experimentally we observe the changes shown in Fig. 17, several of these dehydration processes are metastable with respect to other phase assemblages. This has to be considered when predicting the drying behaviour of cementitious systems.

4. Conclusions

The Cemdata18 database summarised in this paper can reliably calculate the type, composition, amount and volume of hydrates formed and the pH and composition of the pore solution during hydration and degradation of cementitious systems. The Cemdata18 database, as compiled in Table 1 to Table 4, includes carefully selected thermodynamic data published in the literature based on critical reviews supplemented with new experimental data. Data for solids commonly encountered in cement systems in the temperature range 0–100 °C, including C-S-H, M-S-H, hydrogarnet, hydrotalcite-like phases, some zeolite, AFm and AFt phases and their respective solid solutions has been compiled. The Cemdata18 database is an update of the Cemdata07 and Cemdata14 databases, and is compatible with the GEMS version of the PSI/Nagra 12/07 TDB [22,23]. Cemdata18 TDB is freely downloadable (http://www.empa.ch/cemdata) in formats supporting the computer programs GEM-Selektor [13,14] and PHREEQC [18]. Further details are available in Appendices A and B.

The most important additions to the Cemdata18 TDB include:

- C-S-H:
  - CSHQ model for Portland and blended cements, the uptake of alkalis by C-S-H is modelled by additional Na- and K-containing end members
  - CSH3T model that corresponds to pure defect-tobermorite structure with ordering at Ca/Si ratio close to 1.0, and forms the basis for CNASH-ss model
  - C-(N-)A-S-H model for alkali activated materials (CNASH-ss), which calculates the uptake of aluminium and sodium in low Ca/Si C-S-H
- iron-containing hydrates, in particular for the mixed Fe-Al-hydrogarnet solid solution, $C_3FS_{0.84}H_{4.32}$-$C_3A_{0.5}F_{0.5}S_{0.84}H_{4.32}$, which takes up iron and a part of the aluminium in hydrated cements
- AFm and AFt-phases with different water contents to describe the effect of water activity and drying on hydrates
- amorphous, microcrystalline AH_3 and gibbsite to study the effect of AH_3 solubility on the hydrates in calcium aluminate and calcium sulfoaluminate cements
- chloride, nitrate and nitrate-containing AFm phases
- thaumasite and the uptake of carbonates in SO_4-ettringite.
- description of the variation in Mg/Al in layered double hydroxides (hydrotalcite-like phases) observed in alkali activated materials
- data for M-S-H and some Na- and Ca-based zeolites, which can form at the interaction zone of cement with clays, rocks or seawater and in alkali activated materials.

These additions improve the reliability of thermodynamic modelling of cement systems, in particular for alkali activated materials and for processes at cement/environment interfaces, where hydrates such as thaumasite, Friedel's salt, M-S-H, and zeolites may form.

The consideration of siliceous hydrogarnet solid solution in Cemdata18 leads to a quite significant redistribution of alumina and iron within the phase assemblage in PC; the predictions based on Cemdata18 suggest that alumina is bound not only in AFt, AFm phases and hydrotalcite but also in siliceous hydrogarnet phase while all hydrated iron is present in siliceous hydrogarnet.

Several C-S-H solubility models as well two models for hydroxide-hydrotalcite are available (Table 4, Appendices A and B). The CSHQ and the OH-hydrotalcite with Mg/Al = 2 are well adapted for PC systems. Although CSHQ is able to describe the entire range of Ca/Si ratios encountered, it is best used for high Ca/Si C-S-H as it lacks the ability to predict aluminium uptake, however, this is less important in PC where the aluminium content is relatively low. For alkali activated binders, the CNASH model has been developed for C-S-H type calcium (alkali) aluminosilicate hydrate gels with lower calcium but higher aluminium and alkali content. An Mg-Al layered double hydroxide model with variable Mg/Al ratio is also available for use in alkali activated cement systems.

Despite significant additions to the Cemdata18 TDB, several important gaps still exist in the database. In particular, reliable thermodynamic data for alkali, aluminium and water uptake in C-S-H applicable to high and low Ca/Si C-S-H and M-S-H, data for hydrotalcite-like phases of variable composition and for different interlayer ions, data for further zeolites derived from experimental solubility measurements, data for aqueous complexes which possibly form at high pH values as well as data for the reaction products of alkali silica reaction are needed. However, these data gaps should be viewed as possible future improvements rather than barriers to use thermodynamic modelling: Cemdata18 database has already been successfully applied to model hydrated PC, calcium aluminate, calcium sulfoaluminate and blended cements, and also alkali activated materials. Cemdata18, therefore, enables improved characterisation and understanding of the chemistry and related in-service performance properties of a wide range of cement systems, including the most common types.

Acknowledgements

The partial financial support from the NANOCEM consortium (www.nanocem.org), the Swiss National Foundation (SNF grants No. 117605, 132559, 130419 and 200021_169014), from Nagra, Wettingen, Switzerland, and from the BMBF ThermAc3 Verbundprojekt (Germany) are gratefully acknowledged. The authors thank also Tres Thoenen, Ravi Patel and Andres Idiart for their support on the PHREEQC version.

Appendix A. Cemdata18 dataset in GEMS format

Cemdata18 database in GEM-Selektor v.3 format can be freely downloaded (http://www.empa.ch/cemdata) and is fully compatible with the GEMS version of the PSI/Nagra 12/07 TDB [22,23] (http://gems.web.psi.ch). As several alternative C-S-H models, as well as two models for hydroxide-hydrotalcite are available, the user needs to select the appropriate models during the generation of new projects, as illustrated in Fig. A.1. The CSHQ and the OH-hydrotalcite with Mg/Al = 2 are well adapted for Portland cement systems (select cemdata, pc, ht. and cshq as indicated at the left hand side of Fig. A.1).

For alkali activated binders, the CNASH model has been developed for C-S-H type calcium (alkali) aluminosilicate hydrate gels with lower calcium but higher aluminium and alkali content. An Mg-Al layered double hydroxide model with variable Mg/Al ratio is also available for use in alkali activated cement systems. For alkali activated binders, the selection of cemdata and aam and deselection of pc, including ht and csh is recommended as illustrated at the right hand side of Fig. A.1.

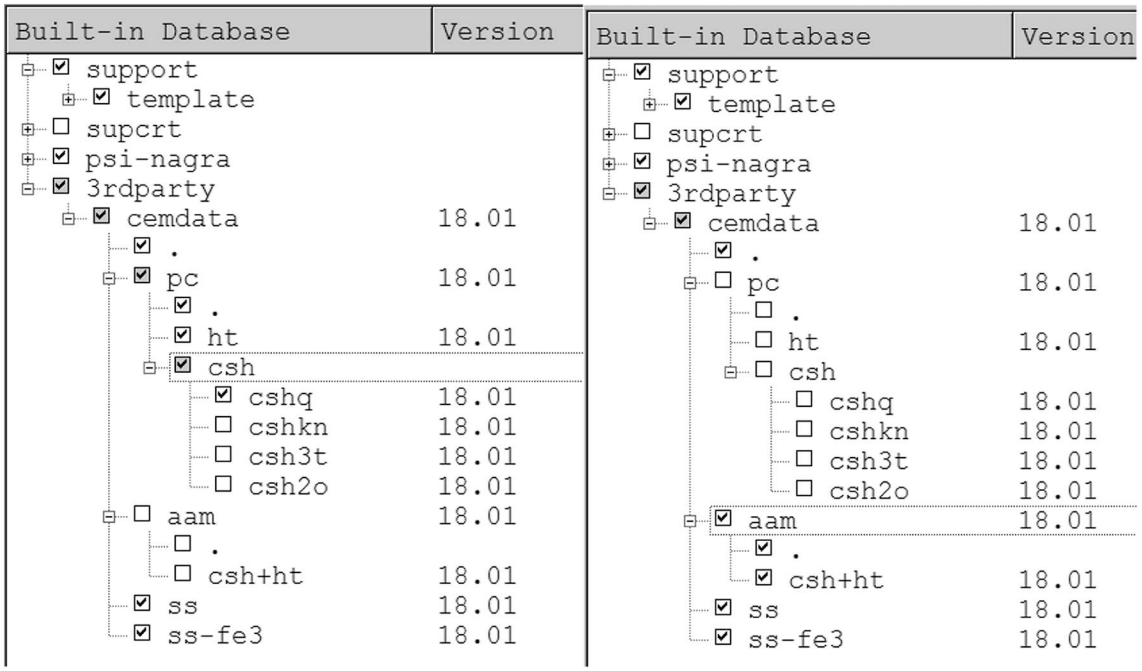

Fig. A.1. Selection of modules of Cemdata18 and related databases in GEM-Selektor to model PC (Portland-cement) systems (left) and to model AAM (alkali-activated materials). For PC systems, one of four alternative solid solution models of C-S-H should be selected (see Section 2.7); selection of Fe-containing solid solutions ("ss-fe3" module) is also optional.

Appendix B. Cemdata18 dataset in PHREEQC format

To enable users to model cementitious systems using the Cemdata18 dataset with the popular PHREEQC geochemical speciation code [18], a PHREEQC ".dat" format database of the Cemdata18 dataset (CEMDATA18.dat) is provided for download from http://www.empa.ch/cemdata. This LMA (Law of Mass Action) type dataset has been generated using the reaction generator module of the ThermoMatch code (Miron et al. in preparation) and exported into the PHREEQC format ".dat" file using the ThermoMatch database export module. The reaction generator algorithm is based on the matrix "row reduce" method described by Smith and Missen [128]. In this process, all aqueous and solid species from the Cemdata18 GEM-Selektor database were considered. The supplementary data for aqueous, gaseous and solid species corresponding to the list of elements covered by Cemdata18 were selected from the GEMS version of the PSI/Nagra TDB [22,23]. The latter and the Cemdata18 GEM database are mutually consistent, and should be used together in GEMS codes for modelling cementitious systems.

To generate PHREEQC-style reactions for product species, firstly the following master species were selected based on their generic predominance: Ca^{+2}, Mg^{+2}, Sr^{+2}, Na^{+}, K^{+}, H^{+}, CO_3^{-2}, SO_4^{-2}, Cl^{-}, NO_3^{-}, AlO_2^{-}, FeO_2^{-}, SiO_2^{0}, H_2O^{0}, and e^{-}(electron). Using selected master species, the reactions were automatically generated for the remaining (product) species, and their properties at 25 °C and 1 bar were calculated. Formation reactions were generated for aqueous product species, and dissolution reactions - for gaseous and solid product species. The LMA dataset of reactions was then exported into a PHREEQC "dat" file (CEMDATA18.dat) using the ThermoMatch database export module. Parameters for the $\log K^{o} = f(T)$ analytical expressions were calculated for the 3-term extrapolation method that assumes the $\Delta_r Cp^{o}$ to be not zero and independent of temperature. These reported parameters are used by PHREEQC for calculating the $\log_{10} K^{o}$ as a function of temperature. Such temperature extrapolations of $\log_{10} K^{o}$ should be valid at least up to 100 °C.

Table B.1 contains the generated formation reactions for the aqueous product species, together with the values for reaction standard effects at 25 °C and 1 bar. Table B.2 contains the generated dissolution reactions for gaseous and solid product species, together with the reaction standard effects at 25 °C and 1 bar. Table B.2 contains, in addition to the Cemdata18 database as detailed in Table 1 to Table 4, also the thermodynamic data of all solids composed of Al, C, Ca, Cl, Fe, H, K, Mg, N, Na, S, Si or Sr compiled in the GEMS version of the PSI/Nagra 12/07 TDB [22,23], needed to allow the generation of a compatible dataset in PHREEQC. Figs. B.1, B.2, and B.3 show comparisons of cement-related modelling problems between GEM-Selektor (using GEM-type Cemdata18) and PHREEQC (using LMA-type Cemdata18 CEMDATA18.dat). For the PHREEQC calculations, PHREEQC for Windows version 2.18.00 (uses PHREEQC-2 source version 2.18.3-5570) was used. In all three cases, the considered solid solutions were modelled in PHREEQC using the simple ideal mixing model.

Table B.1
Product aqueous species reactions from master species, together with their reaction properties at 25 °C and 1 bar.

