53)	-	-	-	-
5. $H_2Se°$	22.17 (5.30)	22.17 (5.30)		-	-	-
6. $HSeO_4^-$	-452.16 (-108.07)	-450.87 (-107.76)	-	-	-	-
7. $H_2SeO_3°$	-426.14 (-101.85)	-426.14 (-101.85)	-	-	-	-
8. $H_2SeO_4°$	-	-	-	-	-	-441.08 (-105.42)
9. $BaSeO_3$	-968.18 (-231.40)	-	-971.95 (-232.30)	-	-	-
10. $CaSe$	-363.17 (-86.80)	-	75.32 (18.00)	-	-	-
11. $CaSe_3 \cdot 2H_2O$	-1428.84 (-341.50)	-1423.40 (-340.20)	-1428.84 (-341.50)	-	-	-

Table 13. Summary of Collected Standard Free Energies of Formation ($\Delta G°f$, kJ/mole) of Se Species. Values in the Parenthesis are kcal/mole.

| Species | Source* | | | | | |
	1	2	3	4	5	6
12. $CaSeO_4$	–	–	–	-1013.50 (-242.23)	–	–
13. $CaSeO_4 \cdot 2H_2O$	-1486.80 (-355.35)	-1486.16 (-355.20)	-1402.40 (-335.18)	–	–	–
14. $CuSe$	–	–	–	-79.50 (-19.00)	–	–
15. Cu_2Se	–	–	–	-116.44 (-27.83)	–	–
16. $CuSeO_3$	-348.07 (-83.19)	–	–	–	–	–
17. $CuSe_3O_3 \cdot 2H_2O$	–	-817.39 (-195.36)	-827.60 (-197.80)	-823.00 (196.70)	–	–
18. $FeSe$	–	–	-58.16 to -74.06 (-13.90 to -17.70)	-110.29 (-26.36)	–	-58.16 (-13.90)
19. $Fe_2(SeO_3)_3$	–	–	–	–	–	-1331.56 (-318.25)
20. $Fe_3(OH)_4SeO_3$	–	–	–	–	–	-1390.56 (-332.35)
21. $MnSe$	-111.71 (-26.70)	-153.55 (-36.70)	-122.30 (-157.73)	-166.94 (-39.90)	–	–

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Table 13. Summary of Collected Standard Free Energies of Formation ($\Delta G°f$, kJ/mole) of Se Species. Values in the Parenthesis are kcal/mole.

Species	Source* 1	2	3	4	5	6
22. PbSe	–	–	−64.43 to −73.64 (−15.40 to −17.60	−131.88 (−31.52)	–	−64.43 (−15.40)
23. $PbSeO_3$	–	–	−463.80 (−110.85)	–	–	–
24. $PbSeO_4$	−504.88 (−120.67)	−504.84 (−120.88)	−497.90 (−119.00)	–	–	–
25. ZnSe	−163.00 (−38.96)	–	−145.18 (−34.70)	−185.72 (−44.39)	–	−145.18 (−34.00)
26. $ZnSe_3 \cdot H_2O$	−729.80	–	–	–	–	–
27. $ZnSeO_4$	–	–	–	−601.12 (−143.67)	–	–

*Source
1. Wagman et al. (1982)
2. Naumov et al. (1971)
3. Karapet'yants and Karapet'yants (1970)
4. Smith and Martell (1976)
5. Lindsay (1979)
6. Garrels and Christ (1965)

Table 14. Selected Standard Free Energies of Formation ($\Delta G°f$) of Se Species.

	Species	$\Delta G°f$ (kJ/mole)	(kcal/mole)	Source	Remarks
1.	Se^{2-}	-129.30	-30.90	Wagman et al. (1982)	$\Delta H°f$ and $s°$
2.	SeO_3^{2-}	-369.78	-88.38	Wagman et al. (1982)	$\Delta H°f$ and $s°$
3.	SeO_4^{2-}	-441.28	-105.47	Wagman et al. (1982)	$\Delta H°f$ and $s°$
4.	HSe^-	43.93	10.50	Wagman et al. (1982)	$\Delta H°f$ and $s°$
5.	H_2Se	22.17	5.30	Wagman et al. (1982)	$\Delta H°f$ and $s°$
6.	$HSeO_4^-$	-452.16	-108.07	Wagman et al. (1982)	$\Delta H°f$ and $s°$
7.	$H_2SeO_4°$	-441.08	-105.42	Garrels and Christ (1965)	$\Delta H°f$ and $s°$
8.	$BaSeO_3$	-968.13	-231.40	Wagman et al. (1982)	$\Delta H°f$ and $s°$
9.	$CaSe$	-363.17	-86.80	Wagman et al. (1982)	$\Delta H°f$ and $s°$
10.	$CaSe_3 \cdot 2H_2O$	-1428.84	-341.50	Wagman et al. (1982)	$\Delta H°f$ and $s°$
11.	$CaSeO_4$	-1013.50	-242.23	Smith and Martell (1976)	pk
12.	$CaSeO_4 \cdot 2H_2O$	-1486.80	-355.35	Wagman et al. (1982)	$\Delta H°f$ and $s°$
13.	$CuSe$	-79.50	-19.00	Smith and Martell (1976)	pk
14.	Cu_2Se	-116.44	-27.83	Smith and Martell (1976	pk
15.	$CuSeO_3$	-348.07	-83.19	Wagman et al. (1982)	$\Delta H°f$ and $s°$
16.	$CuSeO_3 \cdot 2H_2O$	-827.60	-197.80	Karapet'yants & Karapet'yants (1970)	$\Delta H°f$ and $s°$
17.	$FeSe$	-110.29	-26.36	Smith and Martell (1976)	pk

Table 14. Selected Standard Free Energies of Formation ($\Delta G°f$) of Se Species. (cont.)

