Exploration of new water stable pronton-conducting materials in the amino acid-templated metal phosphate system

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Physical measurements:

Powder X-ray diffraction (XRD) data were obtained using a Rigaku D/MAX-rA diffractometer with Cu-Kα radiation (λ = 1.5418 Å). IR spectra (KBr pellets) were recorded on a Nicolet Impact 410 FTIR spectrometer. The thermogravimetric analyses were performed on a Netzsch STA 449c analyzer in a flow of N_2 with a heating rate of 10 ºC/min. Single crystal X-ray diffraction data were collected on a New Gemini, Dual, Cu at zero, EosS2 diffractometer at room temperature. The crystal structures were solved by direct methods. The structures were refined on F^2 by full-matrix least-squares methods using the *SHELXTL* program package.[1]

Reference

1. G. M. Sheldrick, Acta Cryst., Sect. A, 2008, 64, 112.

Table S1. Hydrogen bond information for SCU-4

D-H···A[a]	d(D-H) (Å)	d(H···A) (Å)	d(D···A) (Å)	<(DHA) (deg)
O4-H4···O3#1	0.82	2.00	2.758(4)	154.3
N1-H1A···O6#2	0.89	1.98	2.763(4)	146.1
N1-H1B···O3#2	0.89	2.18	3.068(4)	179.0
N1-H1C···O1#3	0.89	2.17	2.870(4)	135.2

[a] Symmetry transformations used to generate equivalent atoms: #1 -x, 1-y, -z; #2 1-x, -1/2+y, 1/2-z; #3 1-x, 1/2+y, 1/2-z.

Table S2. Hydrogen bond information for SCU-12

D-H···A[a]	d(D-H) (Å)	d(H···A) (Å)	d(D···A) (Å)	<(DHA) (deg)
O4-H4···O10#1	0.82	1.80	2.622(7)	175.9
N4-H7···O10#2	0.82	1.85	2.632(7)	160.4
O8-H8···O3#3	0.82	1.77	2.549(6)	158.8
N1-H1A···O5#4	0.89	2.11	2.943(7)	155.8
N1-H1B···O8#5	0.89	2.13	2.890(8)	143.0
N2-H1C···O2	0.89	2.11	2.981(8)	165.3

[a] Symmetry transformations used to generate equivalent atoms: #1 1+x, +y, +z; #2 -x, 1-y, 1-z; #3 -1+x, 2/3-y, -1/2+z; #4 1-x, -1/2+y, 3/2-z; #5 -x, -1/2+y, 2/3-z.

Table S3. CHN elemental analysis results

	SCU-4	SCU-12
anal. found	C 13.98%, H 3.07%, N 5.56%	C 8.79%, H 2.48%, N 3.37%
calc:	C 14.39%, H 3.22%, N 5.59 %	C 9.08%, H 2.54%, N 3.53 %

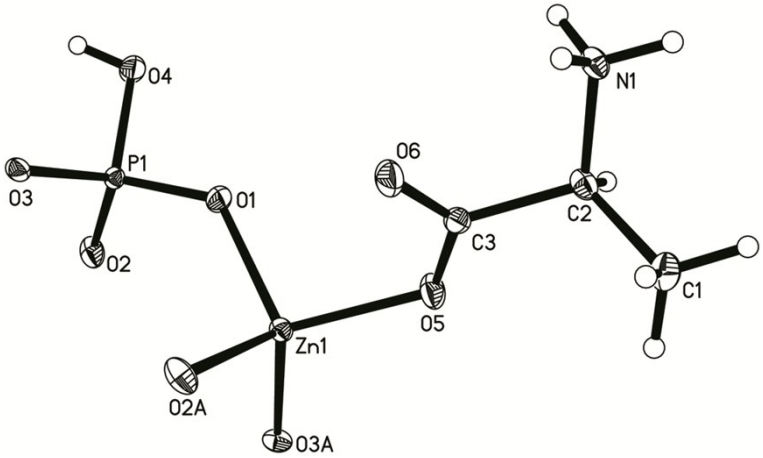

Fig. S1. ORTEP plot of the asymmetric unit of SCU-4, showing the labeling scheme and the 30% probability displacement ellipsoid. Atom labels having "A" refer to symmetry-generated atoms.

