CEMDATA07 data base, to be used with auxiliary data from Nagra/PSI TDB only! [6,7]

Version 07.2, released 14. August 2008

If you use the CEMDATA07 data base please do cite the relevant papers [1], [2], [3], [4], [5], [6], or [7] and NOT this homepage!

	log K_{S0}	$\Delta_f G°$ [kJ/mol]	$\Delta_f H°$ [kJ/mol]	S° [J/K/mol]	a_0 [J/K/mol]	a_1	a_2	a_3	V° [cm^3/mol]	Ref
(Al-)ettringite[a]	-44.9	-15205.94	-17535	1900	1939	0.789			707	[1,2]
tricarboaluminate[a]	-46.5	-14565.64	-16792	1858	2042	0.559	-7.78e6		650	[2,1]
Fe-ettringite[a]	-44.0	-14282.36	-16600	1937	1922	0.855	2.02e6		717	[3,1]
Thaumasite	-49.4	-15128.46	-17373	1883	1860	0.703	-3.94e6	1600	663	[9]
C_3AH_6[b]	-20.84	-5010.09	-5540	419	292	0.561			150	[2,1]
$C_3AS_{0.8}H_{4.4}$[*]	-29.87	-5368.01	-5855	369	109	0.631	-1.95e6	2560	143	[2,1]
C_3FH_6[** b]	-25.16	-4116.29	-4640	439	275	0.627	2.02e6		155	[1]
C_4AH_{13}[c,d]	-25.40	-7326.56	-8302	700	711	1.047		-1600	274	[1,2]
C_2AH_8[e]	-13.56	-4812.76	-5433	440	392	0.714		-800	184	[1,2]
$C_4A\bar{S}H_{12}$[d,f]	-29.26	-7778.50	-8750	821	594	1.168			309	[2,1]
$C_4A\bar{C}H_{11}$[g]	-31.47	-7337.46	-8250	657	618	0.982	-2.59e6		262	[2,1]
$C_4A\bar{C}_{0.5}H_{12}$[h]	-29.13	-7335.97	-8270	713	664	1.014	-1.30e6	-800	285	[2,1]
C_2ASH_8[i]	-19.70	-5705.15	-6360	546	438	0.749	-1.13e6	-800	216	[2,1]
C_4FH_{13}[** c]	-29.4	-6430.94	-7395	737	694	1.113	2.02e6	-1600	286	[1]
C_2FH_8[** e]	-17.6	-3917.38	-4526	476	375	0.780	2.02e6	-800	194	[1]
$C_4F\bar{S}H_{12}$[f]	-33.2	-6882.55	-7843	858	577	1.234	2.02e6		322	[3,1]
$C_4F\bar{C}H_{12}$[** g]	-35.5	-6679.20	-7637	737	612	1.157	-5.73e5		290	[3,1]
$C_4F\bar{C}_{0.5}H_{12}$[** h]	-33.1	-6440.19	-7363	749	648	1.080	7.24e5	-800	296	[1]
C_2FSH_8[** i]	-23.7	-4809.53	-5453	583	422	0.815	8.91e5	-800	227	[1]
CAH_{10}	-7.50	-4622.39	-5320	501	151	1.113		3200	194	[2]
M_4AH_{10}[** k]	-56.02	-6394.56	-7196	549	-364	4.21	3.75e6	629	220	[1,4]
$M_4A\bar{C}H_9$[**]	-51.14	-6580.15	-7374	551	-382	4.24	4.32e6	629	220	[1,4]
M_4FH_{10}[** k]	-60.0	-5498.84	-6289	586	-381	4.27	5.78e6	629	232	[1]
$C_{1.67}SH_{2.1}$(jen.)[l]	-13.17	-2480.81	-2723	140	210	0.120	-3.07e6		78	[1]
$C_{0.83}SH_{1.3}$(tob.)[l,m]	-8.0	-1744.36	-1916	80	85	0.160			59	[1]
$SiO_{2,am}$[m]	1.476	-848.90	-903	41	47	0.034	-1.13e6		29	[1]
syngenite	-7.20	-2884.91	-3172	326	201	0.308	-1.78e6		128[n]	[4]
$Al(OH)_3$(am)	0.24	-1143.21	-1281	70	36	0.191			32	[1]
$Fe(OH)_3$(mic)	-4.60	-711.61	-844	88	28	0.052			34	[1]
C_3S		-2784.33	-2931	169	209	0.036	-4.25e6		73	[1,2,5]
C_2S		-2193.21	-2308	128	152	0.037	-3.03e6		52	[1,2,5]
C_3A		-3382.35	-3561	205	261	0.019	-5.06e6		89	[1,2,5]
C_4AF		-4786.50	-5080	326	374	0.073			130	[1,2,5]

