APPENDIX A
TABLES OF THERMODYNAMIC DATA

Table A.1
Standard Heats of Formation, Standard Entropies, Melting (M.P.) and Boiling (B.P.) Points.

Solid < >, Liquid [ ], Gas ( ).
P^0 = 1 atm (1 bar for References 1 and 5 below). Standard T = 298 K.

Substance	$\Delta H^{0,f}_{298}$ (kJ/mol)	S^0_{298} [J/(mol·K)]	M.P. (K)	B.P. (K)	Ref.*
<Al>	0	28.33	933	2773	4
<Al_2O_3>$_\alpha$	−1675.73	50.90	—	—	1
<Al_2SiO_5>[a]	−2591.27	91.40	—	—	1
<B>	0	5.86	2323	—	4
<B_4C>	−57.70	27.07	2623	—	4
<C>$_{Graphite}$	0	5.69	—	—	4
<Ca>$_\alpha$	0	41.63	1123	1623	4
<$CaAl_2Si_2O_8$>	−4232.74	199.30	—	—	1
<$CaCO_3$>[b]	−1207.43	87.99	—	—	5
<$CaCO_3$>[c]	−1206.70	88.70	—	—	5
Tremolite[d]	−12302.50	0.55	—	—	1
<CaO>	−633.88	39.75	2873	—	4
<$CaSiO_3$>	−1635.22	82.01	—	—	5
(CH_4)	−74.81	186.26	—	—	1
(CO_2)	−393.51	213.80	—	—	3
<Cr>	0	23.77	2123	2773	4
<Cr_2O_3>	−1129.00	81.18	2673	—	3
<Cu>	0	33.35	1356	2843	4
<Cu>	0	33.15	1356	—	5
<Cu_2O>	−167.38	93.94	1503	—	4
<Cu_2S>$_\alpha$	−80.115	120.75	—	—	2
<Fe>	0	27.28	1809	—	3
<FeO(OH)>	−545.59	75.73	—	—	6
<Fe_2O_3>	−823.41	89.96	—	—	7
<Fe_2P>	−160.25	72.38	—	—	4
<FeS_2>	−177.40	53.14	—	—	4
<Fe_2SiO_4>	−1479.36	148.32	1490	1800	5
<$FeTiO_3$>	−1233.26	108.50	—	—	1
(H_2)	0	130.68	—	—	5
[H_2O]	−285.90	70.09	273	373	4
(H_2O)	−241.81	188.80	—	—	3
(H_2S)	−20.627	205.80	—	—	5
(HCl)	−92.32	186.80	159	265	3
[Hg]	0	75.91	234	630	3
<HgO>	90.80	70.30	—	—	4

Table A.1 Continued
Standard Heats of Formation, Standard Entropies, Melting (M.P.) and Boiling (B.P.) Points.
Solid < >, Liquid [ ], Gas ( ).
P^0 = 1 atm (1 bar for References 1 and 5 below). Standard T = 298 K.

<Mg>	0	32.51	923	1378	4
<MgO>	–601.30	27.41	3043	—	4
<$Mg(OH)_2$>	–925.50	63.00	—	—	1
<$Mg_3Si_2O_5(OH)_4$>	–4361.66	221.30	—	—	5
<$Mg_3Si_4O_{10}(OH)_2$>	–5915.90	260.83	—	—	5
(N_2)	0	191.52	—	—	3
<$NaAlSi_2O_6$>	–3029.40	133.47	—	—	5
<$NaAlSi_3O_8$>	–3935.12	207.40	—	—	5
Glaucophane[e]	–11963.86	535.00	—	—	1
(NH_3)	–46.02	192.34	—	—	4
<Ni>	0	29.79	1726	3183	4
<NiO>	–240.60	38.08	2233	—	4
(O_2)	0	205.02	—	—	3
(P_2)	143.85	218.00	—	—	3
(S_2)	128.49	228.17	—	—	5
<Si>	0	18.83	1693	2873	4
($SiCl_4$)	–662.81	330.86	203	331	3
[Si_3N_4]	–749.00	96.24	—	2173	4
<SiO_2>$_\alpha$	–910.70	41.46	—	—	5
(SO_2)	–296.81	248.22	—	—	5
<Ti>$_\alpha$	0	30.54	—	—	3
<TiC>	–183.70	24.27	3423	—	3
<W>	0	33.48	3653	—	4
<WO_2>	–560.70	66.95	—	—	4
<WO_3>	–836.90	83.27	1746	—	4
<W_3O_8>	–2232.20	—	—	—	4

