

**CEM DATA07 data base, to be used with auxiliary data from Nagra/PSI TDB only! [6,7]**

**Version 07.3, released 28. September 2013**

**If you use the CEM DATA07 data base please do cite the relevant papers [1], [2], [3], [4], [5], [6], or [7] and NOT this homepage!**

	log K <sub>SO</sub>	Δ <sub>f</sub> G° [kJ/mol]	Δ <sub>f</sub> H° [kJ/mol]	S° [J/K/mol]	a <sub>0</sub> [J/K/mol]	a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	V° [cm <sup>3</sup> /mol]	Ref
(Al-)jettringite <sup>a</sup>	-44.9	-15205.94	-17535	1900	1939	0.789			707	[1,2]
tricarboaluminate <sup>a</sup>	-46.5	-14565.64	-16792	1858	2042	0.559	-7.78e6		650	[2,1]
Fe-ettringite <sup>a</sup>	-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 <sub>3</sub> AH <sub>6</sub> <sup>b</sup>	-20.84	-5010.09	-5540	419	292	0.561			150	[2,1]
C <sub>3</sub> AS <sub>0.8</sub> H <sub>4.4</sub> <sup>*</sup>	-29.87	-5368.01	-5855	369	109	0.631	-1.95e6	2560	143	[2,1]
C <sub>3</sub> FH <sub>6</sub> <sup>**b</sup>	-25.16	-4116.29	-4640	439	275	0.627	2.02e6		155	[1]
C <sub>4</sub> AH <sub>13</sub> <sup>c,d</sup>	-25.40	-7326.56	-8302	700	711	1.047		-1600	274	[1,2]
C <sub>2</sub> AH <sub>8</sub> <sup>e</sup>	-13.56	-4812.76	-5433	440	392	0.714		-800	184	[1,2]
C <sub>4</sub> A $\bar{S}$ H <sub>12</sub> <sup>d,f</sup>	-29.26	-7778.50	-8750	821	594	1.168			309	[2,1]
C <sub>4</sub> A $\bar{C}$ H <sub>11</sub> <sup>g</sup>	-31.47	-7337.46	-8250	657	618	0.982	-2.59e6		262	[2,1]
C <sub>4</sub> A $\bar{C}$ <sub>0.5</sub> H <sub>12</sub> <sup>h</sup>	-29.13	-7335.97	-8270	713	664	1.014	-1.30e6	-800	285	[2,1]
C <sub>2</sub> ASH <sub>8</sub> <sup>i</sup>	-19.70	-5705.15	-6360	546	438	0.749	-1.13e6	-800	216	[2,1]
C <sub>4</sub> FH <sub>13</sub> <sup>**c</sup>	-29.4	-6430.94	-7395	737	694	1.113	2.02e6	-1600	286	[1]
C <sub>2</sub> FH <sub>8</sub> <sup>**e</sup>	-17.6	-3917.38	-4526	476	375	0.780	2.02e6	-800	194	[1]
C <sub>4</sub> F $\bar{S}$ H <sub>12</sub> <sup>f</sup>	-33.2	-6882.55	-7843	858	577	1.234	2.02e6		322	[3,1]
C <sub>4</sub> F $\bar{C}$ H <sub>12</sub> <sup>**g</sup>	-35.5	-6679.20	-7637	737	612	1.157	-5.73e5		290	[3,1]
C <sub>4</sub> F $\bar{C}$ <sub>0.5</sub> H <sub>12</sub> <sup>**h</sup>	-33.1	-6440.19	-7363	749	648	1.080	7.24e5	-800	296	[1]
C <sub>2</sub> FSH <sub>8</sub> <sup>**i</sup>	-23.7	-4809.53	-5453	583	422	0.815	8.91e5	-800	227	[1]
CAH <sub>10</sub>	-7.50	-4622.39	-5320	501	151	1.113		3200	194	[2]
M <sub>4</sub> AH <sub>10</sub> <sup>**k</sup>	-56.02	-6394.56	-7196	549	-364	4.21	3.75e6	629	220	[1,4]
M <sub>4</sub> A $\bar{C}$ H <sub>9</sub> <sup>**</sup>	-51.14	-6580.15	-7374	551	-382	4.24	4.32e6	629	220	[1,4]
M <sub>4</sub> FH <sub>10</sub> <sup>**k</sup>	-60.0	-5498.84	-6289	586	-381	4.27	5.78e6	629	232	[1]
C <sub>1.67</sub> SH <sub>2.1</sub> (jen.) <sup>l</sup>	-13.17	-2480.81	-2723	140	210	0.120	-3.07e6		78	[1]
C <sub>0.83</sub> SH <sub>1.3</sub> (tob.) <sup>l,m</sup>	-8.0	-1744.36	-1916	80	85	0.160			59	[1]
SiO <sub>2,am</sub> <sup>m</sup>	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 <sup>n</sup>	[4]
Al(OH) <sub>3</sub> (am)	0.24	-1143.21	-1281	70	36	0.191			32	[1]
Fe(OH) <sub>3</sub> (mic)	-4.60	-711.61	-844	88	28	0.052			34	[1]
C <sub>3</sub> S		-2784.33	-2931	169	209	0.036	-4.25e6		73	[1,2,5]
C <sub>2</sub> S		-2193.21	-2308	128	152	0.037	-3.03e6		52	[1,2,5]
C <sub>3</sub> A		-3382.35	-3561	205	261	0.019	-5.06e6		89	[1,2,5]
C <sub>4</sub> AF		-4786.50	-5080	326	374	0.073			130	[1,2,5]

