

Supporting Information for

The Monetite Structure Probed by Advanced Solid-State NMR Experimentation at Fast Magic-Angle Spinning

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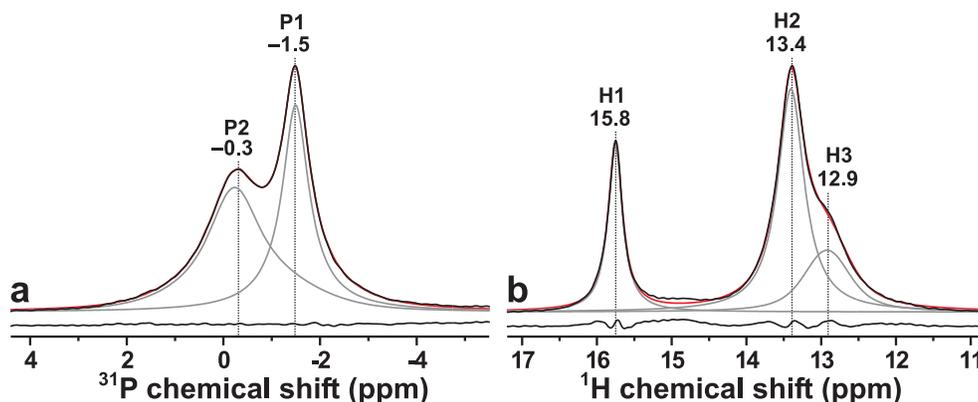


Figure S1. Deconvoluted (a) ³¹P and (b) ¹H MAS NMR spectra (obtained at $\nu_r = 66$ kHz for ¹H). The experimental NMR spectra (black traces) are shown together with the best-fit result (red traces), as well as the component NMR peaks (grey traces). The curve beneath each NMR spectrum represents the difference between the experiment and best-fit. Note that each ³¹P resonance (grey traces) from the respective P1 and P2 sites in (a) represents the sum of two signals: one narrow (fitted with the constraint FWHM < 1.5 ppm) and one broad (FWHM < 4.2 ppm) NMR peak, which were necessary to emulate the structural disorder of the monetite structure. We refer to refs. [S1] and [S2] for details about the deconvolution procedure. Each of the three ¹H NMR resonances from the ¹H1, ¹H2, and ¹H3 sites in (b) were accounted for by one peak.

References

- [S1] Yu, Y.; Guo, H.; Pujari-Palmer, M.; Stevansson, B.; Grins, J.; Engqvist, H.; Edén, M. Advanced Solid-State ¹H/³¹P NMR Characterization of Pyrophosphate-Doped Calcium Phosphate Cements for Biomedical Applications: The Structural Role of Pyrophosphate. *Ceram. Int.* **2019**, *45*, 20642–20655.
- [S2] Guo, H.; Pujari-Palmer, M.; Yu, Y.; Stevansson, B.; Engqvist, H.; Edén, M. Quantitative Phase Analyses of Pyrophosphate-Bearing Monetite and Brushite Biocements by Solid-State NMR and Powder XRD. *Ceram. Int.* **2019**, submitted.