Supporting Information for

Alkaline Earth Metal-Organic Frameworks with Tailorable Ion Release: A Path for Supporting Biomineralization

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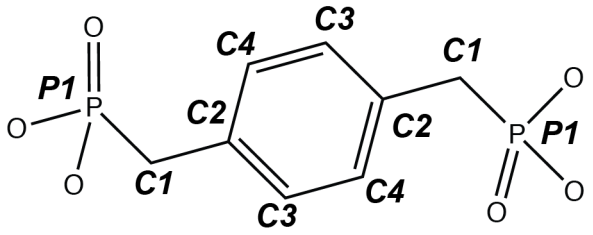
Table S1. *Crystallographic Data*

sample name	CaPAEM	SrCaPAEM	SrPAEM
sample content	$CaP_2C_8O_9H_{16}$	$Sr_{1-x}Ca_xP_2C_8O_9H_{16}$	$SrP_2C_8O_9H_{16}$
formula mass (amu)	358.23	386.75	405.77
metal site occupancy	Ca, 0.9(1)	Sr, 0.6(1) Ca, 0.4(1)	Sr, 1.0 (1)
space group	*C*2/*c* (No. 15)	*C*2/*c* (No. 15)	*C*2/*c* (No. 15)
a (Å)	22.604(2)	23.045(2)	23.189(3)
b(Å)	7.0629(6)	7.2353(9)	7.3137(9)
c (Å)	9.1011(9)	9.304(1)	9.379(1)
β°	103.865(6)	103.823(6)	103.723(9)
V (Å^3)	1410.7(2)	1506.5(3)	1545.2(4)
Z	4	4	4
ρ_{calcd} (g cm^{-3})	1.594(5)	1.667(9)	1.79(2)
T (K)	296	296	296
radiation	Cu Kα, λ=1.5406 Å	Cu Kα, λ=1.5406 Å	Cu Kα, λ=1.5406 Å
2θ limits	10.00–50.00°	10.00–50.00°	10.00–50.00°
refinement method	Rietveld	Rietveld	Rietveld
no. of data collected	1379 data points	1379 data points	1379 data points
no. of Bragg reflections	115	115	116
no. of variables	24	24	24
residuals[a]	R_{wp} = 0.1235	R_{wp} = 0.1064	R_{wp} = 0.1122
	R_{exp} = 0.0110	R_{exp} = 0.0093	R_{exp} = 0.0084
Goodness of fit	1.1691	1.2133	1.1394

[a] $R_{wp} = \left[\sum[w(y_o - y_c)]/\sum w y_o^2\right]^{1/2}$ R_{exp} = [(N-P+C)/ Σ (wy_o^2)]$^{1/2}$; R_{wp} = [Σ[$w(y_o - y_c)$] / Σwy_o^2]$^{1/2}$; N is the total number of observations, P is the number of parameters refined, C is the number of constraints used in the refinement.

Table S2: *GIPAW DFT Calculations* on CaPAEM and SrPAEM*

Chemical Environment	CaPAEM; Calculated Shielding (σ_{iso}, ppm)	SrPAEM; Calculated Shielding (σ_{iso}, ppm)
P	251.87	254.37
C1	135.12	137.45
C2	36.07	35.29
C3	35.98	36.57
C4	38.20	34.46



**GIPAW DFT (CASTEP ver. 4.4); Coarse with a cut-off of 449.9947 eV, a grid size of 2x1x1, geometry optimized.*

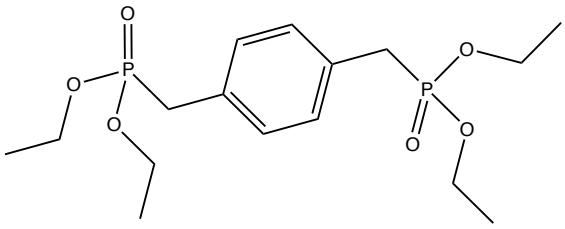


Figure S1. *Molecular structure of the tetraethyl p-xylylenediphosphonate linker.*