*References:

(1) Holland, 1990, Table 7, p. 103–104.
(2) Kelley, 1960.
(3) Kubaschewski and Alcock, 1979, Table A, p. 267.
(4) Kubaschewski and Evans, 1958, Table A, p. 226.
(5) Robie et al., 1979.
(6) Schmalz, 1959.
(7) Wicks and Block, 1963.

Footnotes:

(a) Andalusite polymorph
(b) Aragonite polymorph
(c) Calcite polymorph
(d) Tremolite: <$Ca_2Mg_5Si_8O_{22}(OH)_2$>
(e) Glaucophane: <$Na_2Mg_3Al_2(Si_4O_{11})_2(OH)_2$>

Table A.2
Heats of Transformation and Fusion at Specified Transformation (Tr. Pt.) and Melting (M.P.) Points.
P^0 = 1 atm (1 bar for Reference 5 below).
s = solid, l = liquid, g = gas; α, β, δ, and γ are polymorphic solids.

Substance	ΔH^{Tr} (kJ/mol)	Tr. Pt. (K)	M.P. (K)	Ref.*
Al	10.461 ($s \rightarrow l$)	—	933	3
Au	12.760 ($s \rightarrow l$)	—	1336	3
Bi	10.879 ($s \rightarrow l$)	—	544	3
Cr	19.25 ($s \rightarrow l$)	—	2123	4
Cu	12.972 ($s \rightarrow l$)	—	1356	3
Cu	13.054 ($s \rightarrow l$)	—	1356	5
Cu_2S	3.849 ($\alpha \rightarrow \beta$)	376	—	2
Cu_2S	0.8368 ($\beta \rightarrow \gamma$)	623	—	2
Cu_2S_γ	10.878 ($s \rightarrow l$)	—	1403	2
Fe	0.669 ($\alpha \rightarrow \gamma$)	1187	—	3
Fe	13.770 ($s \rightarrow l$)	—	1809	4
Fe_2SiO_4	92.173 ($s \rightarrow l$)	—	1490	5
H_2O	41.09 ($l \rightarrow g$)	373	—	4
Li	2.929 ($s \rightarrow l$)	—	453	3
Mn	2.009 ($\alpha \rightarrow \beta$)	993	—	4
Mn	2.301 ($\beta \rightarrow \gamma$)	1373	—	4
Mn	1.800 ($\gamma \rightarrow \delta$)	1409	—	4
Mn_δ	13.390 ($s \rightarrow l$)	—	1517	4
Pb	4.812 ($s \rightarrow l$)	—	600	3
S	0.368 ($\alpha \rightarrow \beta$)	369	—	1

Table A.2 Continued
Heats of Transformation and Fusion at Specified Transformation (Tr. Pt.) and Melting (M.P.) Points.
P^0 = 1 atm (1 bar for Reference 5 below).
s = solid, l = liquid, g = gas; α, β, δ, and γ are polymorphic solids.

S	1.226 ($\beta \rightarrow l$)	392	—	1
S	20.92 ($l \rightarrow g$)	718	—	1
Sb	19.876 ($s \rightarrow l$)	—	903	3
Si	50.630 ($s \rightarrow l$)	—	1693	4
SO_2	24.937 ($l \rightarrow g$)	263	—	5
Ta	24.558 ($s \rightarrow l$)	—	3253	4
Ti	3.473 ($\alpha \rightarrow \beta$)	1155	—	4
Ti_β	18.830 ($s \rightarrow l$)	—	1933	4

*References

(1) Handbook of Chemistry and Physics, 1989, p. D-45.
(2) Kelley, 1960.
(3) Kubaschewski and Alcock, 1979, Table B, p. 326.
(4) Kubaschewski and Evans, 1958, Table B, p. 286.
(5) Robie et al., 1979.

