Cemdata14 data base, to be used with general PSI-Nagra TDB only! [6,7,7a]

Version 14.01: Oct 2014

Based on the CEMDATA07 data base [1-8]. New data [9-19] are indicated **in bold**

	log K_{S0}	$\Delta_fG°$ [kJ/mol]	$\Delta_fH°$ [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,b]	-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[b]	-44.0	-14282.36	-16600	1937	1922	0.855	2.02e6		717	[3,1]
Thaumasite	**-24.75**	**-7564.52**	**-8700**	**897.1**	**1031**	**0.263**	**-3.40e6**		**330**	**[9]**
C_3AH_6 [c]	**-20.50**	**-5008.2**	**-5537.3**	**422**	**290**	**0.644**	**-3.25e6**		**150**	**[10]**
$C_3AS_{0.41}H_{5.18}$ [*c]	***-25.35***	***-5192.9***	***-5699***	***399***	***310***	***0.566***	***-4.37e6***		***146***	***[11]***
$C_3AS_{0.84}H_{4.32}$ [*e]	***-26.70***	***-5365.2***	***-5847***	***375***	***331***	***0.484***	***-5.55e6***		***142***	***[11]***
C_3FH_6 [d**]	***-26.30***	***-4122.8***	***-4518***	***870***	***330***	***1.237***	***-4.74e6***		***155***	***[11]***
$C_3FS_{0.84}H_{4.32}$ [d,e]	**-32.50**	**-4479.9**	**-4823**	**840**	**371**	**0.478**	**-7.03e6**		**149**	**[11]**
$C_3FS_{1.34}H_{3.32}$	**-34.20**	**-4681.1**	**-4994**	**820**	**395**	**0.383**	**-8.39e6**		**145**	**[11]**
C_4AH_{19} [f]	**-25.45**	**-8749.9**	**-10017.9**	**1120**	**1163**	**1.047**		**-1600**	**371**	**[10]**
C_4AH_{13}	**-25.00**	**-7324.3**	**-8300.2**	**700**	**711**	**1.047**		**-1600**	**274**	**[10]**
$C_2AH_{7.5}$	**-13.80**	**-4695.5**	**-5277.6**	**450**	**323**	**0.728**			**180**	**[10]**
CAH_{10}	**-7.60**	**-4623.0**	**-5288.2**	**610**	**151**	**1.113**		**3200**	**193**	**[10]**
C_4AsH_{12} [f,g]	-29.26	-7778.50	-8750	821	594	1.168			309	[2,1]
C_4AcH_{11}	-31.47	-7337.46	-8250	657	618	0.982	-2.59e6		262	[2,1]
$C_4Ac_{0.5}H_{12}$	-29.13	-7335.97	-8270	713	664	1.014	-1.30e6	-800	285	[2,1]
C_2ASH_8	-19.70	-5705.15	-6360	546	438	0.749	-1.13e6	-800	216	[2,1]
$C_4ACl_2H_{10}$	**-27.27**	**-6810.90**	**-7604**	**731**	**498**	**0.895**	**-2.04e6**	**1503**	**272**	**[15,16]**
$C_4As_{0.5}ClH_{12}$	**-28.53**	**-7533.97**	**-8472[***]**	**820**	**557**	**1.141**	**-1.02e6**	**751**	**289**	**[16,17]**
C_4FH_{13} [**]	***-30.75***	***-6438.6***	***-7435***	***630***	***694***	***1.113***	***2.02e6***	***-1600***	***286***	***[11]***
C_4FsH_{12} [g]	**-31.57**	**-6873.2**	**-7663**	**1430**	**577**	**1.234**	**2.02e6**		**321**	**[12]**
C_4FcH_{12}	**-34.59**	**-6674.0**	**-7485**	**1230**	**612**	**1.157**	**-5.73e5**		**292**	**[13]**
$C_4Fc_{0.5}H_{10}$	**-30.83**	**-5952.9**	**-6581**	**1270**	**308**	**1.201**	**-9.08e5**	**3200**	**273**	**[13]**
M_4AH_{10} [**]	*-56.02*	*-6394.56*	*-7196*	*549*	*-364*	*4.21*	*3.75e6*	*629*	*220*	*[1,4]*
$1/2M_6A\bar{C}H_{13}$ [h]	**-33.29 [v]**	**-4339.85**	**-4875.89**	**411**	**512.6**				**115**	**[18]**
$1/2M_6F\bar{C}H_{13}$ [h]	**-33.64 [v]**	**-3882.60**	**-4415.09**	**423**	**521.7**				**119**	**[18]**
Cs (anhydrite)	-4.357	-1322.12	-1434.60	106.7	70.2	-0.099			46	[6,7]
CsH_2 (gypsum)	-4.581	-1797.76	-2023.36	193.8	91.4	-0.318			75	[6,7]
β-$CsH_{0.5}$(hemihyd)	**-3.59[*v]**	**-1436.34[*v]**	**-1575.3[*v]**	**134.3**	**124.1**				**62**	**[19]**
syngenite	-7.20	-2884.91	-3172	326	201	0.308	-1.78e6		128[k]	[4]
$Al(OH)_3$(gibbsite)	-1.12	-1151.0	-1288.7	70	36	0.191			32	[6,7]
$Al(OH)_3$(mic)	**-0.67**	**-1148.4**	**-1265.3**	**140**	**36**	**0.191**			**32**	**[10]**
FeOOH(mic)	**-5.6**	**-480.14**	**-509.3**	**200**	**101**	**-0.008**	**-2.12E6**		**21**	**[11]**
CH (portlandite)	-5.2	-897	-985	83	187	-0.022		-1600	33	[6,7]
$SiO_{2,am}$	1.476	-848.90	-903	41	47	0.034	-1.13e6		29	[1]

