Supplementary Material for PCCP

Supporting information for manuscript

Natural abundance high field ^{43}Ca solid state NMR in cement science

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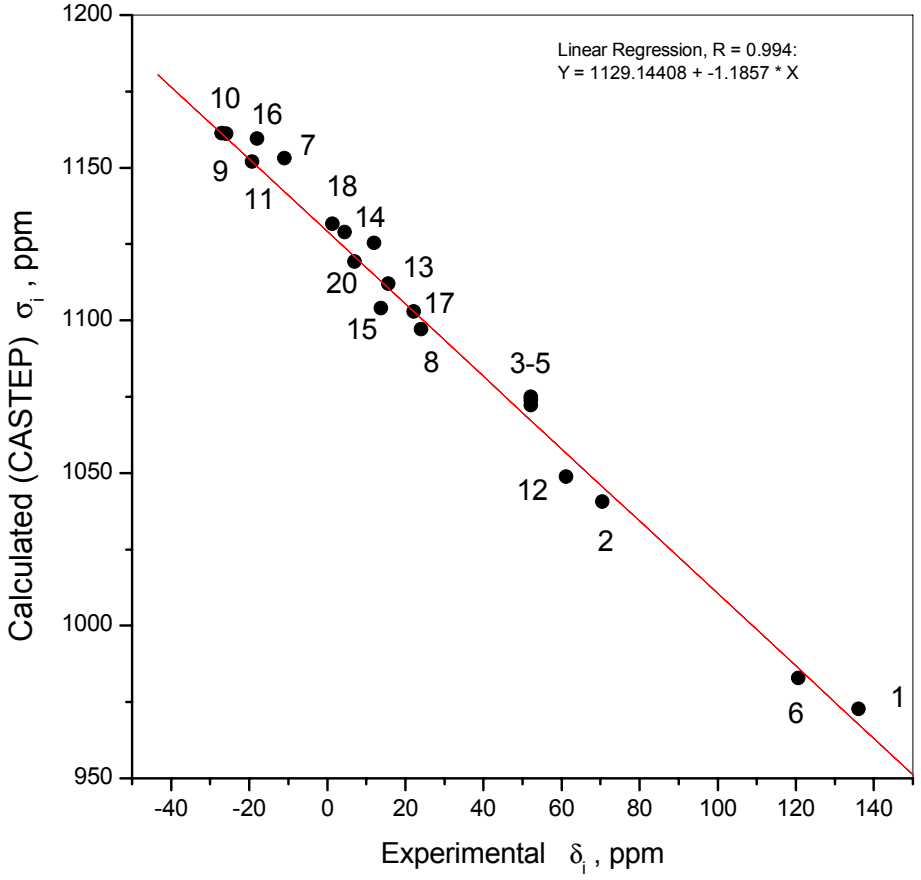

	Compound	$\delta_i^{exp.}$, ppm	$\sigma_i^{calc.}$, ppm
1	CaO	136.1	972.7
2	Ca(OH)2	70.5	1040.7
3	CaSiO3, Wollastonite, Ca1	52.1	1072.2
4	CaSiO3, Wollastonite, Ca2	52.1	1073.8
5	CaSiO3, Wollastonite, Ca3	52.1	1075.1
6	CaS (cubic)	120.7	982.9
7	CaMoO4	-11	1153.1
8	CaCO3, Calcite	22.1	1102.9
9	CaCO3, Aragonite	-25.9	1161.2
10	CaSO4	-27	1161.3
11	CaSO4x2H2O, Gypsum	-19.3	1152.1
12	CaCl2	61.2	1048.9
13	a-Ca(BH4)2	13.7	1104.0
14	b-Ca(BH4)2	4.5	1128.9
15	a-Ca2P2O7, Ca1	12	1125.3
16	a-Ca2P2O7, Ca2	-18	1159.6
17	CaMg(CO3)2, Dolomite	15.6	1112.1
18	CaMgSi2O7, Akermanite	1.3	1131.7
19	CaMgSi2O6, Diopside	24	1097.1
20	CaSiO3, pseudo-wollastonite	7	1119.3

Figure S1: Correlation between calculated isotropic shieldings and experimental ^{43}Ca isotropic chemical shifts in diamagnetic compounds of calcium. All experimental data except for $CaCl_2$ were obtained at 21.1T. The chemical for $CaCl_2$ is taken from Ref. 29 and corrected for the difference in the references.

Table S1. CASTEP calculated ^{43}Ca NMR parameters in triclinic C_3S.

Ca site [1]	σ_i, ppm	C_q, MHz	η	$\delta_i^{Calc.}$ [2], ppm
1	969.14	7.2	0.39	134.9
2	1039.49	5.3	0.23	75.6
3	1019.5	-3.9	0.75	92.5
4	1005.13	3.8	0.59	104.6
5	1028.49	4.5	0.71	84.9
6	1028.47	-3.4	0.92	84.9
7	1017.15	2.2	0.82	94.5
8	1016.3	-2.6	0.42	95.2
9	1019.54	-3.8	0.89	92.4
10	1031.41	-3.1	0.10	82.4
11	1018.8	-3.3	0.29	93.1
12	1018.04	-2.5	0.95	93.7
13	1042.42	-3.9	0.51	73.1
14	1033.41	4.3	0.84	80.7
15	1023.43	-2.1	0.21	89.2
16	982.45	-31.9	0.02	123.7
17	1040.84	-3.1	0.61	74.5
18	1017.29	-2.2	0.49	94.3
19	1013.39	1.2	0.72	97.6
20	1027.19	2.7	0.22	86.0
21	963.78	-2.9	0.35	139.5
22	1075.6	-2.4	0.23	45.2
23	955.56	-3.4	0.17	146.4
24	1009.16	-1.9	0.19	101.2
25	1010.32	-3.5	0.63	100.2
26	1020.14	4.6	0.90	91.9
27	1019.15	3.4	0.67	92.8
28	1004.67	4.6	0.85	105.0
29	978.88	-5.1	0.69	126.7

[1] A structure from Ref. 46 was used in calculations. Sites numbering follows the original reference.

[2] $\delta_i^{Calc.}$ are converted from the absolute shielding constants s using an empirical relationship σ_i=1129.1 -1.1857*δ_i (see Fig. S1).