

C-A-S-H end-member model:

Phases	V° (cm ³ mol ⁻¹)	ΔH_f° (kJ mol ⁻¹)	ΔG_f° (kJ mol ⁻¹)	S° (J mol ⁻¹ K ⁻¹)	C_p° (J mol ⁻¹ K ⁻¹)	Reference
5CA , C _{1.25} A _{0.125} S ₁ H _{1.625}	57.3	-2491	-2293	163	177	[1]
INFCA , C ₁ A _{0.15625} S _{1.1875} H _{1.65625}	59.3	-2551	-2343	154	181	[1]
JenD , C _{1.5} S _{0.67} H _{2.5} ^a	80.6	-2401	-2169	173	209	[2]
T2C* , C _{1.5} S ₁ H _{2.5} ^b	80.6	-2721	-2298	167	237	[3]
T5C , C _{1.25} S _{1.25} H _{2.5}	79.3	-2780	-2517	160	234	[1]
TobH , C ₁ S _{1.5} H _{2.5}	85.0	-2831	-2560	153	231	[1]

*Adapted from Myers et al 2014.

Pitzer parameters used for C-A-S-H modelling in presence of NaOH and KOH:

Species A	Species B	Parameter_type	Interaction Value	Reference
AlO2-	K+	B0	0.094	[4]
AlO2-	K+	B1	0.32	[4]
AlO2-	K+	C0	-0.0012	[1]
Ca+2	AlO2-	B0	0.315098	[5]
Ca+2	AlO2-	B1	1.687621	[2]
Ca+2	HSiO3-	B0	0.342599	[2]
Ca+2	HSiO3-	B1	1.710847	[2]
Ca+2	OH-	B1	-0.3727	[6]
Ca+2	OH-	B2	-11.052	[3]
Ca+2	OH-	C0	-0.0092	[3]
Ca+2	SiO3-2	B0	0.1960	[2]
Ca+2	SiO3-2	B1	2.4181	[2]
K+	HSiO3-	B0	0.1160	[2]
K+	HSiO3-	B1	0.4546	[2]
K+	OH-	C0	0.0041	[7]
K+	SiO3-2	B0	0.0783	[2]
K+	SiO3-2	B1	0.5166	[2]
Na+	AlO2-	B0	-0.0083	[8]
Na+	AlO2-	B1	0.071	[5]
Na+	AlO2-	C0	9.77E-03	[5]
Na+	HSiO3-	B0	0.1391	[2]
Na+	HSiO3-	B1	0.4681	[2]
Na+	OH-	C0	0.0044	[5]
Na+	SiO3-2	B0	0.0877	[2]
Na+	SiO3-2	B1	0.5304	[2]
OH-	Ca+2	B0	-0.1421	[3]
OH-	K+	B0	0.1611	[9]
OH-	K+	B1	0.137	[9]
OH-	Na+	B0	0.0864	[5]
OH-	Na+	B1	0.253	[5]

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