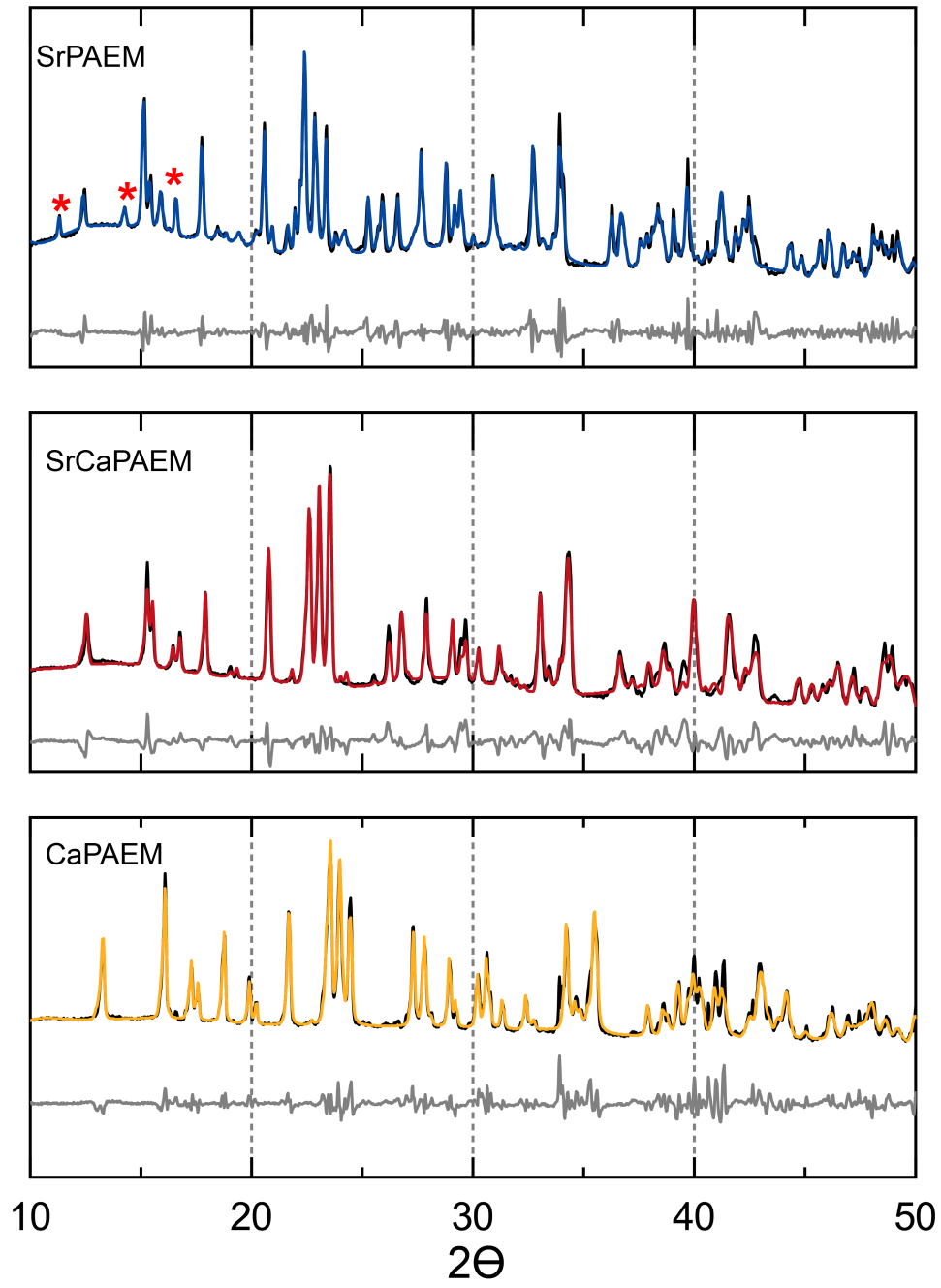


Figure S2. *Powder XRD data (experimental, fitted and difference) of CaPAEM (yellow), SrCaPAEM (red) and SrPAEM (blue).*

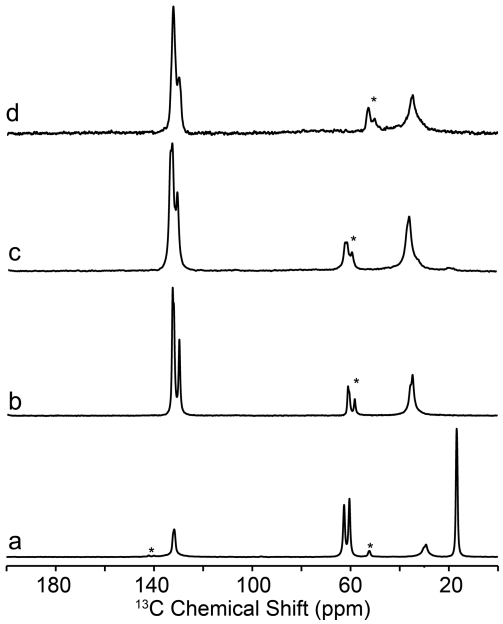


Figure S3. *Carbon-13 CP MAS NMR spectra of PXBP (a); CaPAEM (b); SrPAEM (c) and SrCaPAEM (d).*