Product Substance	Reaction	$\log_{10}K^{o}_{298}$	$\Delta_r G^{o}_{298}$ [J/mol]	$\Delta_r H^{o}_{298}$ [J/mol]	$\Delta_r S^{o}_{298}$ [J/K/mol]	$\Delta_r Cp^{o}_{298}$ [J/K/mol]	$\Delta_r V^{o}_{298}$ [J/bar]
Al(SO4)+	S|6|O4–2 + AlO2- + 4H + = Al(SO4)+ + 2H2O@	26.8	−152,857	−159,164	−21.2	261.8	0.8
Al(SO4)2-	2S|6|O4–2 + AlO2- + 4H + = Al(SO4)2- + 2H2O@	28.8	−164,272	−165,197	−3.1	463.6	3.2
Al+3	AlO2- + 4H + = Al+3 + 2H2O@	22.9	−130,595	−176,821	−155.0	71.1	−1.9
AlHSiO3+2	AlO2- + 3H+ + SiO2 = AlHSiO3+2 + H2O	20.5	−116,839	−106,764	33.8	−136	3.3
AlO+	AlO2- + 2H+ = AlO+ + H2O@	12.3	−70,124	−73,951	−12.8	−0.7	0.9
AlO2H@	AlO2- + H + = AlO2H@	6.4	−36,798	−21,554	51.1	−160.2	0.4
AlOH+2	AlO2- + 3H+ = Al(OH) + 2 + H2O@	17.9	−102,299	−127,582	−84.8	180.4	0.6
AlSiO5–3	AlO2- + H2O@ + SiO2@ = AlSiO5–3 + 2H+	−22.6	129,059	71,975	−191.5	0.0	−7.8
Ca(CO3)@	CO3–2 + Ca+2 = CaCO3@	3.2	−18,405	16,462	116.9	196.4	0.9
Ca(HCO3)+	CO3–2 + Ca+2 + H+ = Ca(HCO3)+	11.4	−65,269	−13,562	173.4	554.0	3.8
Ca(HSiO3)+	Ca+2 + H2O@ + SiO2@ = Ca(HSiO3)+ + H+	−8.6	49,143	30,328	−63.1	48.9	−2.2
Ca(SO4)@	Ca+2 + S|6|O4–2 = CaSO4@	2.3	−13,128	4336	58.6	192.4	1.0
CaOH+	Ca+2 + H2O@ = Ca(OH)+ + H+	−12.8	72,950	77,301	14.6	−38.4	0.6
CaSiO3@	Ca+2 + H2O@ + SiO2@ = CaSiO3@ + 2H+	−18.5	105,827	48,743	−191.5	0.0	−1.6
CH4@	CO3–2 + 8e- + 10H+ = C|-4|H4@ + 3H2O@	38.2	−217,923	−270,138	−175.1	677.3	9.8
ClO4-	Cl- + 4H2O@ = Cl|7|O4– + 8e- + 8H+	−187.7	1,071,500	1,181,308	368.3	−87.6	−4.6
CO2@	CO3–2 + 2H + = CO2@ + H2O@	16.7	−95,216	−24,408	237.5	607.8	5.7
Fe(CO3)@	CO3–2 + e- + 4H+ + Fe|3|O2– = FeCO3@ + 2H2O@	39.0	−222,615	−216,144	21.7	537.5	2.5
Fe(HCO3)+	CO3–2 + e- + 5H+ + Fe|3|O2– = FeHCO3+ + 2H2O@	46.9	−267,988	−246,735	71.3	892.0	5.0
Fe(HSO4)+	S|6|O4–2 + e- + 5H+ + Fe|3|O2– = FeHSO4+ + 2H2O@	37.7	−215,125	−208,704	21.5	975.6	4.2
Fe(HSO4)+2	S|6|O4–2 + 5H+ + Fe|3|O2– = Fe|3|HSO4+2 + 2H2O@	26.1	−148,798	−200,163	−172.3	1078.5	2.5
Fe(SO4)@	S|6|O4–2 + e- + 4H+ + Fe|3|O2– = Fe(SO4)@ + 2H2O@	36.9	−210,456	−212,106	−5.5	535.7	2.4
Fe(SO4)+	S|6|O4–2 + 4H+ + Fe|3|O2– = Fe|3|(SO4)+ + 2H2O@	25.6	−146,355	−160,671	−48.0	505.8	2.0
Fe(SO4)2-	2S|6|O4–2 + 4H+ + Fe|3|O2– = Fe|3|(SO4)2- + 2H2O@	27.0	−154,003	−162,930	−29.9	707.5	4.0
Fe+2	e- + 4H+ + Fe|3|O2– = Fe+2 + 2H2O@	34.6	−197,613	−220,183	−75.7	338.8	1.3
Fe+3	4H+ + Fe|3|O2– = Fe|3|+3 + 2H2O@	21.6	−123,295	−177,529	−181.9	308.9	−0.2
FeHSiO3+2	FeO2- + 3H+ + SiO2 = Fe|3|HSiO3+2 + H2O@	21.5	−122,665	−148,472	−86.5	101.9	3.5
FeCl+	Cl- + e- + 4H+ + Fe|3|O2– = FeCl+ + 2H2O@	34.8	−198,413	−218,887	−68.7	580.2	1.9
FeCl+2	Cl- + 4H+ + Fe|3|O2– = Fe|3|Cl+2 + 2H2O@	23.1	−131,742	−173,502	−140.1	523.0	−0.5
FeCl2+	2Cl- + 4H+ + Fe|3|O2– = Fe|3|Cl2+ + 2H2O@	23.7	−135,453	−179,471	−147.6	931.3	1.1
FeCl3@	3Cl- + 4H+ + Fe|3|O2– = Fe|3|Cl3@ + 2H2O@	22.7	−129,649	−190,999	−205.8	1121.3	2.0
FeO+	2H+ + Fe|3|O2– = Fe|3|O+ + H2O@	15.9	−90,930	−97,152	−20.9	109.3	−2.4
FeO2H@	H+ + Fe|3|O2– = Fe|3|O2H@	9.0	−51,601	−37,130	48.5	−77.2	0.7
FeOH+	e- + 3H+ + Fe|3|O2– = FeOH+ + H2O@	25.1	−143,387	−167,718	−81.6	358.9	0.1
FeOH+2	3H+ + Fe|3|O2– = Fe|3|(OH)+2 + H2O@	19.4	−110,794	−134,855	−80.7	276.6	−0.8
Fe2(OH)2+4	2FeO2- + 6H + = Fe|3|2(OH)2+4 + 2H2O@	40.3	−229,747	−298,572	−230.8	617.9	7.5
Fe3(OH)4+5	3FeO2- + 8H + = Fe|3|3(OH)4+5 + 2H2O@	58.5	−333,918	−472,753	−465.6	926.8	7.6

(*continued on next page*)

Table B.1 (*continued*)

Product Substance	Reaction	$\log_{10}K^{o}_{298}$	$\Delta_r G^{o}_{298}$ [J/mol]	$\Delta_r H^{o}_{298}$ [J/mol]	$\Delta_r S^{o}_{298}$ [J/K/mol]	$\Delta_r Cp^{o}_{298}$ [J/K/mol]	$\Delta_r V^{o}_{298}$ [J/bar]
H2@	2e- + 2H+ = H|0|2@	−3.1	17,729	−4018	−72.9	138.0	2.5
H2S@	S|6|O4–2 + 8e- + 10H+ = H2S|-2|@ + 4H2O@	40.7	−232,203	−272,852	−136.3	631.4	9.4
HCN@	CO3–2 + NO3- + 10e- + 13H+ = HC|-1|N|0|@ + 6H2O@	117.4	−669,854	−729,336	−199.5	664.1	8.6
HCO3-	CO3–2 + H+ = HCO3-	10.3	−58,959	−14,699	148.4	254.5	3.0
HS-	S|6|O4–2 + 8e- + 9H+ = HS|-2|- + 4H2O@	33.7	−192,305	−250,044	−193.7	358.3	8.0
HSiO3-	H2O@ + SiO2@ = HSiO3- + H+	−9.8	55,992	29,057	−90.3	−207.0	−3.0
HSO3-	S|6|O4–2 + 2e- + 3H+ = HS|4|O3– + H2O@	3.8	−21,822	−3885	60.2	307.2	3.8
HSO4-	S|6|O4–2 + H+ = HS|6|O4-	2.0	−11,346	20,464	106.7	288.8	2.2
K(SO4)-	S|6|O4–2 + K+ = KSO4-	0.9	−4851	3070	26.6	212.6	0.6
KOH@	H2O@ + K+ = KOH@ + H+	−14.5	82,538	63,874	−62.6	−168.8	−1.2
Mg(CO3)@	CO3–2 + Mg+2 = Mg(CO3)@	3.0	−17,009	9124	87.7	194.5	1.1
Mg(HCO3)+	CO3–2 + Mg + 2 + H + = Mg(HCO3)+	11.4	−65,056	−12,725	175.5	565.4	3.7
Mg(HSiO3)+	Mg+2 + H2O@ + SiO2@ = Mg(HSiO3)+ + H+	−8.3	47,429	25,758	−72.7	60.5	−2.3
MgOH+	Mg+2 + H2O@ = Mg(OH)+ + H+	−11.4	65,300	61,792	−11.8	75.5	0.6
MgSiO3@	Mg+2 + H2O + SiO2 = MgSiO3@ + 2H+	−17.4	99,548	85,125	−48.4	−363.0	1.0
MgSO4@	S|6|O4–2 + Mg + 2 = Mg(SO4)@	2.4	−13,529	6855	68.4	197.4	1.1
N2@	2NO3- + 10e- + 12H + = N|0|2@ + 6H2O@	207.3	−1.183,095	−1.311,876	−431.9	675.7	8.4
Na(CO3)-	CO3–2 + Na+ = NaCO3-	1.3	−7251	−22,969	−52.7	199.9	0.7
Na(HCO3)@	CO3–2 + Na+ + H+ = NaHCO3@	10.1	−57,533	−13,909	146.3	451.5	4.0
Na(SO4)-	S|6|O4–2 + Na + = Na(SO4)-	0.7	−3996	3314	24.5	197.9	0.7
NaOH@	Na+ + H2O@ = NaOH@ + H+	−14.2	80,940	56,026	−83.6	−126.9	−1.3
NH3@	NO3- + 8e- + 9H + = N|-3|H3@ + 3H2O@	109.9	−627,314	−732,284	−352.1	254.4	5.0
NH4+	NO3- + 8e- + 10H + = N|-3|H4+ + 3H2O@	119.1	−680,039	−784,011	−348.7	244.6	4.4
O2@	2H2O@ = O|0|2@ + 4e- + 4H+	−86.0	490,812	559,525	230.5	141.1	−0.6
OH-	H2O@ = OH– + H+	−14.0	79,913	55,872	−80.6	−211.7	−2.3
S-2	S|6|O4–2 + 8e- + 8H + = S|-2|-2 + 4H2O@	14.7	−83,851	−250,044	−557.4	358.3	5.9
S2O3–2	2S|6|O4–2 + 8e- + 10H + = S|2|2O3–2 + 5H2O@	38.0	−216,987	−259,866	−143.8	555.2	9.2
SCN-	CO3–2 + NO3- + S|6|O4–2 + 16e- + 20H + = S|0|C|0|N|-1|- + 10H2O@	156.9	−895,711	−990,513	−318.0	1105.5	18.1
Si4O10–4	2H2O@ + 4SiO2@ = Si4O10–4 + 4H+	−36.3	207,202	207,202	0.0	0.0	−10.0
SiO3–2	H2O@ + SiO2@ = SiO3–2 + 2H+	−23.1	132,084	75,000	−191.5	0.0	−3.4
SO3–2	S|6|O4–2 + 2e- + 2H+ = S|4|O3–2 + H2O@	−3.4	19,390	−13,070	−108.9	31.6	0.1
Sr(CO3)@	CO3–2 + Sr+2 = Sr(CO3)@	2.8	−16,013	18,891	117.1	196.6	0.9
Sr(HCO3)+	CO3–2 + Sr+2 + H + = SrHCO3+	11.5	−65,721	−12,816	177.4	541.0	3.8
Sr(SO4)@	S|6|O4–2 + Sr+2 = Sr(SO4)@	2.3	−13,072	9071	74.3	197.1	1.0
SrOH+	Sr+2 + H2O@ = Sr(OH)+ + H+	−13.3	75,860	82,619	22.7	−65.5	0.7
SrSiO3@	Sr+2 + H2O@ + SiO2@ = SrSiO3@ + 2H+	−18.8	107,136	107,184	0.2	0.1	0.0

e- - represents one electron.
|| - is used for specifying a different valence for the element.
@ - is used to represent a neutral aqueous species.

Table B.2
Product solid and gaseous species reactions from master species, together with their reaction properties at 25 °C and 1 bar.

