

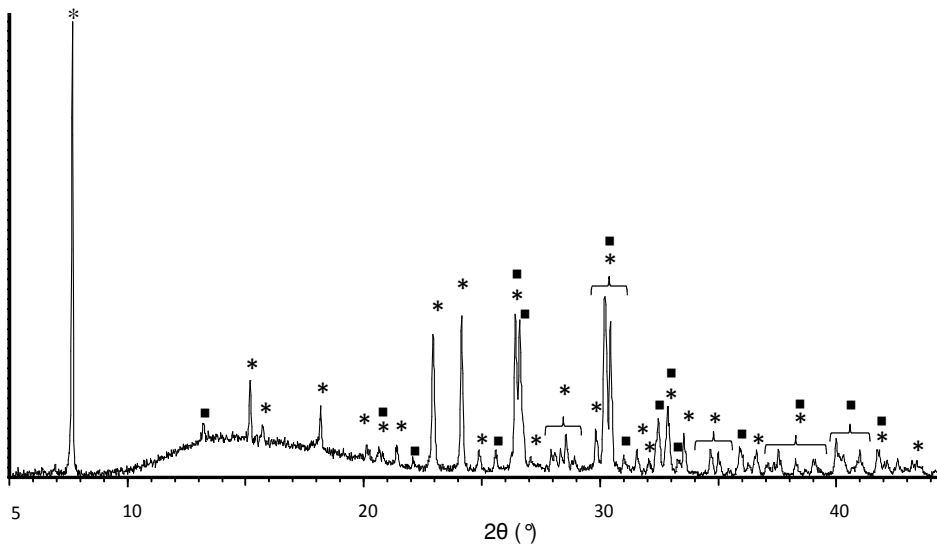
High resolution solid state NMR experiments

for the characterization of calcium phosphate biomaterials and biominerals

SUPPLEMENTARY MATERIALS

Figure S1.

XRD powder pattern of ^{17}O labeled MCPM-monetite



* MCPM ($\text{Ca}(\text{H}_2\text{PO}_4)_2 \cdot \text{H}_2\text{O}$)

■ Monetite (CaHPO_4)

Figure S2.

Experimental ^{17}O MAS NMR spectra of ^{17}O -labeled MCPM-monetite (in black), recorded on 600 and 750 MHz NMR spectrometers, together with their simulation (in red).

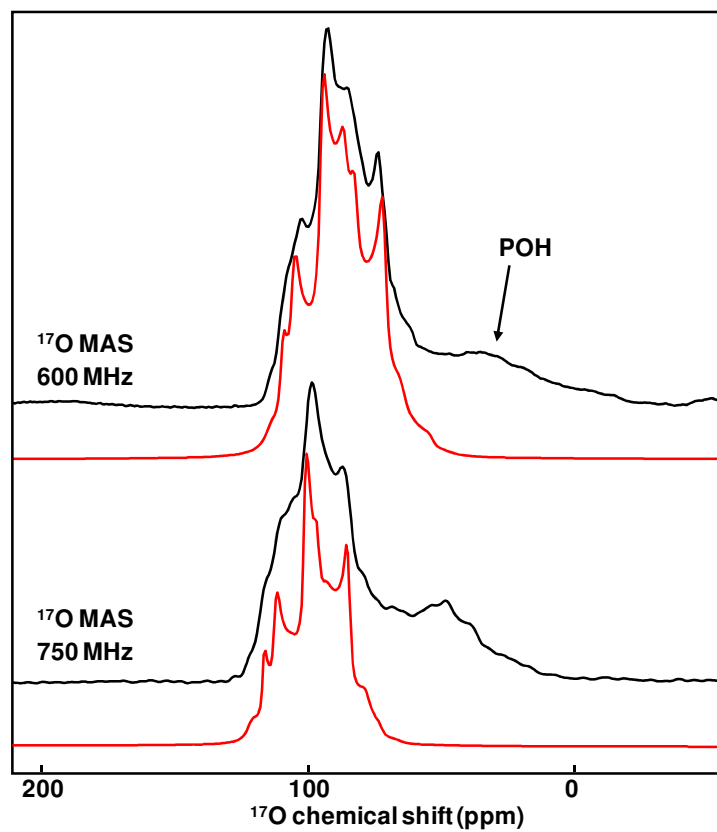


Table S1GIPAW calculated ^{17}O NMR parameters for MCPM and Monetite.

	Oxygen site	$\delta_{\text{iso.}}$ (ppm)	C_Q (MHz)	η_Q
MCPM JCPDS 700090	O1 (PO)	96.1	4.58	0.08
	O2 (PO)	98.9	4.57	0.07
	O3 (POH)	74.9	6.75	0.83
	O4 (POH)	67.0	7.06	0.75
	O5 (PO)	91.4	4.70	0.32
	O6 (POH)	65.8	7.43	0.80
	O7 (POH)	64.5	7.46	0.69
	O8 (PO)	99.4	4.67	0.12
	O9 (H ₂ O)	-0.9	7.63	0.82
Monetite (Catti <i>et al.</i> , 1977)	O1 (POH)	91.5	6.74	0.91
	O1' (POH)	84.1	6.59	0.92
	O2 (PO)	110.6	4.59	0.11
	O2' (PO)	115.2	4.89	0.16
	O3 (PO)	113.2	4.68	0.19
	O3' (PO)	112.2	4.95	0.29
	O4 (PO)	106.7	4.84	0.14
	O4' (PO)	108.0	4.72	0.19
	O5 (PO)	109.0	4.61	0.57
	O5' (PO)	110.6	4.95	0.51
	O6 (POH)	83.3	6.82	0.59
	O6' (PO)	121.7	5.27	0.34
	O7 (PO)	116.4	4.91	0.13
	O7' (POH)	58.8	-6.32	0.93
	O8 (PO)	124.9	5.19	0.24
O8' (PO)	125.0	4.37	0.47	