Table A.3A

Heat Capacities: $C_p = a + bT + cT^{-2} + dT^{-0.5}$. Units: J/(mol·K), T is in degrees K, M.P. denotes melting point. $P^0 = 1$ atm (1 bar for References 2 and 6 below). Solid < >, Liquid [ ], Gas ( ).

Substance	a	$b \times 10^3$	$c \times 10^{-5}$	$d \times 10^{-3}$	Temp. Range (K)	Ref.*
<Al>	20.67	12.39	—	—	298–M.P.	4
[Al]	29.29	—	—	—	M.P.–1273	5
<Al_4C_3>	100.76	132.23	—	—	298–600	5
<Au>	23.68	5.19	—	—	298–M.P.	4
[Au]	29.29	—	—	—	M.P.–1600	4
<BN>	7.62	15.15	—	—	298–1200	5
<C>[a]	17.15	4.27	–8.79	—	298–2300	5
<Ca>$_\alpha$	21.92	14.64	—	—	298–723	1
<Trem>[b]	1214.40	26.53	–123.62	–7.39	298–	2
(CH_4)	23.64	47.87	–1.92	—	298–1500	4
<Cr>	24.44	9.88	–3.68	—	298–M.P.	4
[Cr]	39.33	—	—	—	M.P.–	4
<Cr_2O_3>	119.40	9.21	–15.65	—	350–1800	4
<Cu_2S>$_\alpha$	81.588	—	—	—	298–376	3
<Cu_2S>$_\beta$	97.278	—	—	—	376–623	3
<Cu_2S>$_\gamma$	85.019	—	—	—	623–M.P.	3
<Fe>$_\alpha$	17.49	24.77	—	—	273–1181	5
<Fe>$_\gamma$	7.70	19.50	—	—	1181–1674	5
<FeS_2>	74.81	5.52	–12.76	—	298–1000	4
<$FeTiO_3$>	116.61	18.24	–20.04	—	298–1640	4
[H_2O]	75.44	—	—	—	273–373	4
(H_2O)	30.00	10.71	0.33	—	298–2500	4
(H_2S)	29.37	15.40	—	—	298–1800	5
<Jd>[c]	301.13	10.143	–22.393	–2.055	298–1300	6
<MgO>	42.59	7.28	–6.19	—	298–2100	5
<$Mg(OH)_2$>	158.40	–4.076	–10.523	–1.1713	298–	2
<Mn>$_\alpha$	21.59	15.94	—	—	298–1000	5
<Mn>$_\beta$	34.86	2.76	—	—	1000–1374	5
<Mn>$_\gamma$	44.77	—	—	—	1374–1410	5
<Mn>$_\delta$	47.28	—	—	—	1410–M.P.	5
(N_2)	27.87	4.27	—	—	298–2500	4
Glauc.[d]	1717.50	–121.07	70.75	–19.272	298–	2
<PbS>	44.60	16.40	—	—	298–900	4
<S>$_\alpha$	14.98	26.12	—	—	298–369	1
<S>$_\beta$	14.90	29.08	—	—	369–392	1
(S_2)	8.54	0.28	–0.79	—	298–2000	5
[S]	22.59	20.92	—	—	392–718	1
<Si>	24.10	2.34	–4.56	—	298–M.P.	5
[Si]	25.61	—	—	—	M.P.–1873	5
<Si_3N_4>	70.42	98.75	—	—	298–900	5
<SiO_2>$_\alpha$	44.60	37.754	–10.018	—	298–844	6

Table A.3A Continued

Heat Capacities: $C_p = a + bT + cT^{-2} + dT^{-0.5}$. Units: J/(mol·K), T is in degrees K, M.P. denotes melting point. P^0 = 1 atm (1 bar for References 2 and 6 below). Solid < >, Liquid [ ], Gas ( ).

Substance	a	$b \times 10^3$	$c \times 10^{-5}$	$d \times 10^{-3}$	Temp. Range (K)	Ref.*
<Ti>$_\alpha$	22.09	10.04	—	—	298–1155	4
<Ti>$_\beta$	28.91	—	—	—	1155–1350	5
<Ti>$_\beta$	28.91	—	—	—	1155–1350	5
<TiC>	49.50	3.35	–14.98	—	298–1800	4

*References:

(1) Handbook of Chemistry and Physics, 1989, p. D-44.
(2) Holland, 1990, Table 7, p. 103–104.
(3) Kelley, 1960.
(4) Kubaschewski and Alcock, 1979, Tables C_1 and C_2, p. 336.
(5) Kubaschewski and Evans, 1958, Table C, p. 310.
(6) Robie et al., 1979.