Product Substance	Reaction	$^{log}10^{\circ}$ 298	$^{A}r^{G}$ 298 [J/mol]	$^{A}r^{H}$ 298 [J/mol]	$^{A}r\$$ 298 [J/K/mol]	$^{A}r^{Cp}$ 298 [J/K/mol]	$^{A}r^{\circ}$ 298 [J/bar]
5CA	(CaO)1.25(SiO2)1(Al2O3)0.125(H2O)1.625 + 2.25H+ = 0.25AlO2- + 1.25Ca+2 + 2.75H2O@ + SiO2@	15.9	-90709	-92987	-7.6	23.7	-1.2
5CNA	(CaO)1.25(SiO2)1(Al2O3)0.125(Na2O)0.25(H2O)1.375 + 2.75H+ = 0.25AlO2- + 1.25Ca+2 + 0.5Na+ + 2.75H2O@ + SiO2@	23.2	-132663	-135750	-10.4	43.6	-2.0
AlOHam	Al(OH)3 = AlO2- + H+ + H2O@	-13.8	78536	69482	-30.4	-66.8	-0.4
AlOHmic	Al(OH)3 = AlO2- + H+ + H2O@	-14.7	83730	53830	-100.3	-66.8	-0.4
Amor-Sl	SiO2 = SiO2@	-2.7	15492	15492	0.0	0.0	-1.3
Anh	CaSO4 = Ca+2 + S|6|O4-2	-4.4	24872	-18165	-144.3	-396.7	-5.1
Arg	CaCO3 = CO3-2 + Ca+2	-8.3	47583	-11060	-196.7	-401.5	-5.9
Brc	Mg(OH)2 + 2H+ = Mg+2 + 2H2O@	16.8	-96124	-114419	-61.4	51.8	-1.1
C12A7	(CaO)12(Al2O3)7 + 10H+ = 14AlO2- + 12Ca+2 + 5H2O@	167.2	-954361	-1489798	-1795.9	-1765.7	-51.6
C2AClH5	Ca2AlCl(OH)6(H2O)2 + 2H+ = AlO2- + 2Ca+2 + Cl- + 6H2O@	14.4	-82445	-92106	-32.4	-195.7	-3.8
C2AH65	Ca2Al(OH)7(H2O)3 + 3H+ = AlO2- + 2Ca+2 + 8H2O@	29.4	-167699	-167567	0.4	-79.0	-2.0
C2AH7.5	Ca2Al2(OH)10(H2O)2.5 + 2H+ = 2AlO2- + 2Ca+2 + 8.5H2O@	14.2	-81085	-89743	-29.0	-55.2	-4.4
C2S	(CaO)2SiO2 + 4H+ = 2Ca+2 + 2H2O@ + SiO2@	38.5	-219567	-237276	-59.4	4.7	-3.6
C3A	(CaO)3Al2O3 + 4H+ = 2AlO2- + 3Ca+2 + 2H2O@	70.7	-403436	-491527	-295.5	-249.5	-8.9
C3AFS0.84H4.32	(AlFe|3|O3)[Ca3O3(SiO2)0.84(H2O)4.32] + 4H+ = AlO2- + 3Ca+2 + 6.32H2O@ + 0.84SiO2@ + Fe|3|O2-	22.3	-127203	-215980	-297.8	-286.9	-6.3
C3AH6	Ca3Al2O6(H2O)6 + 4H+ = 2AlO2- + 3Ca+2 + 8H2O@	35.5	-202666	-230152	-92.2	-33.6	-4.2
C3AS0.41H5.18	Ca3Al2O6(SiO2)0.41(H2O)5.18 + 4H+ = 2AlO2- + 3Ca+2 + 7.18H2O@ + 0.41SiO2@	28.9	-165175	-197973	-110.0	-61.6	-4.6
C3AS0.84H4.32	Ca3Al2O6(SiO2)0.84(H2O)4.32 + 4H+ = 2AlO2- + 3Ca+2 + 6.32H2O@ + 0.84SiO2@	25.8	-147182	-185475	-128.4	-90.9	-5.1
C3FH6	Ca3Fe 13| 2O6(H2O)6 + 4H+ = 3Ca+2 + 8H2O@ + 2Fe|3|O2-	29.7	-169558	-286244	-391.4	-426.6	-6.5
C3FS0.84H4.32	(Fe|3|Fe|3|O3)[Ca3O3(SiO2)0.84(H2O)4.32] + 4H+ = 3Ca+2 + 6.32H2O@ + 0.84SiO2@ + 2Fe|3|O2-	20.0	-114074	-246486	-444.1	-482.9	-7.5
C3FS1.34H3.32	Ca3Fe|3|2O6(SiO2)1.34(H2O)3.32 + 4H+ = 3Ca+2 + 5.32H2O@ + 1.34SiO2@ + 2Fe|3|O2-	16.2	-92409	-233544	-473.4	-516.4	-8.5
C3S	(CaO)3SiO2 + 6H+ = 3Ca+2 + 3H2O@ + SiO2@	73.3	-418180	-444107	-87.0	6.2	-5.8
C4AClH10	Ca4Al2Cl2(OH)12(H2O)4 + 4H+ = 2AlO2- + 4Ca+2 + 2Cl- + 12H2O@	28.9	-164890	-184212	-64.8	-391.5	-7.6
C4AF	(CaO)4(Al2O3)(Fe|3|2O3) + 4H+ = 2AlO2- + 4Ca+2 + 2H2O@ + 2Fe|3|O2-	50.5	-288060	-402597	-384.2	-937.0	-14.8
C4AH11	Ca4Al2(OH)14(H2O)4 + 6H+ = 2AlO2- + 4Ca+2 + 14H2O@	60.5	-345302	-369182	-80.1	-228.6	-5.9
C4AH13	Ca4Al2(OH)14(H2O)6 + 6H+ = 2AlO2- + 4Ca+2 + 16H2O@	58.8	-335407	-335144	0.9	-158.0	-4.0
C4AH19	Ca4Al2(OH)14(H2O)12 + 6H+ = 2AlO2- + 4Ca+2 + 22H2O@	58.6	-334271	-294930	132.0	53.7	-2.6
C4AsClH12	Ca4Al2Cl(SO4)0.5(OH)12(H2O)6 + 4H+ = 2AlO2- + 4Ca+2 + Cl- + 0.5S|6|O4-2 + 14H2O@	27.6	-157430	-175702	-61.3	-351.3	-6.7
C4FH13	Ca4Fe|3|2(OH)14(H2O)6 + 6H+ = 4Ca+2 + 16H2O@ + 2Fe|3|O2-	53.3	-304002	-199193	351.5	-343.7	-7.0
CA	CaOAl2O3 = 2AlO2- + Ca+2	-0.3	1756	-67154	-231.1	-254.7	-5.3
CA2	CaO(Al2O3)2 + H2O@ = 4AlO2- + Ca+2 + 2H+	-30.1	171600	44867	-425.1	-502.0	-8.8
CAH10	CaOAl2O3(H2O)10 = 2AlO2- + Ca+2 + 10H2O@	-7.6	43348	35098	-27.7	-43.2	-1.3
Cal	CaCO3 = CO3-2 + Ca+2	-8.5	48404	-10975	-199.2	-402.1	-6.1
CH4	C|-4|H4 + 3H2O@ = CO3-2 + 10H+ + 8e-	-41.0	234277	257142	76.7	-435.8	-
Cls	SrSO4 = S|6|O4-2 + Sr+2	-6.6	37855	-854	-129.8	-415.5	-5.1

(*continued on next page*)

Table B.2 (*continued*)

Product Substance	Reaction	$^{log}10^{\circ}$ 298	$^{A}r^{G}$ 298 [J/mol]	$^{A}r^{H}$ 298 [J/mol]	$^{A}r\$$ 298 [J/K/mol]	$^{A}r^{Cp}$ 298 [J/K/mol]	$^{A}r^{\circ}$ 298 [J/bar]
CO2	CO2 + H2O@ = CO3-2 + 2H+	-18.1	103560	4079	-333.7	-401.8	-
CSH3T-T2C	((CaO)0.75(SiO2)0.5(H2O)1.25)2 + 3H+ = 1.5Ca+2 + 4H2O@ + SiO2@	25.3	-144257	-123574	69.4	62.5	-2.0
CSH3T-T5C	((CaO)1(SiO2)1(H2O)2)1.25 + 2.5H+ = 1.25Ca+2 + 3.75H2O@ + 1.25SiO2@	18.1	-103538	-78676	83.4	65.4	-1.4
CSH3T-TobH	(CaO)1(SiO2)1.5(H2O)2.5 + 2H+ = Ca+2 + 3.5H2O@ + 1.5SiO2@	12.5	-71524	-42463	97.5	68.4	-1.6
CSHQ-JenD	(CaO)1.5(SiO2)0.6667(H2O)2.5 + 3H+ = 1.5Ca+2 + 4H2O@ + 0.6667SiO2@	28.7	-164004	-149357	49.1	51.9	-2.6
CSHQ-JenH	(CaO)1.3333(SiO2)1(H2O)2.1667 + 2.6666H+ = 1.3333Ca+2 + 3.5H2O@ + SiO2@	22.2	-126609	-106258	68.3	59.1	-2.1
CSHQ-TobD	((CaO)1.25(SiO2)1(H2O)2.75)0.6667 + 1.66675H+ = 0.833375Ca+2 + 2.6668H2O@ + 0.6667SiO2@	13.7	-77952	-64488	45.2	37.9	-0.4
CSHQ-TobH	(CaO)0.6667(SiO2)1(H2O)1.5 + 1.3334H+ = 0.6667Ca+2 + 2.1667H2O@ + SiO2@	8.3	-47306	-27842	65.3	45.5	-1.2
Dis-Dol	CaMg(CO3)2 = 2CO3-2 + Ca+2 + Mg+2	-16.5	94412	-43108	-461.2	-789.0	-11.7
ECSH1-KSH	((KOH)2.5SiO2H2O)0.2 + 0.5H+ = 0.7H2O@ + 0.2SiO2@ + 0.5K+	5.5	-31394	-13703	59.3	25.2	0.8
ECSH1-NaSH	((NaOH)2.5SiO2H2O)0.2 + 0.5H+ = 0.5Na+ + 0.7H2O@ + 0.2SiO2@	5.4	-30883	-17398	45.2	42.8	0.5
ECSH1-SH	(SiO2H2O)1 = H2O@ + SiO2@	-2.6	14839	14839	0.0	0.0	0.0
ECSH1-SrSH	((Sr(OH)2)1SiO2H2O)1 + 2H+ = Sr+2 + 3H2O@ + SiO2@	15.4	-87911	-64744	77.7	54.2	-1.1
ECSH1-TobCa	((Ca(OH)2)0.8333SiO2H2O)1 + 1.6666H+ = 0.8333Ca+2 + 2.6666H2O@ + SiO2@	11.0	-62909	-43194	66.1	49.3	-1.9
ECSH2-JenCa	((Ca(OH)2)1.6667SiO2H2O)0.6 + 2.00004H+ = 1.00002Ca+2 + 2.60004H2O@ + 0.6SiO2@	17.6	-100489	-77495	77.1	77.2	0.2
ECSH2-KSH	((KOH)2.5SiO2H2O)0.2 + 0.5H+ = 0.7H2O@ + 0.2SiO2@ + 0.5K+	6.0	-34250	-16559	59.3	25.2	0.8
ECSH2-NaSH	((NaOH)2.5SiO2H2O)0.2 + 0.5H+ = 0.5Na+ + 0.7H2O@ + 0.2SiO2@	5.9	-33732	-20247	45.2	42.8	0.5
ECSH2-SrSH	((Sr(OH)2)1SiO2H2O)1 + 2H+ = Sr+2 + 3H2O@ + SiO2@	16.2	-92473	-69306	77.7	54.2	-1.1
ECSH2-TobCa	((Ca(OH)2)0.8333SiO2H2O)1 + 1.6666H+ = 0.8333Ca+2 + 2.6666H2O@ + SiO2@	11.0	-62909	-43194	66.1	49.3	-1.9
ettringite	((H2O)2)Ca6Al2(SO4)3(OH)12(H2O)24 + 4H+ = 2AlO2- + 6Ca+2 + 3S|6|O4-2 + 34H2O@	11.2	-63708	-23594	134.5	-694.0	-14.6
ettringite03_ss	(SO4)Ca2Al0.6666667(OH)4(H2O)8.6666667 + 1.3333332H+ = 0.6666667AlO2- + 2Ca+2 + S|6|O4-2 + 11. 3333333H2O@	3.7	-21231	-7860	44.8	-231.3	-4.9
ettringite05	Ca3Al(SO4)1.5(OH)6(H2O)13 + 2H+ = AlO2- + 3Ca+2 + 1.5S|6|O4-2 + 17H2O@	5.6	-31852	-11795	67.3	-347.0	-7.3
ettringite13	Ca6Al2(SO4)3(OH)12(H2O)7 + 4H+ = 2AlO2- + 6Ca+2 + 3S|6|O4-2 + 15H2O@	39.0	-222527	-596572	-1254.6	-1364.4	-19.3
Ettringite13_des	Ca6Al2(SO4)3(OH)12(H2O)7 + 4H+ = 2AlO2- + 6Ca+2 + 3S|6|O4-2 + 15H2O@	39.0	-222527	-596572	-1254.6	-1364.4	-19.3
ettringite30	Ca6Al2(SO4)3(OH)12(H2O)24 + 4H+ = 2AlO2- + 6Ca+2 + 3S|6|O4-2 + 32H2O@	11.8	-67136	-36633	102.3	-764.6	-18.3
ettringite9	Ca6Al2(SO4)3(OH)12(H2O)3 + 4H+ = 2AlO2- + 6Ca+2 + 3S|6|O4-2 + 11H2O@	48.0	-273943	-339631	-220.3	-1505.6	-21.5
Ettringite9_des	Ca6Al2(SO4)3(OH)12(H2O)3 + 4H+ = 2AlO2- + 6Ca+2 + 3S|6|O4-2 + 11H2O@	48.0	-273943	-339631	-220.3	-1505.6	-21.5
Fe	Fe|0| + 2H2O@ = 4H+ + 3e- + Fe|3|O2-	-18.6	106109	127947	73.2	-367.4	-4.3
Fe-ettringite	Ca6Fe|3|2(SO4)3(OH)12(H2O)26 + 4H+ = 6Ca+2 + 3S|6|O4-2 + 34H2O@ + 2Fe|3|O2-	12.1	-68843	4803	247.0	-1091.4	-17.4
Fe-ettringite05	Ca3Fe|3|(SO4)1.5(OH)6(H2O)13 + 2H+ =3Ca+2 + 1.5S|6|O4-2 + 17H2O@ + Fe|3|O2-	6.0	-34420	2403	123.5	-545.7	-8.7
Fe-hemicarbonate	Ca3O3Fe|3|2O3(CaCO3)0.5(CaO2H2)0.5(H2O)9.5 + 5H+ = 0.5CO3-2 + 4Ca+2 + 12.5H2O@ + 2Fe|3|O2-	39.2	-223627	-390054	-558.2	-637.4	-12.3
Femonocarbonate	Ca4O4Fe|3|2O3CO2(H2O)12 + 4H+ = CO3-2 + 4Ca+2 + 14H2O@ + 2Fe|3|O2-	21.4	-122258	-252941	-438.3	-778.2	-11.8
Fe-monosulph05	Ca2Fe|3|S0.5O5(H2O)6 + 2H+ = 2Ca+2 + 0.5S|6|O4-2 + 7H2O@ + Fe|3|O2-	12.2	-69792	-154688	-284.7	-386.3	-6.4
Fe-monosulphate	Ca4Fe|3|2SO10(H2O)12 + 4H+ = 4Ca+2 + S|6|O4-2 + 14H2O@ + 2Fe|3|O2-	24.5	-139576	-309368	-569.5	-772.7	-12.8
FeOOHmic	Fe|3|OOH = H+ + Fe|3|O2-	-19.6	111875	65468	-155.7	-309.3	-3.4
Gbs	Al(OH)3 = AlO2- + H+ + H2O@	-15.1	86323	77269	-30.4	-66.8	-0.4