a<sub>0</sub>, a<sub>1</sub>, a<sub>2</sub>, a<sub>3</sub> are the empirical coefficients of the heat capacity equation: C<sub>p</sub>° = a<sub>0</sub> + a<sub>1</sub>T + a<sub>2</sub>T<sup>-2</sup> + a<sub>3</sub>T<sup>-0.5</sup>; no value = 0.

All solubility products refer to the solubility with respect to the species Al(OH)<sub>4</sub><sup>-</sup>, Fe(OH)<sub>4</sub><sup>-</sup>, SiO(OH)<sub>3</sub><sup>-</sup>, OH<sup>-</sup>, H<sub>2</sub>O, Ca<sup>2+</sup>, K<sup>+</sup>, Mg<sup>2+</sup>, CO<sub>3</sub><sup>2-</sup>, or SO<sub>4</sub><sup>2-</sup>; Cement shorthand notation is used: A = Al<sub>2</sub>O<sub>3</sub>; C = CaO; F = Fe<sub>2</sub>O<sub>3</sub>; H = H<sub>2</sub>O; M = MgO; S =

SiO<sub>2</sub>;  $\bar{C}$  = CO<sub>2</sub>;  $\bar{S}$  = SO<sub>3</sub>;

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

## References

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- [3] Möschner, G., Lothenbach, B., Rose, J., Ulrich, A., Figi, R., Kretzschmar R. (2008) Solubility of Fe-ettringite (Ca<sub>6</sub>[Fe(OH)<sub>6</sub>]<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>·26H<sub>2</sub>O), *Geochimica et Cosmochimica Acta* 72(1), 1-18.
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- [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<sup>3</sup>/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
- Improper handling of entropy and heat capacity of dissolved SiO<sub>2</sub>@ and SiO<sub>3</sub>-2 in GEMS projects corrected (only important for T ≠ 25°C)
- Wording "strätlingite" changed to "straetlingite"