Footnotes

(a) Graphite polymorph
(b) Tremolite: <$Ca_2Mg_5Si_8O_{22}(OH)_2$>
(c) Jadeite: <$NaAlSi_2O_6$>
(d) Glaucophane: <$Na_2Mg_3Al_2(Si_4O_{11})_2(OH)_2$>

Table A.3B*

Heat Capacities: $C_p = a + bT + cT^{-2} + dT^{-0.5} + eT^{-2}$.

Units: J/(mol·K), T is in degrees K, M.P. denotes melting point. P^0 = 1 bar. Solid < >, Liquid [ ], Gas ( ).

Substance	a	$b \times 10^3$	$c \times 10^7$	$d \times 10^{-2}$	$e \times 10^{-4}$	Temp. Range (K)
Ab[a]	583.94	–92.852	227.22	–64.242	167.80	298–1500
Arag[b]	81.533	45.673	—	—	–114.05	298–1000
Calc.[c]	99.715	26.920	—	—	–215.76	298–1200
(CO_2)	87.820	–2.6442	—	–9.9886	70.641	298–1800
<Cu>	29.764	1.6124	3.411	–1.0067	—	298–1356
(H_2)	7.4424	11.707	–13.899	4.1017	–51.041	298–1800
(H_2O)	7.368	27.468	–48.117	3.6174	–22.316	298–1800
(O_2)	48.318	–0.6913	—	–4.2066	49.923	298–1800
(S_2)	47.069	–3.4459	6.9404	–2.3124	–2.2639	298–1800
Serp.[d]	899.60	–144.76	—	–109.32	449.99	298–900
Talc[e]	5653.6	–5271.7	27.291	–769.26	4021.1	298–800
Woll.[f]	111.25	14.373	—	0.1694	–277.79	298–1400

*Robie et al., 1979.

(a) Albite: <$NaAlSi_3O_8$>
(b) Aragonite: <$CaCO_3$> polymorph
(c) Calcite: <$CaCO_3$> polymorph
(d) Serpentine: <$Mg_3Si_2O_5(OH)_4$>
(e) Talc: <$Mg_3Si_4O_{10}(OH)_2$>
(f) Wollastonite: <$CaSiO_3$>

Table A.4
Standard Gibbs Free Energy Changes of Selected Reactions:

$\Delta G_T^0 = A + BT \log(T) + CT$ (ΔC_p assumed constant).
Units: J/mol, T is in degrees K. $P^0 = 1$ atm.
Solid < >, Liquid [ ], Gas ( ).