(*continued on next page*)

Table B.2 (*continued*)

Product Substance	Reaction	$^{log}10^{\circ}$ 298	$^{A}r^{G}$ 298 [J/mol]	$^{A}r^{H}$ 298 [J/mol]	$^{A}r\$$ 298 [J/K/mol]	$^{A}r^{Cp}$ 298 [J/K/mol]	$^{A}r^{\circ}$ 298 [J/bar]
Gp	CaSO4(H2O)2 = Ca+2 + S|6|O4-2 + 2H2O@	-4.6	26147	-1167	-91.6	-332.5	-4.4
Gr	C|0| + 3H2O@ = CO3-2 + 6H+ + 4e-	-32.2	183569	182332	-4.1	-466.4	-6.6
Gt	Fe|3|O(OH) = H+ + Fe|3|O2-	-22.6	128995	124419	-15.4	-309.2	-2.0
H2	H|0|2 = 2H+ + 2e-	0.0	0	0	0.0	0.0	-
H2O	H2O = H2O@	1.5	-8500	-43481	-117.3	35.3	-
H2S	H2S|-2| + 4H2O@ = S|6|O4-2 + 10H+ + 8e-	-41.7	237742	254458	56.1	-486.4	-
Hem	Fe|3|2O3 + H2O@ = 2H+ + 2Fe|3|O2-	-42.1	240195	219672	-68.8	-650.0	-4.7
hemicarbonat10.5	(CaO)3Al2O3(CaCO3)0.5(CaO2H2)0.5(H2O)10 + 5H+ = 2AlO2- + 0.5CO3-2 + 4Ca+2 + 13H2O@	42.6	-243220	-264276	-70.6	-232.4	-8.4
hemicarbonate	(CaO)3Al2O3(CaCO3)0.5(CaO2H2)0.5(H2O)11.5 + 5H+ = 2AlO2- + 0.5CO3-2 + 4Ca+2 + 14.5H2O@	40.9	-233337	-236348	-10.1	-179.5	-8.0
hemicarbonate9	(CaO)3Al2O3(CaCO3)0.5(CaO2H2)0.5(H2O)8.5 + 5H+ = 2AlO2- + 0.5CO3-2 + 4Ca+2 + 11.5H2O@	45.6	-260338	-299005	-129.7	-285.4	-9.9
hemihydrate	CaSO4(H2O)0.5 = Ca+2 + S|6|O4-2 + 0.5H2O@	-3.6	20413	-20432	-137.0	-383.4	-5.8
hydrotalcite	Mg4Al2O7(H2O)10 + 6H+ = 2AlO2- + 4Mg+2 + 13H2O@	28.0	-159755	-235072	-252.6	146.4	-5.4
INFCA	(CaO)1(SiO2)1.1875(Al2O3)0.15625(H2O)1.65625 + 1.6875H+ = 0.3125AlO2- + Ca+2 + 2.5H2O@ + 1.1875SiO2@	9.0	-51116	-50080	3.5	14.1	-1.1
INFCN	(CaO)1(SiO2)1.5(Na2O)0.3125(H2O)1.1875 + 2.625H+ = Ca+2 + 0.625Na+ + 2.5H2O@ + 1.5SiO2@	18.8	-107089	-97770	31.3	64.3	-2.1
INFCNA	(CaO)1.25(SiO2)1(Al2O3)0.125(Na2O)0.25(H2O)1.375 + 2.75H+ = 0.25AlO2- + 1.25Ca+2 + 0.5Na+ + 2.75H2O@ + SiO2@	23.2	-132663	-135750	-10.4	43.6	-2.0
Jennite	(SiO2)1(CaO)1.666667(H2O)2.1 + 3.333334H+ = 1.666667Ca+2 + 3.766667H2O@ + SiO2@	29.3	-167347	-146306	70.6	66.0	-2.5
K2O	K2O + 2H+ = H2O@ + 2K+	84.1	-480020	-426988	177.9	8.0	-0.4
K2SO4	K2SO4 = S|6|O4-2 + 2K+	-1.8	10214	23725	45.3	-379.3	-3.5
Kln	Al2Si2O5(OH)4 = 2AlO2- + 2H+ + H2O@ + 2SiO2@	-38.3	218758	185703	-110.9	-173.4	-3.0
*KSiOH	((KOH)2.5SiO2H2O)0.2 + 0.5H+ = 0.7H2O@ + 0.2SiO2@ + 0.5K+	5.8	-32604	-13463	65.3	20.7	0.8
Lim	CaO + 2H+ = Ca+2 + H2O@	32.6	-186017	-193861	-26.3	1.6	-1.7
M4A-OH-LDH	Mg4Al2(OH)14(H2O)3 + 6H+ = 2AlO2- + 4Mg+2 + 13H2O@	34.3	-195826	-271137	-252.6	147.4	-5.3
M6A-OH-LDH	Mg6Al2(OH)18(H2O)3 + 10H+ = 2AlO2- + 6Mg+2 + 17H2O@	68.0	-388083	-499991	-375.3	250.0	-11.1
M8A-OH-LDH	Mg8Al2(OH)22(H2O)3 + 14H+ = 2AlO2- + 8Mg+2 + 21H2O@	101.7	-580340	-728838	-498.1	353.5	-17.0
Mag	FeFe|3|2O4 + 2H2O@ = 4H+ + e- + 3Fe|3|O2-	-67.8	387007	361013	-87.2	-992.8	-7.9
Melanterite	FeSO4(H2O)7 = S|6|O4-2 + 4H+ + e- + 5H2O@ + Fe|3|O2-	-36.8	210222	230774	68.9	-109.8	-4.3
Mg2AlC0.5OH	Mg2Al(OH)6(CO3)0.5(H2O)2 + 2H+ = AlO2- + 0.5CO3-2 + 2Mg+2 + 6H2O@	5.9	-33755	-100890	-225.2	-182.5	-4.0
Mg2FeC0.5OH	Mg2Fe|3|(OH)6(CO3)0.5(H2O)2 + 2H+ = 0.5CO3-2 + 2Mg+2 + 6H2O@ + Fe|3|O2-	5.8	-33224	-81424	-161.7	-377.1	-5.6
Mg3AlC0.5OH	Mg3Al(OH)8(CO3)0.5(H2O)2.5 + 4H+ = AlO2- + 0.5CO3-2 + 3Mg+2 + 8.5H2O@	22.7	-129680	-215112	-286.5	-130.7	-2.1
Mg3FeC0.5OH	Mg3Fe|3|(OH)8(CO3)0.5(H2O)2.5 + 4H+ = 0.5CO3-2 + 3Mg+2 + 8.5H2O@ + Fe|3|O2-	22.4	-127660	-194156	-223.0	-325.3	-3.4
Mgs	MgCO3 = CO3-2 + Mg+2	-8.3	47310	-28349	-253.8	-386.8	-5.6
monocarbonate	Ca4Al2CO9(H2O)11 + 4H+ = 2AlO2- + CO3-2 + 4Ca+2 + 13H2O@	24.5	-140067	-165182	-84.2	-412.8	-8.8
monocarbonate05	Ca2AlC0.5O4.5(H2O)5.5 + 2H+ = AlO2- + 0.5CO3-2 + 2Ca+2 + 6.5H2O@	12.3	-70033	-82591	-42.1	-206.4	-4.4
monocarbonate9	Ca4Al2CO9(H2O)9 + 4H+ = 2AlO2- + CO3-2 + 4Ca+2 + 11H2O@	28.5	-162891	-224860	-207.8	-483.4	-9.6
mononitrate	Ca4Al2(OH)12N|5|2O6(H2O)4 + 4H+ = 2AlO2- + 4Ca+2 + 2NO3- + 12H2O@	27.3	-156023	-148389	25.6	-356.1	-7.7
mononitrite	Ca4Al2(OH)12N|3|2O4(H2O)4 = 2AlO2- + 4Ca+2 + 2NO3- + 4e- + 10H2O@	-25.7	146749	197173	169.1	-420.1	-9.2

(*continued on next page*)

Table B.2 (*continued*)