## Equations

Mineral	Dissolution reactions used to calculate solubility products $\log K_{S0}$
ettringite	$\text{Ca}_6\text{Al}_2(\text{SO}_4)_3(\text{OH})_{12} \cdot 26\text{H}_2\text{O} \rightarrow 6\text{Ca}^{2+} + 2\text{Al}(\text{OH})_4^- + 3\text{SO}_4^{2-} + 4\text{OH}^- + 26\text{H}_2\text{O}$
tricarboaluminate	$\text{Ca}_6\text{Al}_2(\text{CO}_3)_3(\text{OH})_{12} \cdot 26\text{H}_2\text{O} \rightarrow 6\text{Ca}^{2+} + 2\text{Al}(\text{OH})_4^- + 3\text{CO}_3^{2-} + 4\text{OH}^- + 26\text{H}_2\text{O}$
Fe-ettringite	$\text{Ca}_6\text{Fe}_2(\text{SO}_4)_3(\text{OH})_{12} \cdot 26\text{H}_2\text{O} \rightarrow 6\text{Ca}^{2+} + 2\text{Fe}(\text{OH})_4^- + 3\text{SO}_4^{2-} + 4\text{OH}^- + 26\text{H}_2\text{O}$
thaumasite	$\text{Ca}_6(\text{SiO}_3)_2(\text{SO}_4)_2(\text{CO}_3)_2 \cdot 30\text{H}_2\text{O} \rightarrow 6\text{Ca}^{2+} + 2\text{H}_3\text{SiO}_4^- + 2\text{SO}_4^{2-} + 2\text{CO}_3^{2-} + 2\text{OH}^- + 26\text{H}_2\text{O}$
$\text{C}_3\text{AH}_6$	$\text{Ca}_3\text{Al}_2(\text{OH})_{12} \rightarrow 3\text{Ca}^{2+} + 2\text{Al}(\text{OH})_4^- + 4\text{OH}^-$
siliceous hydrogarnet	$\text{Ca}_3\text{Al}_2(\text{SiO}_4)_{0.8}(\text{OH})_{8.8} \rightarrow 3\text{Ca}^{2+} + 2\text{Al}(\text{OH})_4^- + 0.8 \text{SiO}(\text{OH})_3^- + 3.2\text{OH}^- - 2.4\text{H}_2\text{O}$
$\text{C}_3\text{FH}_6$	$\text{Ca}_3\text{Fe}_2(\text{OH})_{12} \rightarrow 3\text{Ca}^{2+} + 2\text{Fe}(\text{OH})_4^- + 4\text{OH}^-$
$\text{C}_4\text{AH}_{13}$	$\text{Ca}_4\text{Al}_2(\text{OH})_{14} \cdot 6\text{H}_2\text{O} \rightarrow 4\text{Ca}^{2+} + 2\text{Al}(\text{OH})_4^- + 6\text{OH}^- + 6\text{H}_2\text{O}$
$\text{C}_2\text{AH}_8$	$\text{Ca}_2\text{Al}_2(\text{OH})_{10} \cdot 3\text{H}_2\text{O} \rightarrow 2\text{Ca}^{2+} + 2\text{Al}(\text{OH})_4^- + 2\text{OH}^- + 3\text{H}_2\text{O}$
monosulfoaluminate	$\text{Ca}_4\text{Al}_2(\text{SO}_4)(\text{OH})_{12} \cdot 6\text{H}_2\text{O} \rightarrow 4\text{Ca}^{2+} + 2\text{Al}(\text{OH})_4^- + \text{SO}_4^{2-} + 4\text{OH}^- + 6\text{H}_2\text{O}$
monocarboaluminate	$\text{Ca}_4\text{Al}_2(\text{CO}_3)(\text{OH})_{12} \cdot 5\text{H}_2\text{O} \rightarrow 4\text{Ca}^{2+} + 2\text{Al}(\text{OH})_4^- + \text{CO}_3^{2-} + 4\text{OH}^- + 5\text{H}_2\text{O}$
hemicarboaluminate	$\text{Ca}_4\text{Al}_2(\text{CO}_3)_{0.5}(\text{OH})_{13} \cdot 5.5\text{H}_2\text{O} \rightarrow 4\text{Ca}^{2+} + 2\text{Al}(\text{OH})_4^- + 0.5\text{CO}_3^{2-} + 5\text{OH}^- + 5.5\text{H}_2\text{O}$
straetlingite	$\text{Ca}_2\text{Al}_2\text{SiO}_2(\text{OH})_{10} \cdot 3\text{H}_2\text{O} \rightarrow 2\text{Ca}^{2+} + 2\text{Al}(\text{OH})_4^- + 1\text{SiO}(\text{OH})_3^- + \text{OH}^- + 2\text{H}_2\text{O}$
$\text{C}_4\text{FH}_{13}$	$\text{Ca}_4\text{Fe}_2(\text{OH})_{14} \cdot 6\text{H}_2\text{O} \rightarrow 4\text{Ca}^{2+} + 2\text{Fe}(\text{OH})_4^- + 6\text{OH}^- + 6\text{H}_2\text{O}$