a_0, a_1, a_2, a_3 are the empirical coefficients of the heat capacity equation: $C°_p = a_0 + a_1T + a_2T^{-2} + a_3T^{-0.5}$; no value = 0.
All solubility products refer to the solubility with respect to the species $Al(OH)_4^-$, $Fe(OH)_4^-$, $SiO(OH)_3^-$, OH^-, H_2O, Ca^{2+}, K^+, Mg^{2+}, CO_3^{2-} ,or SO_4^{2-}; Cement shorthand notation is used: A = Al_2O_3; C = CaO; F = Fe_2O_3; H = H_2O; M = MgO; S = SiO_2; $\bar{C}$ = CO_2; $\bar{S}$ = SO_3;

[*] precipitates very slowly at 20 °C, generally not included in calculations; [**] tentative values; [a,d] non-ideal solid solutions. For details see [1], [2]. [8]. [b, c, e,f,g,h,i, k, l, m]: ideal solid solutions c.f. [1]. [n]: density data from Corazza, E., Sabelli, C. (1967) Zeitschrift für Kristallographie 124, 398-408.

References

[1] Lothenbach, B., Matschei, T., Möschner, G., Glasser, F. (2008) Thermodynamic modelling of the effect of temperature on the hydration and porosity of Portland cement. *Cement and Concrete Research*, 38(1), 1-18.

[2] Matschei, T., Lothenbach, B., Glasser, F. (2007) Thermodynamic properties of Portland cement hydrates in the system $CaO-Al_2O_3-SiO_2-CaSO_4-CaCO_3-H_2O$. *Cement and Concrete Research*, 37(10), 1379-1410.

[3] Möschner, G., Lothenbach, B., Rose, J., Ulrich, A., Figi, R., Kretzschmar R. (2008) Solubility of Fe-ettringite ($Ca_6[Fe(OH)_6]_2(SO_4)_3 \cdot 26H_2O$), *Geochimica et Cosmochimica Acta* 72(1), 1-18.

[4] Lothenbach, B. and F. Winnefeld (2006), Thermodynamic modelling of the hydration of Portland cement. *Cement and Concrete Research* 36, 209-226.

[5] V.I. Babushkin, G.M. Matveyev, O.P. Mchedlov-Petrossyan, Thermodynamics of Silicates, Springer-Verlag, Berlin, 1985.

[6] W. Hummel, U. Berner, E. Curti, F.J. Pearson, T. Thoenen, Nagra/PSI Chemical Thermodynamic Data Base 01/01, Universal Publishers/uPUBLISH.com, USA, also published as Nagra Technical Report NTB 02-16, Wettingen, Switzerland, 2002.

[7] T. Thoenen, D. Kulik, Nagra/PSI chemical thermodynamic database 01/01 for the GEM-Selektor (V.2-PSI) geochemical modeling code, PSI, Villigen; available at http://les.web.psi.ch/Software/GEMS-PSI/doc/pdf/TM-44-03-04-web.pdf, 2003.