Product Substance	Reaction	$^{log}10^{\circ}$ 298	$^{A}r^{G}$ 298 [J/mol]	$^{A}r^{H}$ 298 [J/mol]	$^{A}r\$$ 298 [J/K/mol]	$^{A}r^{Cp}$ 298 [J/K/mol]	$^{A}r^{\circ}$ 298 [J/bar]
monosulphate10.5	Ca4Al2SO10(H2O)10.5 + 4H+ = 2AlO2- + 4Ca+2 + S|6|O4-2 + 12.5H2O@	28.1	-160590	-194728	-114.5	-434.2	-9.8
monosulphate12	Ca4Al2SO10(H2O)12 + 4H+ = 2AlO2- + 4Ca+2 + S|6|O4-2 + 14H2O@	26.8	-152912	-176816	-80.2	-381.2	-7.1
monosulphate1205	Ca2AlS0.5O5(H2O)6 + 2H+ = AlO2- + 2Ca+2 + 0.5S|6|O4-2 + 7H2O@	13.4	-76454	-88406	-40.1	-190.6	-6.0
monosulphate14	Ca4Al2SO10(H2O)14 + 4H+ = 2AlO2- + 4Ca+2 + S|6|O4-2 + 16H2O@	26.8	-152768	-185449	-109.6	-310.6	-8.4
monosulphate16	Ca4Al2SO10(H2O)16 + 4H+ = 2AlO2- + 4Ca+2 + S|6|O4-2 + 18H2O@	26.9	-153259	-148473	16.1	-246.2	-6.7
monosulphate9	Ca4Al2SO10(H2O)9 + 4H+ = 2AlO2- + 4Ca+2 + S|6|O4-2 + 11H2O@	30.2	-172114	-232353	-202.0	-487.1	-11.8
N2	N|0|2 + 6H2O@ = 2NO3- + 12H+ + 10e-	-210.5	1201289	1301508	336.1	-470.7	-
Na2O	Na2O + 2H+ = 2Na+ + H2O@	67.4	-384943	-351639	111.7	82.7	-0.9
Na2SO4	Na2SO4 = S|6|O4-2 + 2Na+	-0.3	1703	-2457	-14.0	-254.9	-4.3
*NaSiOH	((NaOH)2.5SiO2H2O)0.2 + 0.5H+ = 0.5Na+ + 0.7H2O@ + 0.2SiO2@	5.7	-32021	-19201	43.7	34.7	0.5
O2	O|0|2 + 4H+ + 4e- = 2H2O@	83.1	-474371	-571762	-326.7	63.7	-
Ord-Dol	CaMg(CO3)2 = 2CO3-2 + Ca+2 + Mg+2	-17.1	97552	-36538	-449.7	-789.0	-11.7
Portlandite	Ca(OH)2 + 2H+ = Ca+2 + 2H2O@	22.8	-130145	-130156	0.0	32.3	-1.5
Py	FeS|0|S|-2| + 10H2O@ = 2S|6|O4-2 + 20H+ + 15e- + Fe|3|O2-	-120.5	687822	780233	309.9	-1366.5	-17.8
Qtz	SiO2 = SiO2@	-3.7	21386	21386	0.0	0.0	-0.7
Sd	FeCO3 + 2H2O@ = CO3-2 + 4H+ + e- + Fe|3|O2-	-45.5	259775	204566	-185.2	-742.7	-7.1
Str	SrCO3 = CO3-2 + Sr+2	-9.3	52918	-324	-178.6	-413.3	-6.3
straetlingite	Ca2Al2SiO7(H2O)8 + 2H+ = 2AlO2- + 2Ca+2 + 9H2O@ + SiO2@	4.1	-23479	-38065	-48.9	-39.9	-5.5
straetlingite5.5	Ca2Al2SiO7(H2O)5.5 + 2H+ = 2AlO2- + 2Ca+2 + 6.5H2O@ + SiO2@	7.1	-40503	-79963	-132.3	-128.1	-9.7
straetlingite7	Ca2Al2SiO7(H2O)7 + 2H+ = 2AlO2- + 2Ca+2 + 8H2O@ + SiO2@	4.8	-27477	-45434	-60.2	-75.2	-7.3
Sulfur	S|0| + 4H2O@ = S|6|O4-2 + 8H+ + 6e-	-35.8	204198	233827	99.4	-503.8	-7.5
syngenite	K2Ca(SO4)2H2O = Ca+2 + 2S|6|O4-2 + H2O@ + 2K+	-7.2	41078	19412	-72.7	-743.9	-8.4
T2C-CNASHss	(CaO)1.5(SiO2)1(H2O)2.5 + 3H+ = 1.5Ca+2 + 4H2O@ + SiO2@	25.6	-145938	-125275	69.3	62.5	-2.0
T5C-CNASHss	(CaO)1.25(SiO2)1.25(H2O)2.5 + 2.5H+ = 1.25Ca+2 + 3.75H2O@ + 1.25SiO2@	18.4	-105297	-80438	83.4	65.4	-1.5
thaumasite	(CaSiO3)(CaSO4)(CaCO3)(H2O)15 + 2H+ = CO3-2 + 3Ca+2 + S|6|O4-2 + 16H2O@ + SiO2@	-0.9	5236	23833	62.4	-468.7	-7.3
TobH-CNASHss	(CaO)1(SiO2)1.5(H2O)2.5 + 2H+ = Ca+2 + 3.5H2O@ + 1.5SiO2@	12.8	-73056	-44000	97.5	68.3	-1.6
Tob-I	(SiO2)2.4(CaO)2(H2O)3.2 + 4H+ = 2Ca+2 + 5.2H2O@ + 2.4SiO2@	26.7	-152677	-105616	157.8	119.1	-4.5
Tob-II	(SiO2)1(CaO)0.833333(H2O)1.333333 + 1.666666H+ = 0.833333Ca+2 + 2.166666H2O@ + SiO2@	11.1	-63617	-44009	65.8	49.6	-1.9
tricarboalu03	(CO3)Ca2Al0.6666667(OH)4(H2O)8.6666667 + 1.3333332H+ = 0.6666667AlO2- + CO3-2 + 2Ca+2 + 11.3333333H2O@	3.2	-18115	-21090	-10.0	-236.8	-4.9
Tro	Fe|2|S|-2| + 6H2O@ = S|6|O4-2 + 12H+ + 9e- + Fe|3|O2-	-73.6	420228	471331	171.4	-873.9	-11.3

* - reaction properties at 20 °C 1 bar.
e- - represents one electron.
|| - is used for specifying a different valence for the element.
@ - is used to represent a neutral aqueous species.
Standard molar volumes for ideal gases are not listed because they are all equal to 2479 J/bar at 1 bar, 298.15 K.

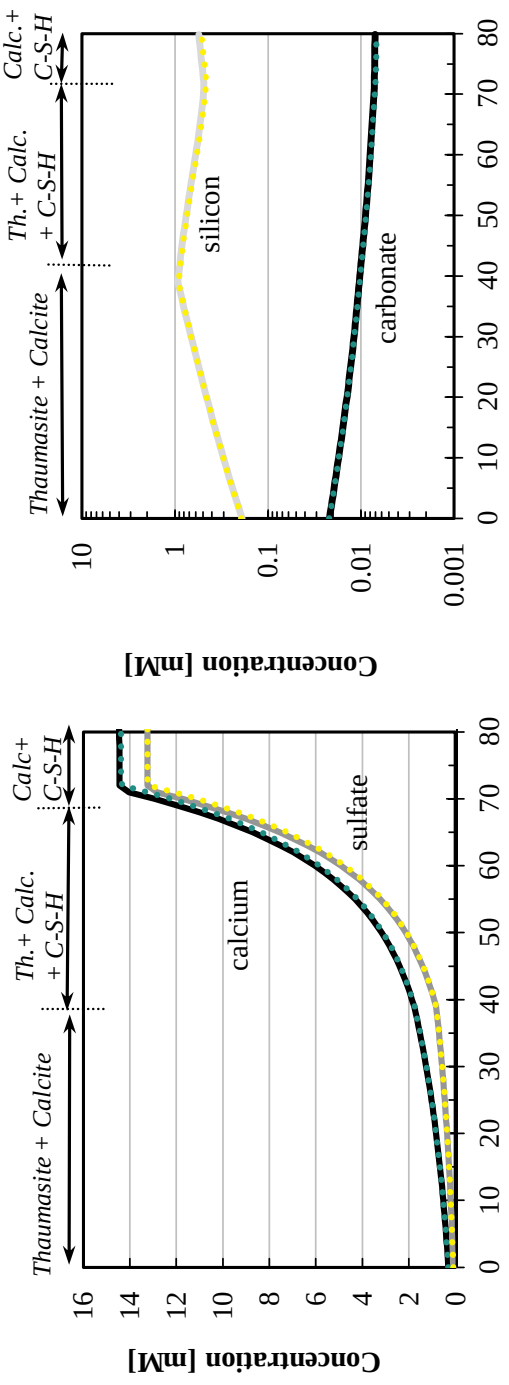

Fig. B.1. Calculated (curves) solubility data for thaumasite, based on the new thermodynamic data for thaumasite complemented with the CSHQ data from Cemdata18 [1,7] in GEM format; Calculated (dotted lines) solubility data for thaumasite, based on data Cemdata18 [1,7] in PHREEQC format.

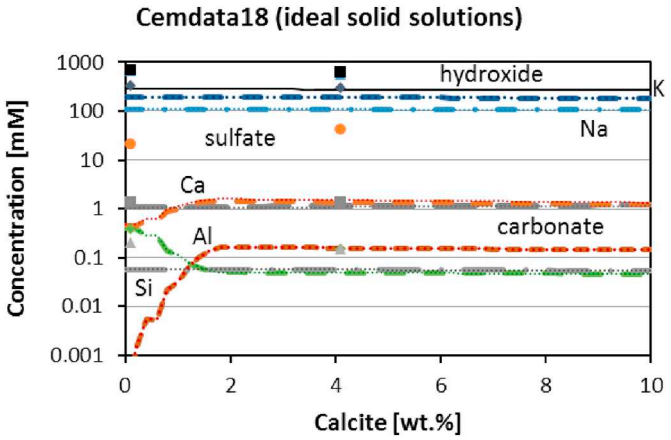

Fig. B.2. Effect of the amount of limestone on the phase assemblage and the distribution of aluminium and iron in hydrated Portland cement calculated using Cemdata18 GEM format (dashed lines) and Cemdata18 PHREEQC format (dotted lines), in both cases using ideal solid solutions.

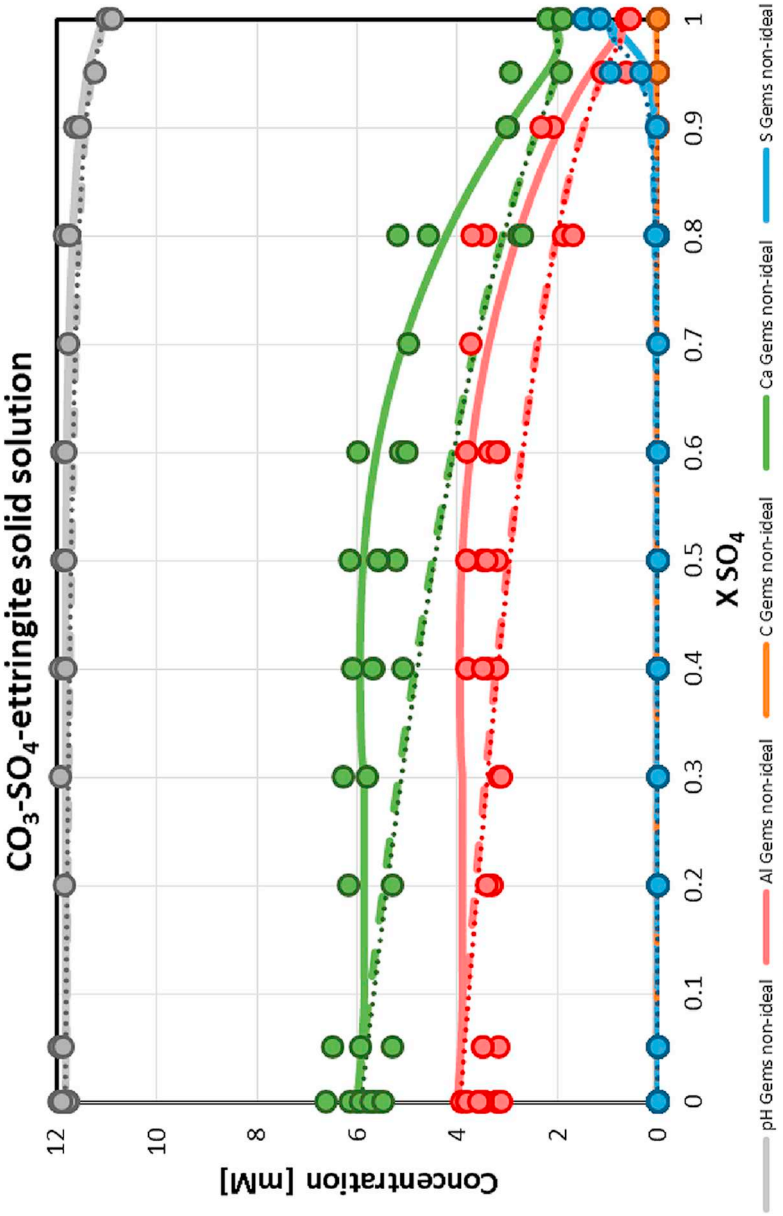

Fig. B.3. Calculated aqueous composition in equilibrium with CO_3-SO_4-ettringite solid solution as a function of SO_4 in the solid. Solid lines calculated using the Cemdata18 GEM format using non ideal solid solution; Dashed lines calculated using the Cemdata18 GEM format using ideal solid solution; Dotted lines calculated using the Cemdata18 PHREEQC format using ideal solid solution; Circles: experimental data [7,129].