	Species	$\Delta G°f$ (kJ/mole)	(kcal/mole)	Source	Remarks
18.	$Fe_2(SeO_3)_3$	−1331.56	−318.25	Smith and Martell (1976)	pk
19.	$Fe_3(OH)_4SeO_3$	−1390.56	−332.35	Smith and Martell (1976)	pk
20.	MnSe	−166.94	−39.90	Smith and Martell (1976)	pk
21.	PbSe	−131.88	−31.52	Smith and Martell (1976)	pk
22.	$PbSeO_3$	−463.80	−110.85	Karapet'yants & Karapet'yants (1970)	$\Delta H°f$ and $s°$
23.	$PbSeO_4$	−504.88	−120.67	Wagman et al. (1982)	$\Delta H°f$ and $s°$
24.	ZnSe	−185.72	−44.39	Smith and Martell (1976)	pk
25.	$ZnSe_3 \cdot H_2O$	−729.80	−174.43	Wagman et al. (1982)	$\Delta H°f$ and $s°$
26.	$ZnSeO_4$	−601.12	−143.67	Smith and Martell (1976)	pk
27.	$H_2SeO_3°$	−426.14	−101.85	Wagman et al. (1982)	$\Delta H°f$ and $s°$

Table 15. Equilibrium Reactions of Selenium.

No.	Equilibrium Reaction	log k°
	Redox Reactions	
1.	$SeO_4^{2-} + 2\bar{e} + 2H^+ \rightleftharpoons SeO_3^{2-} + H_2O$	29.02
2.	$SeO_4^{2-} + 6\bar{e} + 8H^+ \rightleftharpoons Se(c) + 4H_2O$	88.89
3.	$SeO_4^{2-} + 8\bar{e} + 8H^+ \rightleftharpoons Se^{2-} + 4H_2O$	66.24
	Acids	
4.	$H_2SeO_4^\circ \rightleftharpoons H^+ + HSeO_4^-$	1.96
5.	$HSeO_4^- \rightleftharpoons SeO_4^{2-} + H^+$	−1.91
6.	$H_2SeO_3^\circ \rightleftharpoons HSeO_3^- + H^+$	−2.57
7.	$HSeO_3^- \rightleftharpoons H^+ + SeO_3^{2-}$	−7.30
8.	$H_2Se^\circ \rightleftharpoons HSe + H^+$	−3.81
9.	$HSe^- \rightleftharpoons Se^{2-} + H^+$	−14.96
	Selenates	
10.	$BaSeO_4\ (c) \rightleftharpoons Ba^{2+} + SeO_4^{2-}$	−7.46
11.	$CaSeO_4\ (c) \rightleftharpoons Ca^{2+} + SeO_4^{2-}$	−3.03
12.	$CaSeO_4 \cdot 2H_2O\ (c) \rightleftharpoons Ca^{2+} + SeO_4^{2-} + 2H_2O$	−2.94
13.	$PbSeO_4\ (c) \rightleftharpoons Pb^{2+} + SeO_4^{2-}$	−6.82
14.	$ZnSeO_4\ (c) \rightleftharpoons Zn^{2+} + SeO_4^{2-}$	−2.19

Table 15. Equilibrium Reactions of Selenium.

No.	Equilibrium Reaction	logk°
	Selenites	
15.	$BaSeO_3$ (c) $\rightleftharpoons$ $Ba^{2+} + SeO_3^{2-}$	-6.57
16.	$CaSeO_3 \cdot 2H_2O$ (c) $\rightleftharpoons$ $Ca^{2+} + SeO_3^{2-} + 2H_2O$	-4.55
17.	$CuSeO_3$ (c) $\rightleftharpoons$ $Cu^{2+} + SeO_3^{2-}$	-7.68
18.	$Fe_2(SeO_3)_3$ (c) $\rightleftharpoons$ $2Fe^{3+} + 3SeO_3^{2-}$	-33.00
19.	$Fe_2(OH)_4SeO_3$ (c) $\rightleftharpoons$ $2Fe^{3+} + 4\,OH^- + SeO_3^{2-}$	-62.70
20.	$PbSeO_3$ (c) $\rightleftharpoons$ $Pb^{2+} + SeO_3^{2-}$	-12.13
21.	$ZnSeO_3 \cdot H_2O$ $\rightleftharpoons$ $Zn^{2+} + SeO_3^{2-} + H_2O$	-6.77
	Selenides	
22.	$CaSe$ (c) $\rightleftharpoons$ $Ca^{2+} + Se^{2-}$	10.80
23.	$CuSe$ (c) $\rightleftharpoons$ $Cu^{2+} + Se^{2-}$	-48.10
24.	Cu_2Se (c) $\rightleftharpoons$ $2Cu^+ + Se^{2-}$	-60.80
25.	$FeSe$ (c) $\rightleftharpoons$ $Fe^{2+} + Se^{2-}$	-26.00
26.	$MnSe$ (c) $\rightleftharpoons$ $Mn^{2+} + Se^{2-}$	-11.50
27.	$PbSe$ (c) $\rightleftharpoons$ $Pb^{2+} + Se^{2-}$	-42.10
28.	$ZnSe$ (c) $\rightleftharpoons$ $+ Se^{2-}$	-29.40

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