Supplementary Material for PCCP
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Supporting information for manuscript

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

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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 $^{43}\text{Ca}$ NMR parameters in triclinic C$_3$S.

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<th>$C_q$, MHz</th>
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1 A structure from Ref. 46 was used in calculations. Sites numbering follows the original reference.
2 $\delta^{\text{Calc.}}$ are converted from the absolute shielding constants $s$ using an empirical relationship $\sigma = 1129.1 - 1.1857*\delta$ (see Fig. S1).