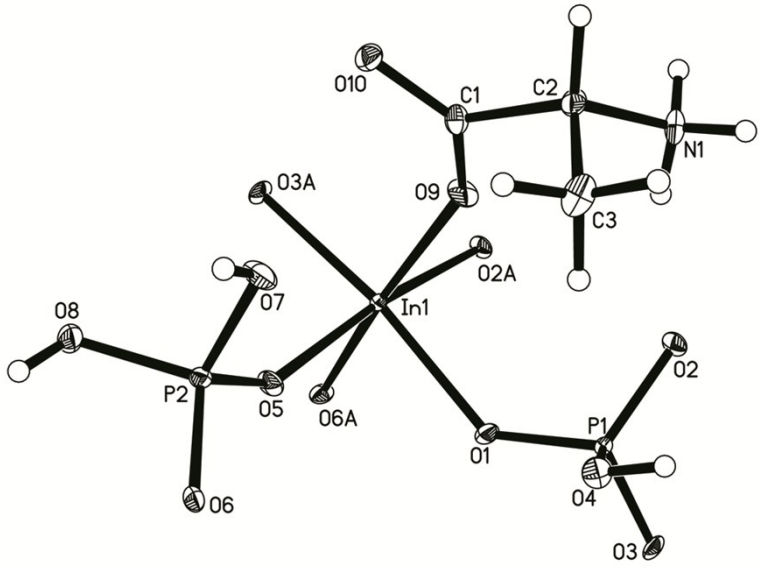

Fig. S2. ORTEP plot of the asymmetric unit of SCU-12, showing the labeling scheme and the 30% probability displacement ellipsoid. Atom labels having "A" refer to symmetry-generated atoms.

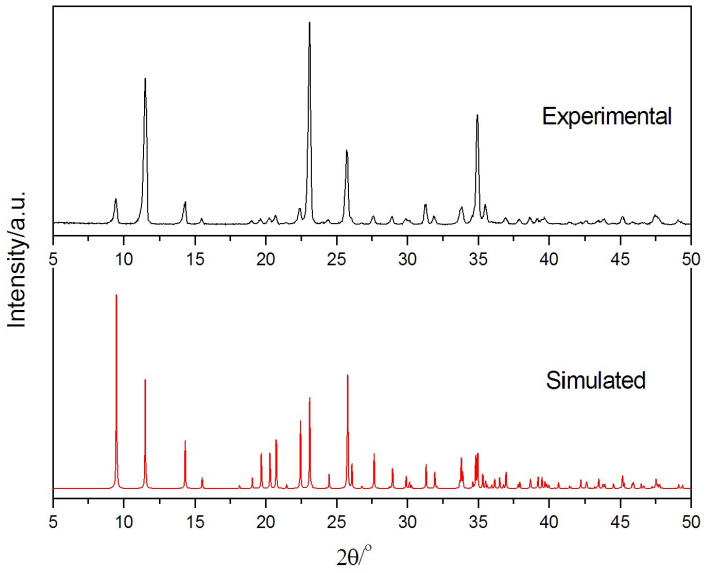

Fig. S3. Experimental and simulated powder XRD patterns of SCU-4.

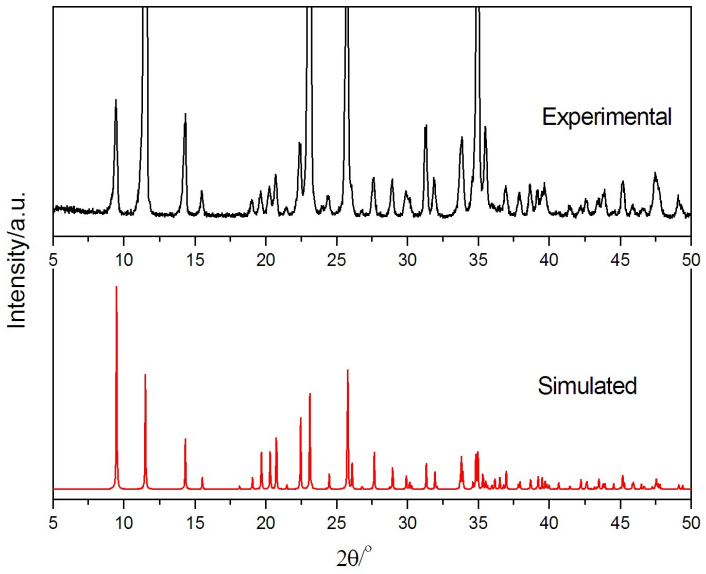

Fig. S4. Experimental and simulated powder XRD patterns of SCU-4. The diffraction peaks of experimental powder XRD pattern are magnified.