[8] G. Möschner, B. Lothenbach, A. Ulrich, R. Figi, R. Kretzschmar, Solid solution between Al-ettringite and Fe-ettringite ($Ca_6[Al_{1-x}Fe_x(OH)_6]_2(SO_4)_3 \cdot 26H_2O$), Cem Concr Res submitted (2008).

[9] Schmidt, T., Lothenbach, B., Romer, M., Scrivener, K., Rentsch, D., Figi, R. (2008) A thermodynamic and experimental study of the conditions of thaumasite formation. *Cement and Concrete Research*, 38, 337-349.

Changes in Cemdata07.2

- Data for thaumasite added [9]: Note: parameters for solid solution formation between ettringite and thaumasite are not yet included!
- Density of syngenite adapted from 126 to 128 cm^3/mol (natural syngenite; Corazza, E., Sabelli, C. (1967) Zeitschrift für Kristallographie 124, 398-408).

The following changes affect the GEMS file only

- 6 digits after the decimal point for jennite and tobermorite
- Inproper handling of entropy and heat capacity of dissolved SiO2@ and SiO3-2 in GEMS projects corrected (only important for $T \neq 25°C$)

Equations

Mineral	Dissolution reactions used to calculate solubility products log K_{S0}
ettringite	$Ca_6Al_2(SO_4)_3(OH)_{12}\cdot 26H_2O \rightarrow 6Ca^{2+} + 2Al(OH)_4^- + 3SO_4^{2-} + 4OH^- + 26H_2O$
tricarboaluminate	$Ca_6Al_2(CO_3)_3(OH)_{12}\cdot 26H_2O \rightarrow 6Ca^{2+} + 2Al(OH)_4^{--} + 3CO_3^{2-} + 4OH^- + 26H_2O$
Fe-ettringite	$Ca_6Fe_2(SO_4)_3(OH)_{12}\cdot 26H_2O \rightarrow 6Ca^{2+} + 2Fe(OH)_4^- + 3SO_4^{2-} + 4OH^- + 26H_2O$
thaumasite	$Ca_6(SiO_3)_2(SO_4)_2(CO_3)_2\cdot 30H_2O \rightarrow 6Ca^{2+} + 2H_3SiO_4^- + 2SO_4^{2-} + 2CO_3^{2-} + 2OH^- + 26H_2O$
C_3AH_6	$Ca_3Al_2(OH)_{12} \rightarrow 3Ca^{2+} + 2Al(OH)_4^- + 4OH^-$
siliceous hydrogarnet	$Ca_3Al_2(SiO_4)_{0.8}(OH)_{8.8} \rightarrow 3Ca^{2+} + 2Al(OH)_4^- + 0.8\ SiO(OH)_3^- + 3.2OH^- - 2.4H_2O$
C_3FH_6	$Ca_3Fe_2(OH)_{12} \rightarrow 3Ca^{2+} + 2Fe(OH)_4^- + 4OH^-$
C_4AH_{13}	$Ca_4Al_2(OH)_{14}\cdot 6H_2O \rightarrow 4Ca^{2+} + 2Al(OH)_4^- + 6OH^- + 6H_2O$
C_2AH_8	$Ca_2Al_2(OH)_{10}\cdot 3H_2O \rightarrow 2Ca^{2+} + 2Al(OH)_4^- + 2OH^- + 3H_2O$