C-S-H (quaternary solid solution):

	log K_{S0}	$\Delta_fG°$ [kJ/mol]	$\Delta_fH°$ [kJ/mol]	S° [J/K/mol]	a_0 [J/K/mol]	a_1	a_2	a_3	V° [cm^3/mol]	Ref
TobH Ca/Si=0.67										
$C_{2/3}SH_{1.5}$ [i]	**-6.19 [v]**	**-1668.56**	**-1841.51**	**89.9**	**141.6**				**55**	**[14]**
TobD Ca/Si =1.25										
$C_{5/6}S_{2/3}H_{1.83}$ [i]	**-6.90 [v]**	**-1570.89**	**-1742.42**	**121.8**	**166.9**				**48**	**[14]**
JenH Ca/Si =1.33										
$C_{1.33}SH_{2.17}$ [i]	**-10.96 [v]**	**-2273.99**	**-2506.27**	**142.5**	**207.9**				**76**	**[14]**
JenD Ca/Si==2.25										
$C_{1.5}S_{0.67}H_{2.5}$ [i]	**-10.47 [v]**	**-2169.56**	**-2400.72**	**173.4**	**232.8**				**81**	**[14]**

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]
$C_{12}A_7$	**-18451.44**	**-19414**	**1145**	**1263**	**0.274**	**-2.31e7**	**518** [l]	**[5]**
CA	**-2207.90**	**-2327**	**114**	**151**	**0.042**	**-3.33e6**	**54** [m]	**[5]**
CA_2	**-3795.31**	**-4004**	**178**	**277**	**0.023**	**-7.45e6**	**89** [n]	**[5]**
C_4AF	-4786.50	-5080	326	374	0.073		130	[1,2,5]
Ks (K_2SO_4 arcanite)	-1319.60	-1438	176	120	0.100	-1.78e6	66	[20]
K (K_2O)	-322.40	-363	94	77	0.036	-3.68e5	40	[21]
Ns (Na_2SO_4 thenardite)	-1269.80	-1387	150	58	0.023		53	[20]
N (Na_2O)	-376.07	-415	75	76	0.020	-1.21e6	25	[21]

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; c = CO_2; s = SO_3;
[*] *precipitates very slowly at 20 °C, generally not included in calculations;* [**] *tentative values*; [***] typing error in [17], recalculated from Gf° and S from [17]. [*v] recalculated from $\Delta G_r°$ of -20500 J/mol [19]. [v] recalculated from $\Delta G_f°$ values; [b, f, g] non-ideal solid solutions. For details see [1], [2]. [8], [12]. [a,c,d,e,h,i]: ideal solid solutions c.f. [11] [14] [18]. [k]: calculated from density data from Corazza, E., Sabelli, C. (1967) Zeitschrift für Kristallographie 124, 398-408, [l]: Boysen, H., Lerch, M., Stys, A., Senyshyn, A. (2007), Acta Cryst. B63, 675–682, [m]: Hörkner W., Müller-Buschbaum H.K. (1976) J Inorganic Nuclear Chemistry, 38(5), 983-984, [n]: Goodwin, D.W., Lindop, A.J. (1970) Acta Cryst. B26, 1230-1235.