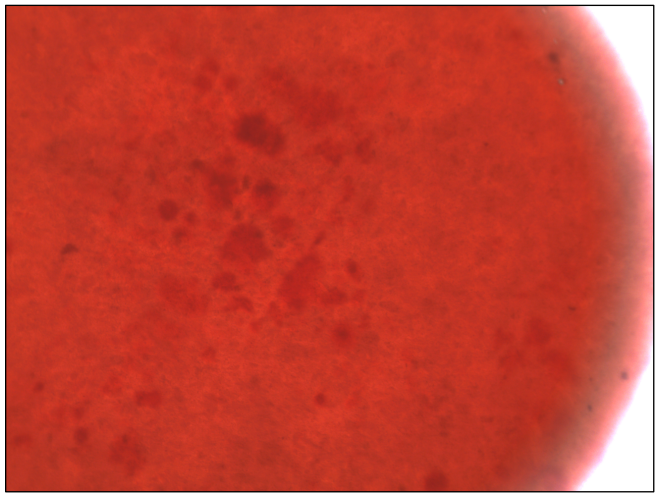


Figure S4. *Human osteosarcoma cells with apparent Alizarin Red S staining (darker spots) indicating calcification caused by CaPAEM, viewed under light microscope.*

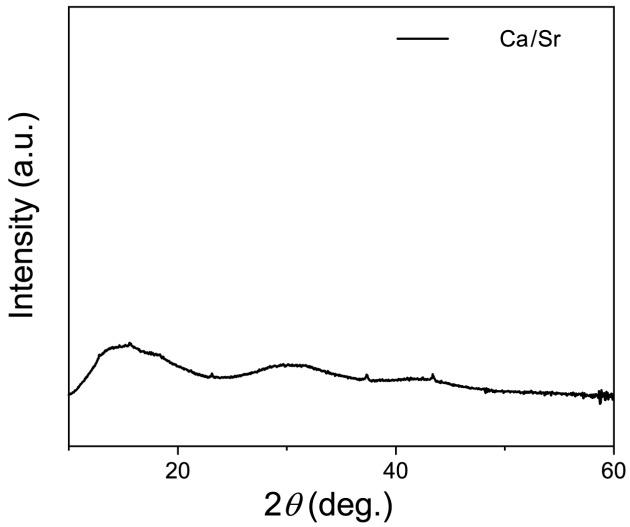


Figure S5. *Powder XRD of post-SBF treated SrCaPAEM (4 days) before final dissolution.*

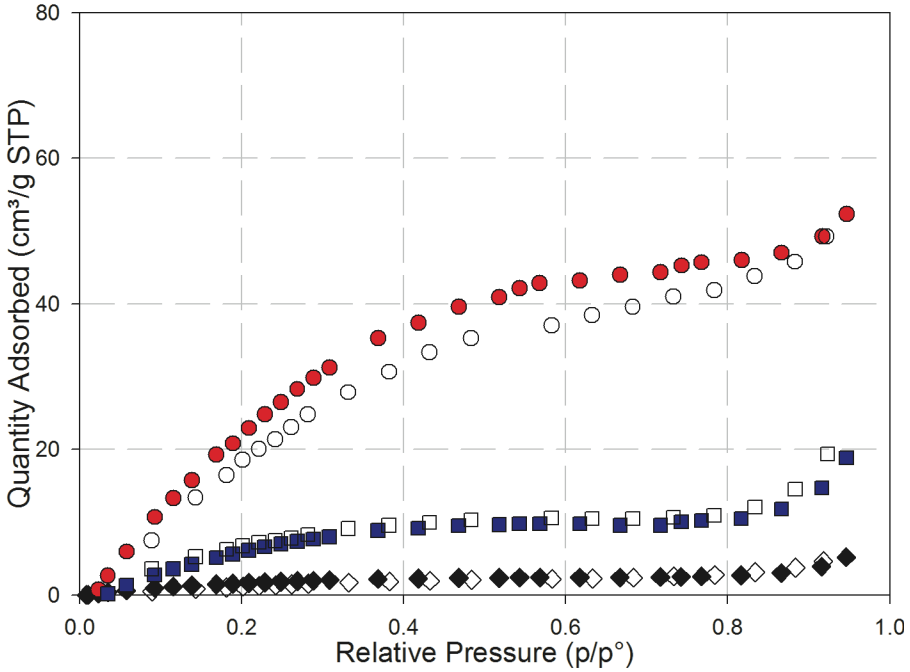


Figure S6. *Nitrogen adsorption isotherms measured at 77 K of SrPAEM (red circles), SrCaPAEM (blue squares) and CaPAEM (black diamonds). Nitrogen desorption white circles, squares, and diamonds respectively.*