monosulfoaluminate	$Ca_4Al_2(SO_4)(OH)_{12}\cdot 6H_2O \rightarrow 4Ca^{2+} + 2Al(OH)_4^- + SO_4^{2-} + 4OH^- + 6H_2O$
monocarboaluminate	$Ca_4Al_2(CO_3)(OH)_{12}\cdot 5H_2O \rightarrow 4Ca^{2+} + 2Al(OH)_4^- + CO_3^{2-} + 4OH^- + 5H_2O$
hemicarboaluminate	$Ca_4Al_2(CO_3)_{0.5}(OH)_{13}\cdot 5.5H_2O \rightarrow 4Ca^{2+} + 2Al(OH)_4^- + 0.5CO_3^{2-} + 5OH^- + 5.5H_2O$
strätlingite	$Ca_2Al_2SiO_2(OH)_{10}\cdot 3H_2O \rightarrow 2Ca^{2+} + 2Al(OH)_4^- + 1SiO(OH)_3^- + OH^- + 2H_2O$
C_4FH_{13}	$Ca_4Fe_2(OH)_{14}\cdot 6H_2O \rightarrow 4Ca^{2+} + 2Fe(OH)_4^- + 6OH^- + 6H_2O$
C_2FH_8	$Ca_2Fe_2(OH)_{10}\cdot 3H_2O \rightarrow 2Ca^{2+} + 2Fe(OH)_4^- + 2OH^- + 3H_2O$
Fe-monosulfate	$Ca_4Fe_2(SO_4)(OH)_{12}\cdot 6H_2O \rightarrow 4Ca^{2+} + 2Fe(OH)_4^- + SO_4^{2-} + 4OH^- + 6H_2O$
Fe-monocarbonate	$Ca_4Fe_2(CO_3)(OH)_{12}\cdot 5H_2O \rightarrow 4Ca^{2+} + 2Fe(OH)_4^- + CO_3^{2-} + 4OH^- + 5H_2O$
Fe-hemicarbonate	$Ca_4Fe_2(CO_3)_{0.5}(OH)_{13}\cdot 5.5H_2O \rightarrow 4Ca^{2+} + 2Fe(OH)_4^- + 0.5CO_3^{2-} + 5OH^- + 5.5H_2O$
Fe-strätlingite	$Ca_2Fe_2SiO_2(OH)_{10}\cdot 3H_2O \rightarrow 2Ca^{2+} + 2Fe(OH)_4^- + 1SiO(OH)_3^- + OH^- + 2H_2O$
CAH_{10}	$CaAl_2(OH)_8\cdot 6H_2O \rightarrow Ca^{2+} + 2Al(OH)_4^- + 6H_2O$
M_4AH_{10}	$Mg_4Al_2(OH)_{14}\cdot 3H_2O \rightarrow 4Mg^{2+} + 2Al(OH)_4^- + 6OH^- + 3H_2O$
$M_4A\overline{C}H_9$	$Mg_4Al_2(OH)_{12}\ CO_3\cdot 3H_2O \rightarrow 4Mg^{2+} + 2Al(OH)_4^- + CO_3^{2-}.+ 4OH^- + 3H_2O$
M_4FH_{10}	$Mg_4Fe_2(OH)_{14}\cdot 3H_2O \rightarrow 4Mg^{2+} + 2Fe(OH)_4^- + 6OH^- + 3H_2O$
jennite-type C-S-H	$(CaO)_{1.6667}(SiO_2)(H_2O)_{2.1} \rightarrow 1.6667Ca^{2+} + SiO(OH)_3^- + 2.3333OH^- - 0.5667\ H_2O$
tobermorite-type C-S-H	$(CaO)_{0.8333}\ (SiO_2)(H_2O)_{1.3333} \rightarrow 0.8333Ca^{2+} + SiO(OH)_3^- + 0.6667OH^- - 0.5H_2O$
$SiO_{2,am}$	$SiO_{2,am} \rightarrow SiO(OH)_3^- - 1OH^- - 1H_2O$
syngenite	$K_2Ca(SO_4)_2\ H_2O \rightarrow 2K^+ + 1Ca^{2+} + 2SO_4^{2-} + 1H_2O$
$Al(OH)_{3,am}$	$Al(OH)_{3,am} \rightarrow Al(OH)_4^- - 1OH^-$
$Fe(OH)_{3,mic}$	$Fe(OH)_{3,am} \rightarrow Fe(OH)_4^- - 1OH^-$