Reaction	A	B	C	Temp. Range (K)	Ref.*
$2<B> + (N_2) = 2<BN>$	–217,590	—	81.18	1200–2300	2
$3<Be> + (N_2) = <Be_3N_2>$	–563,640	—	169.90	298–1000	2
$3<C> + 4[Al] = <Al_4C_3>$	–266,521	—	96.23	932–2000	2
$<C> + 2(H_2) = (CH_4)$	–69,126	51.26	–65.36	298–1200	2
$<C> + 1/2(O_2) = (CO)$	–111,720	—	–87.66	298–2500	2
$<C> + (O_2) = (CO_2)$	–394,170	—	–0.84	298–2000	2
$[Ca] + 2<C> = <CaC_2>$	–57,326	—	–28.45	1123–1963	2
$3<Ca> + (N_2) = <Ca_3N_2>$	–439,360	—	209.20	298–1100	2
$<CaO> + (CO_2) = <CaCO_3>$	–168,420	—	143.94	298–1150	3
$23/6<Cr> + <C> = 1/6<Cr_{23}C_6>$	–68,540	—	–6.44	298–1673	2
$2<Cr> + 3/2(O_2) = <Cr_2O_3>$	–1,120,370	—	259.85	298–2100	3
$2<Cu> + 1/2(O_2) = <Cu_2O>$	–169,470	–16.40	123.44	298–1356	2
$3<Fe> + <C> = <Fe_3C>$	25,940	—	–23.14	298–463	3
$3<Fe> + <C> = <Fe_3C>$	26,700	—	–24.77	463–1115	3
$<Fe> + 1/2(O_2) = <FeO>$	–259,600	—	62.55	298–1642	1
$3<FeCO_3> = <Fe_3O_4> + 2(CO_2) + (CO)$	220,915	—	–46.94	298–700	3
$1/2(H_2) + 1/2(Cl_2) = (HCl)$	–91,094	4.14	–21.84	298–2100	2
$(H_2) + 1/2(O_2) = (H_2O)$	–239,560	18.75	–9.25	298–2500	2
or alternately	–246,460	—	54.82	298–2500	2
$2(H_2) + (S_2) = 2(H_2S)$	–180,600	—	98.79	298–1800	2
$[Mn] + 1/2(S_2) = <MnS>$	–288,770	—	78.92	1517–1803	2
$4<Mo> + (N_2) = 2(Mo_2N)$	–143,940	–38.50	242.30	298–1300	2
$2(N_2) + 3<Si> = <Si_3N_4>$	–753,190	—	336.43	298–1680	3
$2(N_2) + 3[Si] = <Si_3N_4>$	–892,950	—	419.28	1680–1800	3
$<Nb> + <C> = <NbC>$	–130,140	—	1.67	1180–1370	2
$<Ni> + 1/2(O_2) = <NiO>$	–244,580	—	98.54	298–1725	3
$[Pb] + 1/2(O_2) = <PbO>$	–229,930	–33.68	209.64	600–1150	3
$(S_2) + 2(O_2) = 2(SO_2)$	–724,910	—	144.90	298–2000	2
$<Si> + (O_2) = <SiO_2>$	–881,235	–12.55	218.51	298–1700	3
$<Si> + <SiO_2> = 2(SiO)$	697,540	53.98	–518.45	298–1700	3
$2<Ti>_\alpha + (N_2) = 2<TiN>$	–671,600	—	185.80	298–1155	2
$2<Ti>_\beta + (N_2) = 2<TiN>$	–676,620	—	190.20	1155–1500	2
$<W> + <C> = <WC>$	–37,656	—	1.674	298–2000	2

*References:

(1) Gaskell, 1981, Table A-1, p. 585.

(2) Kubaschewski and Alcock, 1979, Table E, p. 378.

(3) Kubaschewski and Evans, 1958, Table E, p. 336.

Table A.5*

Vapor Pressures Over Pure Condensed Phases.

$\log_{10}(P)$ (mm Hg) $= AT^{-1} + B\log_{10}(T) + CT + D$.

T is in degrees K. Solid < >, Liquid [ ].

Substance	A	B	$C \times 10^2$	D	Temp. Range (K)
<Cu>	–17,770	–0.86	—	12.29	298–1356
[Cu]	–17,520	–1.21	—	13.21	1356–2843
<Zn>	–6850	–0.755	—	11.24	298–693
[Zn]	–6620	–1.255	—	12.34	693–1180

*Kubaschewski and Alcock, 1979, Table D, p. 358.

Table A.6*

Activity of Carbon in Austenite Between 800–1200°C.

w/o C	a_C†	w/o C	a_C†
0.05	0.00236	1.1	0.0728
0.10	0.00479	1.2	0.0822
0.20	0.00992	1.3	0.0917
0.30	0.01537	1.4	0.1022
0.40	0.0211	1.5	0.1130
0.50	0.0273	1.6	0.1245
0.60	0.0338	1.7	0.1369
0.70	0.0407	1.8	0.1495
0.80	0.0480	1.9	0.1632
0.90	0.0559	2.0	0.1774
1.00	0.0640	—	—

* Darken and Gurry, 1953, Table 16-4, p. 405-406.

† Standard state is such that $\lim_{X_C \to 0} (a_C / X_C) = 1$. The activity of carbon relative to graphite is obtained from the conversion a_C (graphite) = a_C (w/o C in austenite)/ a_c(w/o C in austenite at saturation) at the same temperature.