Appendix C. Thermodynamic equations and assumptions

The solubility products compiled in Cemdata18 have generally been derived from solutions composition measured at different temperatures, as documented in detail in [1,7–10,12,27,28,30,31,34–37,39–41]. The activity of a species i, a_i, has been calculated with GEMS from the measured concentrations considering the formation of aqueous complexes. By definition $a_i = \gamma_i * m_i$, where γ_i is the activity coefficient and m_i the concentration in mol/kg H_2O. Activity coefficients of aqueous species γ_i were computed using the built-in extended Debye-Hückel equation with the common ion-size parameter a_i of 3.67 Å for KOH and 3.31 Å for NaOH solutions and the common third parameter b_y according to the Eq. (C.1):

$$\log \gamma_i = \frac{-A_y z_i^2 \sqrt{I}}{1 + B_y a_i \sqrt{I}} + b_y I \tag{C.1}$$

where z_i denotes the charge of species i, I is the effective molal ionic strength, b_y is a semi-empirical parameter (~0.123 for KOH and ~0.098 for NaOH electrolyte at 25 °C), and A_y and B_y are P,T-dependent coefficients. For uncharged species, Eq. (C.1) reduces to $\log\gamma_i = b_y I$. This extended Debye-Hückel activity correction is applicable up to approx. 1 m ionic strength [130].

From the solubility products K of solids calculated at different temperatures T, the Gibbs free energy of reaction, $\Delta_r G^\circ$, the Gibbs free energy of formation, $\Delta_f G^\circ$, and the absolute entropy, S°, at T_0 = 298.15 K were obtained according to Eqs. (C.2) and (C.3):

$$\Delta_r G^{o^\circ} = \sum_i \nu_i \Delta_f G^\circ = -RT \ln K \tag{C.2}$$

$$\Delta_a G_T^o = \Delta_f G_{T_0}^o - S_{T_0}^o (T - T_0) + \int_{T_0}^{T} C_p^0 dT - \int_{T_0}^{T} \frac{C_p^o}{T} dT \tag{C.3}$$

Using $C^\circ_p = a_0 + a_1 T + a_2 T^{-2} + a_3 T^{0.5}$ [131], where a_{0-3} are the empirical parameters defined for each mineral, the two integral terms of Eq. (C.3) can be solved to give Eq. (C.4):

$$\Delta_a G_T^o = \Delta_f G_{T_0}^o - S_{T_0}^o (T - T_0) - a_0 \left(T \ln \frac{T}{T_0} - T + T_0 \right) - 0.5 a_1 (T - T_0)^2 - a_2 \frac{(T - T_0)^2}{2T \cdot T_0^2} - a_3 \frac{2(\sqrt{T} - \sqrt{T_0})^2}{\sqrt{T_0}} \tag{C.4}$$

where ν_i are the stoichiometric reaction coefficients, R = 8.31451 J/mol/K, T is the temperature in K, and C°_p is the heat capacity at constant pressure. The apparent Gibbs free energy of formation, $\Delta_a G^\circ_T$, refers to standard Gibbs energies of elements at 298.15 K. A more detailed description of the derivation of the dependence of the Gibbs free energy on temperature is available in [131,132].

Dependence of the solubility product on temperature, consistent to Eq. (C.4) can be expressed as:

$$\log K_T = A_0 + A_1 T + \frac{A_2}{T} + A_3 \ln T + \frac{A_4}{T^2} + A_5 T^2 + A_6 \sqrt{T} \tag{C.5}$$

[131], where A_0, … A_6 are empirical coefficients. If the entropy (S°), the enthalpy ($\Delta_f H^\circ$), and the coefficients (a_0, a_1, …) of the heat capacity equation ($C^\circ_p = a_0 + a_1 T + a_2 T^{-2} + a_3 T^{-0.5} + a_4 T^2$) of the species are available, the coefficients A_0, … A_6 can be calculated directly (see [131]). These calculations involving Eqs. (C.4) and (C.5) are all implemented in the GEM-Selektor.

The heat capacity function, C_p = f(T) is usually obtained from calorimetry experiments. In many cases, the heat capacity has to be estimated by using a reference reaction with a solid having a known heat capacity and similar structure, as described in publications [1,7–10,12,27,28,30,31,34–37,39–41]. Helgeson et al. [43] applied this principle successfully to estimate heat capacities of silicate minerals by formulating reactions involving structurally-related minerals with known heat capacity functions. This method has limitations due to the differing thermodynamic properties of "water" varieties, bound loosely as a hydration water, or structurally as OH-groups. To minimize errors associated with the varying strengths of bonding for "water", reference reactions had been formulated to involve no "free" water as a substituent in reactions, wherever appropriate.

The value of $\Delta_r C_p{}^0$ has little influence on the calculated log K value in the temperature range 0–100 °C and is thus often assumed to be constant in a narrow temperature range: $\Delta_r Cp^0_T = \Delta_r Cp^0_{T0} = \Delta a_o$. This simplifies Eq. (C.5) to the so called 3-term approximation of the temperature dependence, see Eq. (C.6), which can be used to compute the standard thermodynamic properties of each solid [132] to obtain a temperature-dependent "log K" function using Eqs. (C.6)-(C.12) (implemented in GEMS).

$$\log K_T = A_0 + A_2 T^{-1} + A_3 \ln T \tag{C.6}$$

and

$$A_0 = \frac{0.4343}{R} \cdot [\Delta_r S^0_{T_0} - \Delta_r Cp^0_{T_0} (1 + \ln T_0)] \tag{C.7}$$

$$A_2 = \frac{0.4343}{R} \cdot (\Delta_r H^0_{T_0} - \Delta_r Cp^0_{T_0} T_0) \tag{C.8}$$

$$A_3 = \frac{0.4343}{R} \cdot \Delta_r Cp^0_{T_0} \tag{C.9}$$

$$\Delta_r S^0_T = \Delta_r S^0_{T_0} + \Delta_r Cp^0_{T_0} \ln \frac{T}{T_0} \tag{C.10}$$

$$\Delta_r H^0_T = \Delta_r H^0_{T_0} + \Delta_r Cp^0_{T_0} (T - T_0) \tag{C.11}$$

$$\Delta_r G^0_T = \Delta_r H^0_T + T \Delta_r S^0_T \tag{C.12}$$

Within the relatively narrow temperature range of 0 to 100°C, where the Cemdata18 database is valid, this simplification has a negligible influence on the resulting solubility products, also for non-isoelectric reactions as exemplified for ettringite in [20].

Appendix D. Thermodynamic data for aqueous and gaseous species

The thermodynamic data for aqueous and gaseous species compatible with Cemdata18 are summarised in Tables D.1 and D.2.

Table D.1
Standard (partial molal) thermodynamic properties and equation of state parameters of aqueous species at 25 °C, 1 bar used in GEM calculations, as detailed in the GEMS version of the PSI/Nagra 12/07 TDB [22,23]. Numbers referring to the charge of aqueous species are written after the plus or minus signs to avoid any ambiguity; "@" is used to represent a neutral aqueous species.

Species	ΔG^0	ΔH^0	S^0	Cp^0	V^0	$a_1 \cdot 10^*$	$a_2 \cdot 10^{-2*}$	a_3^*	$a_4 \cdot 10^{-4*}$	c_1^*	$c_2 \cdot 10^{-4*}$	$\omega_0 \cdot 10^{-5*}$
	(kJ/mol)	(kJ/mol)	(J/mol·K)	(J/mol·K)	(J/bar)	(cal/mol/bar)	(cal/mol)	(cal·K/mol/bar)	(cal·K/mol)	(cal/mol/K)	(cal·K/mol)	(cal/mol)
$Al(SO_4)^+$	−1250.43	−1422.67	−172.38	−204.01	−6.02	1.3869	−4.3920	7.4693	−2.5974	−11.6742	−12.9914	1.1729
$Al(SO_4)^{2-}$	−2006.30	−2338.40	−135.50	−268.37	31.11	6.8275	8.8925	2.2479	−3.1466	−12.0220	−16.1447	2.1199
Al^{+3}	−483.71	−530.63	−325.10	−128.70	−45.24	−3.3802	−17.0071	14.5185	−2.0758	10.7000	−8.0600	2.7530
AlO^+	−660.42	−713.64	−112.97	−125.11	0.31	2.1705	−2.4811	6.7241	−2.6763	−2.5983	−9.1455	0.9570
AlO_2^-	−827.48	−925.57	−30.21	−49.04	9.47	3.7221	3.9954	−1.5879	−2.9441	15.2391	−5.4585	1.7418
$AlO_2H^@$	−864.28	−947.13	20.92	−209.21	13.01	3.5338	0.8485	5.4132	−2.8140	−23.4129	−13.2195	−0.0300
$AlOH^{+2}$	−692.60	−767.27	−184.93	55.97	−2.73	2.0469	−2.7813	6.8376	−2.6639	29.7923	−0.3457	1.7247
$Ca(CO_3)@$	−1099.18	−1201.92	10.46	−123.86	−15.65	−0.3907	−8.7325	9.1753	−2.4179	−11.5309	−9.0641	−0.0380
$Ca(HCO_3)+$	−1146.04	−1231.94	66.94	233.70	13.33	3.7060	1.2670	5.2520	−2.8310	41.7220	8.3360	0.3080
$Ca(HSiO_3)^+$	−1574.24	−1686.48	−8.33	137.80	−6.74	1.0647	−5.1787	7.7785	−2.5649	30.8048	3.6619	0.5831
$Ca(SO_4)^@$	−1310.38	−1448.43	20.92	−104.60	4.70	2.4079	−1.8992	6.4895	−2.7004	−8.4942	−8.1271	−0.0010
Ca^{+2}	−552.79	−543.07	−56.48	−30.92	−18.44	−0.1947	−7.2520	5.2966	−2.4792	9.0000	−2.5220	1.2366
$CaOH^+$	−717.02	−751.65	28.03	6.05	5.76	2.7243	−1.1303	6.1958	−2.7322	11.1286	−2.7493	0.4496
$CH_4^@$	−34.35	−87.81	87.82	277.26	37.40	6.7617	8.7279	2.3212	−3.1397	42.0941	10.4707	−0.3179
Cl^-	−131.29	−167.11	56.74	−122.49	17.34	4.0320	4.8010	5.5630	−2.8470	−4.4000	−5.7140	1.4560
ClO_4^-	−8.54	−129.33	182.00	−24.00	43.90	8.1411	15.5654	−7.8077	−3.4224	16.4500	−6.5700	0.9699
$CO_2^@$	−386.02	−413.84	117.57	243.08	32.81	6.2466	7.4711	2.8136	−3.0879	40.0325	8.8004	−0.0200
CO_3^{-2}	−527.98	−675.31	−50.00	−289.33	−6.06	2.8524	−3.9844	6.4142	−2.6143	−3.3206	−17.1917	3.3914
e^-	0	0	65.34	14.42	0	0	0	0	0	0	0	0
$Fe(CO_3)^@$	−644.49	−763.51	−58.45	−123.03	−17.23	−0.6069	−9.2604	9.3828	−2.3961	−11.4137	−9.0233	−0.0380
$Fe(HCO_3)^+$	−689.86	−794.10	−8.87	231.41	8.18	3.1064	−0.1934	5.8191	−2.7710	43.9175	8.2195	0.5831
$Fe(HSO_4)^+$	−853.48	−990.45	10.21	338.23	18.81	4.5330	3.2897	4.4500	−2.9149	58.2305	13.4217	0.5121
$Fe(HSO_4)^{+2}$	−787.15	−981.91	−248.95	426.71	2.32	2.8251	−0.8804	6.0891	−2.7426	83.8315	17.6994	1.9551
$Fe(SO_4)^@$	−848.81	−993.86	−16.86	−101.60	1.67	1.9794	−2.9454	6.9007	−2.6572	−8.4131	−7.9804	−0.0380
$Fe(SO_4)^+$	−784.71	−942.42	−124.68	−145.93	−2.64	1.7837	−3.4232	7.0885	−2.6374	−5.1341	−10.1600	0.9986
$Fe(SO_4)_2^-$	−1536.81	−1854.38	−87.78	−210.37	30.49	6.6756	8.5215	2.3937	−3.1312	−5.4923	−13.3173	1.9457
Fe^{+2}	−91.50	−92.24	−105.86	−32.44	−22.64	−0.7867	−9.6969	9.5479	−2.3780	14.7860	−4.6437	1.4382
Fe^{+3}	−17.19	−49.58	−277.40	−76.71	−37.79	−2.4256	−13.6961	11.1141	−2.2127	19.0459	−6.8233	2.5812
$FeCl^+$	−223.59	−258.05	−42.09	86.49	0.85	2.1468	−2.5367	6.7401	−2.6741	24.6912	1.1617	0.7003
$FeCl^{+2}$	−156.92	−212.67	−178.82	14.83	−22.86	−0.7164	−9.5277	9.4878	−2.3851	23.8149	−2.3482	1.7013
$FeCl_2^+$	−291.92	−385.75	−129.66	300.72	10.27	3.5610	0.9165	5.3828	−2.8168	57.6940	11.5846	1.0276
$FeCl_3^@$	−417.51	−564.39	−131.06	368.22	35.94	6.6686	8.5038	2.4024	−3.1304	57.3959	14.8930	−0.0380