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	$Ca_3(SiO_3)(SO_4)(CO_3)\cdot 15H_2O \rightarrow 3Ca^{2+} + H_3SiO_4^- + SO_4^{2-} + CO_3^{2-} + OH^- + 13H_2O$
C_3AH_6	$Ca_3Al_2(OH)_{12} \rightarrow 3Ca^{2+} + 2Al(OH)_4^- + 4OH^-$
$C_3AS_{0.41}H_{5.18}$	$Ca_3Al_2(SiO_4)_{0.41}(OH)_{10.36} \rightarrow 3Ca^{2+} + 2Al(OH)_4^- + 0.41\ SiO(OH)_3^- + 3.59OH^- - 1.23H_2O$
$C_3AS_{0.84}H_{4.32}$	$Ca_3Al_2(SiO_4)_{0.84}(OH)_{8.64} \rightarrow 3Ca^{2+} + 2Al(OH)_4^- + 0.84\ SiO(OH)_3^- + 3.16OH^- - 2.52H_2O$
C_3FH_6	$Ca_3Fe_2(OH)_{12} \rightarrow 3Ca^{2+} + 2Fe(OH)_4^- + 4OH^-$
$C_3FS_{0.84}H_{4.32}$	$Ca_3Fe_2(SiO_4)_{0.84}(OH)_{8.64} \rightarrow 3Ca^{2+} + 2Fe(OH)_4^- + 0.84\ SiO(OH)_3^- + 3.16OH^- - 2.52H_2O$
$C_3FS_{1.34}H_{3.32}$	$Ca_3Fe_2(SiO_4)_{1.34}(OH)_{6.64} \rightarrow 3Ca^{2+} + 2Fe(OH)_4^- + 1.34\ SiO(OH)_3^- + 2.66OH^- - 4.02H_2O$
C_4AH_{19}	$Ca_4Al_2(OH)_{14}\cdot 12H_2O \rightarrow 4Ca^{2+} + 2Al(OH)_4^- + 6OH^- + 12H_2O$
C_4AH_{13}	$Ca_4Al_2(OH)_{14}\cdot 6H_2O \rightarrow 4Ca^{2+} + 2Al(OH)_4^- + 6OH^- + 6H_2O$
$C_2AH_{7.5}$	$Ca_2Al_2(OH)_{10}\cdot 2.5H_2O \rightarrow 2Ca^{2+} + 2Al(OH)_4^- + 2OH^- + 2.5H_2O$
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	$Ca_4Al_2(CO_3)_{0.5}(OH)_{13}\cdot 5.5H_2O \rightarrow 4Ca^{2+} + 2Al(OH)_4^- + 0.5CO_3^{2-} + 5OH^- + 5.5H_2O$
stratlingite	$Ca_2Al_2SiO_2(OH)_{10}\cdot 3H_2O \rightarrow 2Ca^{2+} + 2Al(OH)_4^- + 1SiO(OH)_3^- + OH^- + 2H_2O$
Friedel's salt	$Ca_4Al_2Cl_2(OH)_{12}\cdot 4H_2O \rightarrow 4Ca^{2+} + 2Al(OH)_4^- + 2Cl^- + 4OH^- + 4H_2O$
Kuzel's salt	$Ca_4Al_2Cl(SO_4)_{0.5}(OH)_{12}\cdot 6H_2O \rightarrow 4Ca^{2+} + 2Al(OH)_4^- + Cl^- + 0.5SO_4^{2-} + 4OH^- + 6H_2O$
C_4FH_{13}	$Ca_4Fe_2(OH)_{14}\cdot 6H_2O \rightarrow 4Ca^{2+} + 2Fe(OH)_4^- + 6OH^- + 6H_2O$
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	$Ca_4Fe_2(CO_3)(OH)_{12}\cdot 6H_2O \rightarrow 4Ca^{2+} + 2Fe(OH)_4^- + CO_3^{2-} + 4OH^- + 6H_2O$
Fe-hemicarbonate	$Ca_4Fe_2(CO_3)_{0.5}(OH)_{13}\cdot 3.5H_2O \rightarrow 4Ca^{2+} + 2Fe(OH)_4^- + 0.5CO_3^{2-} + 5OH^- + 3.5H_2O$
CAH_{10}	$CaAl_2(OH)_8\cdot 6H_2O \rightarrow Ca^{2+} + 2Al(OH)_4^- + 6H_2O$
M_4AH_{10}	$Mg_4Al_2(OH)_{14}\cdot 3H_2O \rightarrow 4Mg^{2+} + 2Al(OH)_4^- + 6OH^- + 3H_2O$
$^{1}/_{2}M_6A\bar{C}H_{13}$	$Mg_3Al(OH)_8(CO_3)_{0.5}\ 2.5H_2O \rightarrow 3Mg^{2+} + Al(OH)_4^- + 0.5CO_3^{2-}.+ 4OH^- + 2.5H_2O$
$^{1}/_{2}M_6F\bar{C}H_{13}$	$Mg_3Fe(OH)_8(CO_3)_{0.5}\ 2.5H_2O \rightarrow 3Mg^{2+} + Fe(OH)_4^- + 0.5CO_3^{2-}.+ 4OH^- + 2.5H_2O$
Cs (anhydrite)	$CaSO_4 \rightarrow Ca^{2+} + SO_4^{2-}$
CsH_2 (gypsum)	$Ca\ SO_4\ 2H_2O \rightarrow Ca^{2+} + SO_4^{2-} + 2H_2O$
β-$CsH_{0.5}$	$Ca\ SO_4\ 0.5H_2O \rightarrow Ca^{2+} + SO_4^{2-} + 0.5H_2O$
syngenite	$K_2Ca(SO_4)_2\ H_2O \rightarrow 2K^+ + Ca^{2+} + 2SO_4^{2-} + H_2O$
$Al(OH)_{3,mic}$	$Al(OH)_{3,mic} \rightarrow Al(OH)_4^- - OH^-$
$FeOOH_{mic}$	$FeOOH_{mic} + 2H_2O \rightarrow Fe(OH)_4^- - OH^-$
CH	$Ca(OH)_2 \rightarrow Ca^{2+} + 2OH^-$
$SiO_{2,am}$	$SiO_{2,am} \rightarrow SiO(OH)_3^- - 1OH^- - 1H_2O$
C-S-H quaternary solid solution	
$C_{2/3}SH_{1.5}$(TobH)	$(CaO)_{0.67}SiO_2(H_2O)_{1.5} \rightarrow {}^{2}/_{3}Ca^{2+} + SiO(OH)_3^- + {}^{1}/_{3}OH^- - {}^{1}/_{6}H_2O$
$C_{5/6}S_{2/3}H_{1.83}$(TobD)	$(CaO)_{0.83}(SiO_2)_{0.67}(H_2O)_{1.83} \rightarrow {}^{5}/_{6}Ca^{2+} + {}^{2}/_{3}SiO(OH)_3^- + OH^- + {}^{1}/_{3}H_2O$
$C_{4/3}SH_{2.17}$(JenH)	$(CaO)_{1.33}SiO_2(H_2O)_{2.17} \rightarrow {}^{4}/_{3}Ca^{2+} + SiO(OH)_3^- + {}^{5}/_{3}OH^- - {}^{1}/_{6}H_2O$
$C_{1.5}S_{0.67}H_{2.5}$(JenD)	$(CaO)_{1.5}(SiO_2)_{0.67}(H_2O)_{2.5} \rightarrow {}^{3}/_{2}Ca^{2+} + {}^{2}/_{3}SiO(OH)_3^- + {}^{7}/_{3}OH^- + {}^{1}/_{3}H_2O$