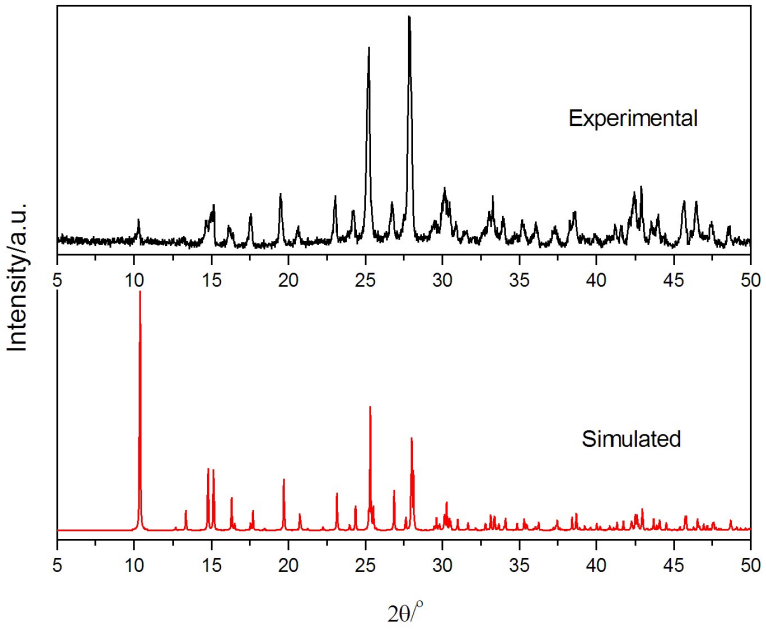

Fig. S5. Experimental and simulated powder XRD patterns of SCU-12.

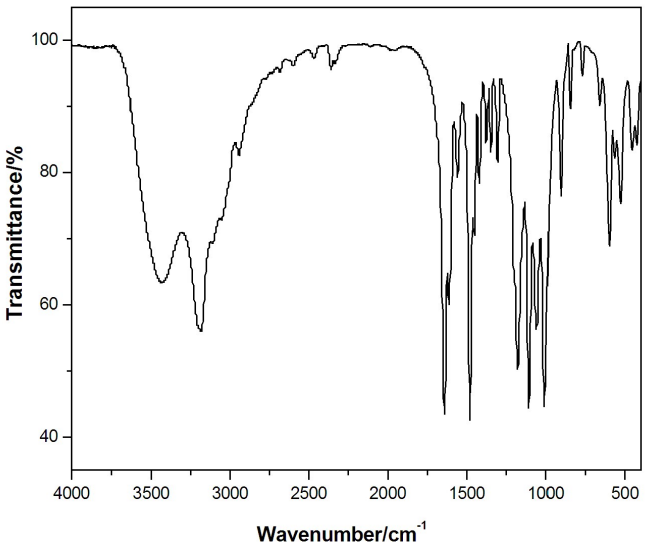

Fig. S6. IR spectrum of SCU-4. The strong bands at 3430 and 1640 cm^{-1} correspond to the NH_3 and C=O stretching vibrations, respectively. The strong band at 1480 cm^{-1} corresponds to the CH_3 bending vibrations.The C–N stretching band is observed at 1350 cm^{-1}. The strong bands in the region 1010-1180 cm^{-1} are assigned to the asymmetric stretch of PO_4 tetrahedra.