(continued on next page)

Table D.1 (*continued*)

Species	ΔG^0	ΔH^0	S^0	Cp^0	V^0	$a_1 \cdot 10^*$	$a_2 \cdot 10^{-2*}$	a_3^*	$a_4 \cdot 10^{-4*}$	c_1^*	$c_2 \cdot 10^{-4*}$	$\omega_0 \cdot 10^{-5*}$
	(kJ/mol)	(kJ/mol)	(J/mol·K)	(J/mol·K)	(J/bar)	(cal/mol/bar)	(cal/mol)	(cal·K/mol/bar)	(cal·K/mol)	(cal/mol/K)	(cal·K/mol)	(cal/mol)
FeO^+	−222.00	−255.09	−46.44	−200.94	−42.02	−3.7118	−16.8408	12.3595	−2.0827	−15.3982	−12.8325	0.7191
FeO_2^-	−368.26	−443.82	44.35	−234.93	0.45	2.3837	−1.9602	6.5182	−2.6979	−13.3207	−14.5028	1.4662
$FeO_2H^@$	−419.86	−480.95	92.88	−312.14	7.21	2.7401	−1.0905	6.1776	−2.7338	−37.8300	−18.2305	−0.0300
$FeOH^+$	−274.46	−325.65	−41.84	63.06	−16.71	−0.2561	−8.4029	9.0457	−2.4315	21.4093	0.0209	0.7003
$FeOH^{+2}$	−241.87	−292.79	−106.27	−33.69	−25.34	−1.1562	−10.6009	9.9077	−2.3407	14.6102	−4.7048	1.4382
H^+	0	0	0	0	0	0	0	0	0	0	0	0
$H_2^@$	17.73	−4.02	57.74	166.85	25.26	5.1427	4.7758	3.8729	−2.9764	27.6251	5.0930	−0.2090
$H_2O^@$	−237.18	−285.88	69.92	75.36	18.07	0	0	0	0	0	0	0
$H_2S^@$	−27.93	−39.03	125.52	179.17	34.95	6.5097	6.7724	5.9646	−3.0590	32.3000	4.7300	−0.1000
$HCN^@$	114.37	103.75	131.30	0	0	0	0	0	0	0	0	0
HCO_3^-	−586.94	−690.01	98.45	−34.85	24.21	7.5621	1.1505	1.2346	−2.8266	12.9395	−4.7579	1.2733
HS^-	11.97	−16.22	68.20	−93.93	20.21	5.0119	4.9799	3.4765	−2.9849	3.4200	−6.2700	1.4410
$HSiO_3^-$	−1014.60	−1144.68	20.92	−87.20	4.53	2.9735	−0.5181	5.9467	−2.7575	8.1489	−7.3123	1.5511
HSO_3^-	−529.10	−627.70	139.75	−5.38	32.96	6.7014	8.5816	2.3771	−3.1338	15.6949	−3.3198	1.1233
HSO_4^-	−755.81	−889.23	125.52	22.68	34.84	6.9788	9.2590	2.1108	−3.1618	20.0961	−1.9550	1.1748
$K(SO_4)^-$	−1031.77	−1158.77	146.44	−45.13	27.46	5.9408	6.7274	3.0989	−3.0571	9.9089	−5.2549	1.0996
K^+	−282.46	−252.14	101.04	8.39	9.01	3.5590	−1.4730	5.4350	−2.7120	7.4000	−1.7910	0.1927
$KOH^@$	−437.11	−474.15	108.37	−85.02	14.96	3.7938	1.4839	5.1619	−2.8402	−6.1240	−7.2104	−0.0500
$Mg(CO_3)^@$	−998.98	−1132.12	−100.42	−116.50	−16.78	−0.5450	−9.1130	9.3320	−2.4020	−10.4990	−8.7060	−0.0380
$Mg(HCO_3)^+$	−1047.02	−1153.97	−12.55	254.42	9.34	3.2710	0.2060	5.6690	−2.7880	47.2840	9.3400	0.5990
$Mg(HSiO_3)^+$	−1477.15	−1613.91	−99.50	158.65	−10.85	0.6289	−6.2428	8.1967	−2.5209	36.7882	4.6702	0.9177
Mg^{+2}	−453.99	−465.93	−138.07	−21.66	−22.01	−0.8217	−8.5990	8.3900	−2.3900	20.8000	−5.8920	1.5372
$MgOH^+$	−625.87	−690.02	−79.91	129.23	1.64	2.3105	−2.1365	6.5827	−2.6906	32.0008	3.2394	0.8449
$MgSO_4^@$	−1211.97	−1368.77	−50.88	−90.31	1.81	1.9985	−2.8987	6.8823	−2.6591	−6.8307	−7.4304	−0.0380
$N_2^@$	18.19	−10.37	95.81	234.16	33.41	6.2046	7.3685	2.8539	−3.0836	35.7911	8.3726	−0.3468
$Na(CO_3)^-$	−797.11	−938.56	−44.31	−51.28	−0.42	2.3862	−1.9521	6.5103	−2.6982	15.3395	−5.5686	1.7870
$Na(HCO_3)^@$	−847.39	−929.50	154.72	200.33	32.32	6.1730	7.2943	2.8760	−3.0805	33.8790	6.7193	−0.0380
$Na(SO_4)$-	−1010.34	−1146.66	101.75	−30.09	18.64	4.7945	3.9284	4.1990	−2.9414	13.4899	−4.5256	1.2606
Na^+	−261.88	−240.28	58.41	38.12	−1.21	1.8390	−2.2850	3.2560	−2.7260	18.1800	−2.9810	0.3306
$NaOH^@$	−418.12	−470.14	44.77	−13.40	3.51	2.2338	−2.3287	6.6683	−2.6826	4.0146	−3.6863	−0.0300
$NH_3^@$	−26.67	−81.53	107.82	76.89	24.45	5.0911	2.7970	8.6248	−2.8946	20.3000	−1.1700	−0.0500
NH_4^+	−79.40	−133.26	111.17	67.11	18.08	3.8763	2.3448	8.5605	−2.8759	17.4500	−0.0210	0.1502
NO_3^-	−110.91	−206.89	146.94	−66.80	28.66	7.3161	6.7824	−4.6838	−3.0594	7.7000	−6.7250	1.0977
$O_2^@$	16.45	−12.24	108.95	234.13	30.50	5.7889	6.3536	3.2528	−3.0417	35.3530	8.3726	−0.3943
OH^-	−157.27	−230.01	−10.71	−136.34	−4.71	1.2527	0.0738	1.8423	−2.7821	4.1500	−10.3460	1.7246
$S_2O_3^{-2}$	−519.99	−649.86	66.94	−238.47	27.59	6.6685	12.4951	−7.7281	−3.2955	−0.0577	−14.7066	2.9694
SCN^-	92.70	76.40	144.01	−39.69	35.36	7.0244	9.3687	2.0708	−3.1662	10.7414	−4.9900	1.1073

(*continued on next page*)

Table D.1 (*continued*)

Species	ΔG^0	ΔH^0	S^0	Cp^0	V^0	$a_1 \cdot 10^*$	$a_2 \cdot 10^{-2*}$	$a_3{}^*$	$a_4 \cdot 10^{-4*}$	$c_1{}^*$	$c_2 \cdot 10^{-4*}$	$\omega_0 \cdot 10^{-5*}$
	(kJ/mol)	(kJ/mol)	(J/mol·K)	(J/mol·K)	(J/bar)	(cal/mol/bar)	(cal/mol)	(cal·K/mol/bar)	(cal·K/mol)	(cal/mol/K)	(cal·K/mol)	(cal/mol)
SO_3^{-2}	−487.89	−636.89	−29.29	−280.99	−4.12	2.4632	−1.7691	6.4494	−2.7058	−2.7967	−16.7843	3.3210
SO_4^{-2}	−744.46	−909.70	18.83	−266.09	12.92	8.3014	−1.9846	−6.2122	−2.6970	1.6400	−17.9980	3.1463
$Sr(CO_3)^@$	−1107.83	−1207.29	35.56	−134.32	−15.23	−0.3332	−8.5922	9.1201	−2.4237	−12.9961	−9.5733	−0.0380
$Sr(HCO_3)^+$	−1157.54	−1239.00	95.94	210.07	14.08	3.7702	1.4274	5.1820	−2.8380	37.4746	7.1883	0.2058
$Sr(SO_4)^@$	−1321.37	−1451.50	61.59	−110.60	5.02	2.4382	−1.8251	6.4604	−2.7035	−9.6731	−8.4183	−0.0380
Sr^{+2}	−563.84	−550.87	−31.51	−41.56	−17.76	0.7071	−10.1508	7.0027	−2.3594	10.7452	−5.0818	1.1363
$SrOH^+$	−725.16	−754.14	61.09	−31.66	7.10	2.8620	−0.7922	6.0586	−2.7462	4.7576	−4.5826	0.3306
Temperature correction using Cp(T) integration						a_0	a_1	a_2	$(Cp^0 = a_0 + a_1T + a_2T^{-2})$			
$SiO_2{}^{@**}$	−833.41	−887.86*	41.34	44.47	1.61	46.94	0.034	−1.13E + 06				
Temperature correction using logK(T)						A_0	A_1	A_2	$(\log K_T = A_0 + A_1T + A_2T^{-1})$			
$SiO_3{}^{-2**}$	−938.51	−1098.74	−80.20	119.83	0	−10.0006	0	−3917.5				
$Si_4O_{10}{}^{-4***}$	−3600.81	−3915.99	305.20	328.58	0	0	0	−10,822.8				
$CaSiO_3{}^{@**}$	−1517.56	−1668.06	−136.68	88.90	0	0	0	1371.49				
$MgSiO_3{}^@$	−1425.03	−1554.54	−75.17	−264.79	0	5.7	0	0				
$AlSiO_5{}^{-3}{}^{***}$	−1769.01	−2027.33	−110.41	70.78	−3.41	0	0	158.02				
$AlHSiO_3{}^{+2}{}^{*v}$	−1540.55	−1634.31	−24.99	−215.896	0	14.5828	0	−2141.57				
$FeHSiO_3{}^{+2}{}^{*v}$	−1087.15	−1194.26	−70.77	−163.91	0	9.7	0	0				
$Fe_2(OH)_2{}^{+4}{}^{*v}$	−491.9	−614.44	−281.97	−2.71	0	6.94586	0	−2950.45				
$Fe_3(OH)_4{}^{+5}{}^{*v}$	−964.33	−1232.44	−472.43	71.30	0	4.1824	0	−3125.33				
$SrSiO_3{}^{@***}$	−1527.29	−1617.43	79.92	78.39	1.64	0	0	1302.92				
S^{-2}	120.42	−16.22	−295.55	−93.93	0	−19	0	0				

*Parameters of the HKF-equation of state; given in original calorimetric units (see [25,26,133]) as used in GEM.