Changes in Cemdata14.01 (compared to Cemdata07)

- Addition of data for C_4AH_{19} [10], $FeOOH_{mic}$, $C_3AS_{0.41}H_{5.18}$, $C_3AS_{0.84}H_{4.32}$, $C_3FS_{0.84}H_{4.32}$, $C_3FS_{1.34}H_{3.32}$ [11], Friedel's salt, Kuzel's salt [15-17], CO_3-hydrotalcite, pyroaurite [18], hemihydrate [19], $C_{12}A_7$, CA, and CA_2 [5], K, N, Ks, Ns [20, 21].
- Updated data for $AH_{3,mic}$, CAH_{10}, $C_2AH_{7.5}$, C_3AH_6, C_4AH_{13} [10], Fe-monosulfate [12], Fe-monocarbonate, Fe-hemicarbonate [13], C_3FH_6, C_4FH_{13} [11], and thaumasite [9]
- Removal of $AH_{3,am}$ [10], C_2FH_8, C_2FSH_8 [14] and Fe-hydrotalcite (inconsistent with Rozov [18]).
- Changes in water content: $C_2AH_{7.5}$ [10], $C_4Fc_{0.5}H_{10}$ [13]
- Use of the quarternary C-S-H model from [16] instead of the "tobermorite-jennite" model used in cemdata07.
- Rescaling within GEMS for all Al-Fe solid solution to 1Al:1Fe

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