$\text{C}_2\text{FH}_8$	$\text{Ca}_2\text{Fe}_2(\text{OH})_{10} \cdot 3\text{H}_2\text{O} \rightarrow 2\text{Ca}^{2+} + 2\text{Fe}(\text{OH})_4^- + 2\text{OH}^- + 3\text{H}_2\text{O}$
Fe-monosulfate	$\text{Ca}_4\text{Fe}_2(\text{SO}_4)(\text{OH})_{12} \cdot 6\text{H}_2\text{O} \rightarrow 4\text{Ca}^{2+} + 2\text{Fe}(\text{OH})_4^- + \text{SO}_4^{2-} + 4\text{OH}^- + 6\text{H}_2\text{O}$
Fe-monocarbonate	$\text{Ca}_4\text{Fe}_2(\text{CO}_3)(\text{OH})_{12} \cdot 5\text{H}_2\text{O} \rightarrow 4\text{Ca}^{2+} + 2\text{Fe}(\text{OH})_4^- + \text{CO}_3^{2-} + 4\text{OH}^- + 5\text{H}_2\text{O}$
Fe-hemicarbonate	$\text{Ca}_4\text{Fe}_2(\text{CO}_3)_{0.5}(\text{OH})_{13} \cdot 5.5\text{H}_2\text{O} \rightarrow 4\text{Ca}^{2+} + 2\text{Fe}(\text{OH})_4^- + 0.5\text{CO}_3^{2-} + 5\text{OH}^- + 5.5\text{H}_2\text{O}$
Fe-straetlingite	$\text{Ca}_2\text{Fe}_2\text{SiO}_2(\text{OH})_{10} \cdot 3\text{H}_2\text{O} \rightarrow 2\text{Ca}^{2+} + 2\text{Fe}(\text{OH})_4^- + 1\text{SiO}(\text{OH})_3^- + \text{OH}^- + 2\text{H}_2\text{O}$
$\text{CAH}_{10}$	$\text{CaAl}_2(\text{OH})_8 \cdot 6\text{H}_2\text{O} \rightarrow \text{Ca}^{2+} + 2\text{Al}(\text{OH})_4^- + 6\text{H}_2\text{O}$
$\text{M}_4\text{AH}_{10}$	$\text{Mg}_4\text{Al}_2(\text{OH})_{14} \cdot 3\text{H}_2\text{O} \rightarrow 4\text{Mg}^{2+} + 2\text{Al}(\text{OH})_4^- + 6\text{OH}^- + 3\text{H}_2\text{O}$
$\text{M}_4\text{A} \overline{\text{C}} \text{H}_9$	$\text{Mg}_4\text{Al}_2(\text{OH})_{12} \text{CO}_3 \cdot 3\text{H}_2\text{O} \rightarrow 4\text{Mg}^{2+} + 2\text{Al}(\text{OH})_4^- + \text{CO}_3^{2-} + 4\text{OH}^- + 3\text{H}_2\text{O}$
$\text{M}_4\text{FH}_{10}$	$\text{Mg}_4\text{Fe}_2(\text{OH})_{14} \cdot 3\text{H}_2\text{O} \rightarrow 4\text{Mg}^{2+} + 2\text{Fe}(\text{OH})_4^- + 6\text{OH}^- + 3\text{H}_2\text{O}$
jennite-type C-S-H	$(\text{CaO})_{1.6667}(\text{SiO}_2)(\text{H}_2\text{O})_{2.1} \rightarrow 1.6667\text{Ca}^{2+} + \text{SiO}(\text{OH})_3^- + 2.3333\text{OH}^- - 0.5667 \text{H}_2\text{O}$
tobermorite-type C-S-H	$(\text{CaO})_{0.8333}(\text{SiO}_2)(\text{H}_2\text{O})_{1.3333} \rightarrow 0.8333\text{Ca}^{2+} + \text{SiO}(\text{OH})_3^- + 0.6667\text{OH}^- - 0.5\text{H}_2\text{O}$
$\text{SiO}_{2,\text{am}}$	$\text{SiO}_{2,\text{am}} \rightarrow \text{SiO}(\text{OH})_3^- - 1\text{OH}^- - 1\text{H}_2\text{O}$
syngenite	$\text{K}_2\text{Ca}(\text{SO}_4)_2 \text{H}_2\text{O} \rightarrow 2\text{K}^+ + 1\text{Ca}^{2+} + 2\text{SO}_4^{2-} + 1\text{H}_2\text{O}$
$\text{Al}(\text{OH})_{3,\text{am}}$	$\text{Al}(\text{OH})_{3,\text{am}} \rightarrow \text{Al}(\text{OH})_4^- - 1\text{OH}^-$
$\text{Fe}(\text{OH})_{3,\text{mic}}$	$\text{Fe}(\text{OH})_{3,\text{mic}} \rightarrow \text{Fe}(\text{OH})_4^- - 1\text{OH}^-$