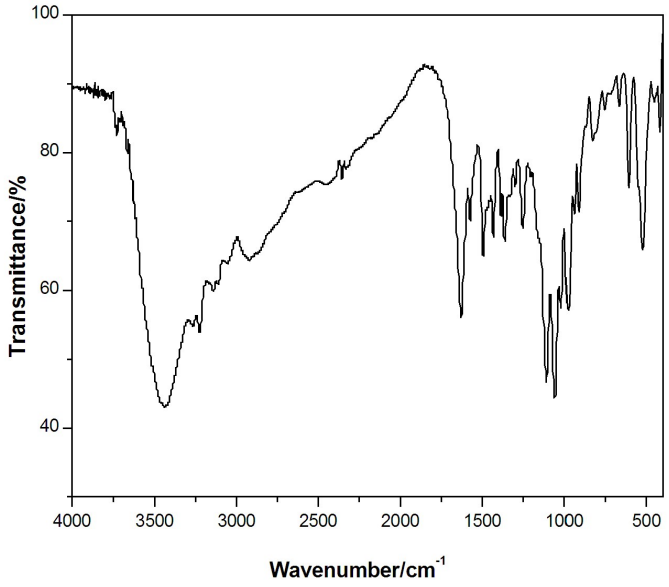

Fig. S7. IR spectrum of SCU-12. The strong bands at 3440 and 1640 cm^{-1} corresponds to the NH_3 and C=O stretching vibrations, respectively. The band at 1490 cm^{-1} corresponds to the CH_3 bending vibrations. The C–N stretching band is observed at 1380 cm^{-1}. The strong bands in the region 970-1110 cm^{-1} are assigned to the asymmetric stretch of PO_4 tetrahedra.

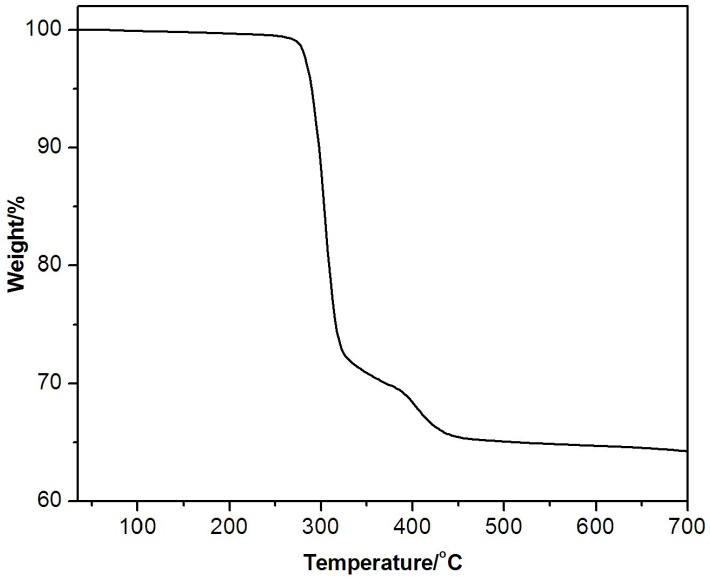

Fig. S8. TGA curve of SCU-4.

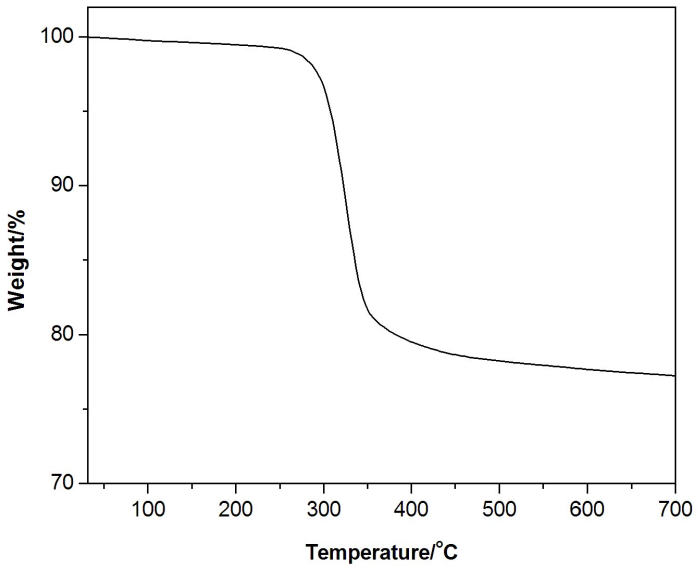

Fig. S9. TGA curve of SCU-12.