**Calculated in Matschei et al. [7] assuming $\Delta_rS^\circ = \Delta_rC^\circ_p = 0$ using S° and C°_p from SiO_2 (quartz) for the reactions: $SiO_2{}^0 -> SiO_2$(quartz) $\Delta_rG^\circ = \Delta_rH^\circ = -21.386$; $SiO_3{}^2 - +2H^+ -> SiO_2{}^0 + H_2O$ $\Delta_rG^\circ = 132.08$, $\Delta_rH^\circ = 75$, $\Delta_rS^\circ = -191.46$, $\Delta_rC^\circ_p = 0$; $SiO_3{}^2 - +Ca^{2+} -> CaSiO_3{}^0$ $\Delta_rG^\circ = \Delta_rH^\circ = -26.257$, $\Delta_rS^\circ = 0$, $\Delta_rC^\circ_p = 0$

***Calculated in this paper assuming $\Delta_rS^\circ = \Delta_rC^\circ_p = 0$ using S° and C°_p from SiO_2 (quartz) for the reactions: $SiO_3{}^2 - +AlO_2{}^- -> AlSiO_5{}^{3-}$ $\Delta_rG^\circ = \Delta_rG^\circ = -3.025$, $\Delta_rS^\circ = 0$, $\Delta_rC^\circ_p = 0$; $Si_4O_{10}{}^4 - +4H^+ -> 4SiO_2{}^0 + 2H_2O$ $\Delta_rG^\circ = \Delta_rH^\circ = 207.2$, $\Delta_rS^\circ = 0$, $\Delta_rC^\circ_p = 0$; $SiO_3{}^2 - +Mg^{2+} -> MgSiO_3{}^0$ $\Delta_rG^\circ = -32.54$, $\Delta_rH^\circ = 0$, $\Delta_rS^\circ = 109.126$, $\Delta_rC^\circ_p = 0$; $SiO_3{}^2 - +Sr^{2+} -> SrSiO_3{}^0$ $\Delta_rG^\circ = \Delta_rH^\circ = -29.944$, $\Delta_rS^\circ = 0$, $\Delta_rC^\circ_p = 0$

*vFrom the GEMS version of the PSI/Nagra 12/07 TDB [22,23]: $Al^{+3} + HSiO_3{}^- -> AlHSiO_3{}^{+2}$ $\Delta_rG^\circ = -42.24$, $\Delta_rH^\circ = 41$, $\Delta_rS^\circ = 279.19$, $\Delta_rC^\circ_p = 0$; $Fe^{+3} + HSiO_3{}^- -> FeHSiO_3{}^{+2}$ $\Delta_rG^\circ = -55.37$, $\Delta_rH^\circ = 0$, $\Delta_rS^\circ = 185.7$, $\Delta_rC^\circ_p = 0$; $2Fe^{+3} + 2H_2O -> Fe_2(OH)_2{}^{+4} + 2H^+$ $\Delta_rG^\circ = 16.84$, $\Delta_rH^\circ = 56.486$, $\Delta_rS^\circ = 132.98$, $\Delta_rC^\circ_p = 0$; $3Fe^{+3} + 4H_2O -> Fe_3(OH)_4{}^{+5} + 4H^+$ $\Delta_rG^\circ = 35.96$, $\Delta_rH^\circ = 59.834$, $\Delta_rS^\circ = 80.07$, $\Delta_rC^\circ_p = 0$

Table D.2
Standard (partial molal) thermodynamic properties and heat capacity coefficients ($Cp^0 = a_0 + a_1T + a_2T^{-2}$) of gaseous species at 25 °C, 1 bar used in GEM calculations, as used in the GEMS version of the PSI/Nagra 12/07 TDB [22,23]. Standard molar volumes for ideal gases are not listed because they are all equal to 2479 J/bar at 1 bar, 298.15 K.

Species	ΔG^0	ΔH^0	S^0	Cp^0	a_0	a_1	a_2
	(kJ/mol)	(kJ/mol)	(J/mol K)	(J/mol K)	(J/mol/K)	(J/mol/K^2)	(J·K/mol)
CH_4	−50.66	−74.81	186.26	35.75	23.64	0.0479	−192,464
CO_2	−394.39	−393.51	213.74	37.15	44.22	0.0088	−861,904
H_2	0	0	130.68	28.82	27.28	0.0033	50,208
H_2O	−228.68	−242.40	187.25	40.07	52.99	−0.0435	5472
H_2S	−33.75	−20.63	205.79	34.20	32.68	0.0124	−192,464
N_2	0	0	191.61	29.13	28.58	0.0038	−50,208
O_2	0	0	205.14	29.32	29.96	0.0042	−167,360

References

[1] B. Lothenbach, T. Matschei, G. Möschner, F.P. Glasser, Thermodynamic modelling of the effect of temperature on the hydration and porosity of Portland cement, Cem. Concr. Res. 38 (2008) 1–18.
[2] T. Matschei, B. Lothenbach, F.P. Glasser, The role of calcium carbonate in cement hydration, Cem. Concr. Res. 37 (2007) 551–558.
[3] M. Moesgaard, D. Herfort, M. Steenberg, L.F. Kirkegard, Y. Yue, Physical performance of blended cements containing calcium aluminosilicate glass powder and limestone, Cem. Concr. Res. 41 (2011) 359–364.
[4] T. Matschei, F.P. Glasser, Temperature dependence, 0 to 40 °C, of the mineralogy of Portland cement paste in the presence of calcium carbonate, Cem. Concr. Res. 40 (2010) 763–777.
[5] B. Lothenbach, F. Winnefeld, C. Alder, E. Wieland, P. Lunk, Effect of temperature on the pore solution, microstructure and hydration products of Portland cement pastes, Cem. Concr. Res. 37 (2007) 483–491.
[6] F. Deschner, B. Lothenbach, F. Winnefeld, J. Neubauer, Effect of temperature on the hydration Portland cement blended with siliceous fly ash, Cem. Concr. Res. 52 (2013) 169–181.
[7] T. Matschei, B. Lothenbach, F.P. Glasser, Thermodynamic properties of Portland cement hydrates in the system CaO-Al_2O_3-SiO_2-$CaSO_4$-$CaCO_3$-H_2O, Cem. Concr. Res. 37 (2007) 1379–1410.
[8] B.Z. Dilnesa, B. Lothenbach, G. Le Saout, G. Renaudin, A. Mesbah, Y. Filinchuk, A. Wichser, E. Wieland, Iron in carbonate containing AFm phases, Cem. Concr. Res. 41 (2011) 311–323.
[9] B.Z. Dilnesa, B. Lothenbach, G. Renaudin, A. Wichser, D. Kulik, Synthesis and characterization of hydrogarnet $Ca_3(Al_xFe_{1-x})_2(SiO_4)_y(OH)_{4(3-y)}$, Cem. Concr. Res. 59 (2014) 96–111.
[10] B.Z. Dilnesa, B. Lothenbach, G. Renaudin, A. Wichser, E. Wieland, Stability of monosulfate in the presence of iron, J. Am. Ceram. Soc. 95 (2012) 3305–3316.
[11] D.A. Kulik, Improving the structural consistency of C-S-H solid solution thermodynamic models, Cem. Concr. Res. 41 (2011) 477–495.
[12] B. Lothenbach, L. Pelletier-Chaignat, F. Winnefeld, Stability in the system CaO–Al_2O_3–H_2O, Cem. Concr. Res. 42 (2012) 1621–1634.
[13] D. Kulik, T. Wagner, S. Dmytrieva, G. Kosakowski, F. Hingerl, K. Chudnenko, U. Berner, GEM-Selektor geochemical modeling package: revised algorithm and GEMS3K numerical kernel for coupled simulation codes, Comput. Geosci. 17 (2013) 1–24.
[14] T. Wagner, D.A. Kulik, F.F. Hingerl, S.V. Dmytrieva, GEM-Selektor geochemical modeling package: TSolMod library and data interface for multicomponent phase models, Can. Mineral. 50 (2012) 1173–1195.
[15] P. Blanc, X. Bourbon, A. Lassin, E. Gaucher, Chemical model for cement-based materials: Temperature dependence of thermodynamic functions for nanocrystalline and crystalline C-S-H phases, Cem. Concr. Res. 40 (2010) 851–866.
[16] P. Blanc, X. Bourbon, A. Lassin, E. Gaucher, Chemical model for cement-based materials: thermodynamic data assessment for phases other than CSH, Cem. Concr. Res. 40 (2010) 1360–1374.
[17] C.M. Bethke, Geochemical and Biogeochemical Reaction Modeling, 2nd Ed., Cambridge University Press, New York, NY, USA, 2008.
[18] D.J. Parkhurst, C.A.J. Appelo, Description of Input and Examples for PHREEQC Version 3 - A Computer Program for Speciation, Batch-reaction, One-dimensional Transport, and Inverse Geochemical Calculations, 6 USGS, Denver, CO, USA, 2013.
[19] J.E. Cross, F.T. Ewart, HATCHES - a thermodynamic database and management system, Radiochim. Acta 52/53 (1991) 421–422.
[20] D. Damidot, B. Lothenbach, D. Herfort, F.P. Glasser, Thermodynamics and cement science, Cem. Concr. Res. 41 (2011) 679–695.
[21] G. Möschner, B. Lothenbach, J. Rose, A. Ulrich, R. Figi, R. Kretzschmar, Solubility of Fe-ettringite ($Ca_6[Fe(OH)_6]_2(SO_4)_3\cdots 26H_2O$), Geochim. Cosmochim. Acta 72 (2008) 1–18.
[22] T. Thoenen, W. Hummel, U. Berner, E. Curti, The PSI/Nagra Chemical Thermodynamic Data Base 12/07, PSI Report 14-04, Villigen PSI, Switzerland, 2014.
[23] T. Thoenen, D.A. Kulik, Nagra/PSI Chemical Thermodynamic Data Base 01/01 for the GEM-Selektor (V.2- PSI) Geochemical Modeling Code: Release 28-02-03. Internal Report TM-44-03-04, available from http://gems.web.psi.ch/TDB/doc/pdf/TM-44-03-04-web.pdf, (2003) (checked 2018-04-19).
[24] 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.
[25] E. Shock, D. Sassani, M. Willis, D. Sverjensky, Inorganic species in geologic fluids: Correlations among standard molal thermodynamic properties of aqueous ions and hydroxide complexes, Geochim. Cosmochim. Acta 61 (1997) 907–950.
[26] D. Sverjensky, E. Shock, H. Helgeson, Prediction of the thermodynamic properties of aqueous metal complexes to 1000 C and 5 kb, Geochim. Cosmochim. Acta 61 (1997) 1359–1412.
[27] M. Balonis, B. Lothenbach, G. Le Saout, F.P. Glasser, Impact of chloride on the mineralogy of hydrated Portland cement systems, Cem. Concr. Res. 40 (2010) 1009–1022.
[28] T. Matschei, F.P. Glasser, The thermal stability of thaumasite, Mater. Struct. 48 (2015) 2277–2289.
[29] B. Lothenbach, F. Winnefeld, Thermodynamic modelling of the hydration of Portland cement, Cem. Concr. Res. 36 (2006) 209–226.
[30] L.G. Baquerizo, T. Matschei, K.L. Scrivener, Impact of water activity on the stability of ettringite, Cem. Concr. Res. 76 (2016) 31–44.
[31] L.G. Baquerizo, T. Matschei, K.L. Scrivener, Hydration states of AFm cement phases, Cem. Concr. Res. 73 (2015) 143–157.
[32] L.G. Baquerizo, T. Matschei, K.L. Scrivener, M. Saeidpour, A. Thorell, L. Wadsö, Methods to determine hydration states of minerals and cement hydrates, Cem. Concr. Res. 65 (2014) 85–95.
[33] M. Balonis, F.P. Glasser, The density of cement phases, Cem. Concr. Res. 39 (2009) 733–739.
[34] M. Balonis, The Influence of Inorganic Chemical Accelerators and Corrosion Inhibitors on the Mineralogy of Hydrated Portland Cement Systems, Thesis University of Aberdeen, Aberdeen, UK, 2010.
[35] M. Balonis, M. Medala, F.P. Glasser, Influence of calcium nitrate and nitrite on the constitution of AFm and AFt cement hydrates, Adv. Cem. Res. 23 (2011) 129–143.
[36] M. Balonis, F.P. Glasser, Calcium nitrite corrosion inhibitor in portland cement: influence of nitrite on chloride binding and mineralogy, J. Am. Ceram. Soc. 94 (2011) 2230–2241.
[37] B.Z. Dilnesa, Fe-containing Hydrates and Their Fate During Cement Hydration: Thermodynamic Data and Experimental Study, Thesis EPFL, Lausanne, 2012.
[38] D. Garvin, V.B. Parker, H.J. White, CODATA Thermodynamic Tables. Selections for Some Compounds of Calcium and Related Mixtures: A Prototype Set of Tables, Springer Verlag, Berlin, 1987.
[39] K.B. Rozov, U. Berner, D.A. Kulik, L.W. Diamond, Solubility and thermodynamic properties of carbonate-bearing hydrotalcite-pyroaurite solid solutions with a 3:1 Mg/(Al + Fe) mole ratio, Clay Clay Miner. 59 (2011) 215–232.
[40] D. Nied, K. Enemark-Rasmussen, E. L'Hôpital, J. Skibsted, B. Lothenbach, Properties of magnesium silicate hydrates (M-S-H), Cem. Concr. Res. 79 (2016) 323–332.
[41] B. Lothenbach, E. Bernard, U. Mäder, Zeolite formation in the presence of cement hydrates and albite, Phys. Chem. Earth 99 (2017) 77–94.
[42] V.J. Babushkin, G.M. Matveyev, O.P. Mchedlov-Petrossyan, Thermodynamics of Silicates, Springer-Verlag, Berlin, H, 1985.
[43] H.C. Helgeson, J.M. Delany, H.W. Nesbitt, D.K. Bird, Summary and critique of the thermodynamic properties of rock-forming minerals, Am. J. Sci. 278-A (1978) 1–229.