

Supporting Information

Switching on the proton transport pathway of a lanthanide metal-organic framework by one-pot loading of tetraethylene glycol for high proton conduction

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Table S1 Crystal data and structure refinement for SmHEDP-H₂O.

Table S2 Selected bond lengths and bond angles for SmHEDP-H₂O.

Fig. S1 Simulated and experimental powder X-ray diffraction (XRD) pattern of SmHEDP-H₂O.

Fig. S2 Thermogravimetric (TG) spectra of SmHEDP-H₂O and SmHEDP-TEG.

Fig. S3 IR spectra of SmHEDP-H₂O and SmHEDP-TEG in the range of 400 and 4000 cm⁻¹. The inset is the detailed IR spectra in the range of 1080 and 1260 cm⁻¹.

Fig. S4 Thermal ellipsoid plot (30% probability) and atomic labeling scheme of SmHEDP-H₂O.

Fig. S5 Hydrogen bond interaction existed in SmHEDP-H₂O (Color code: Sm, purple; P, yellow; O, red; C, green; H, white; hydrogen bond, blue).

Fig. S6 Powder X-ray diffraction (XRD) pattern of SmHEDP-H₂O (a) and SmHEDP-TEG (b) before and after proton conductivity measurements; SEM images of SmHEDP-H₂O (c) and (d) after proton conductivity measurements

Fig. S7 Water adsorption isotherms of SmHEDP-H₂O (a) and SmHEDP-TEG (b) at 298K

Table S1 Crystal data and structure refinement for SmHEDP-H₂O

Empirical formula	C ₂ H ₁₁ SmP ₂ O ₁₀					
Formula weight	407.40					
Temperature	293(2) K					
Wavelength	0.71073 Å					
Crystal system, space group	Orthorhombic, <i>Pbca</i>					
Unit cell dimensions	<i>a</i> = 9.7637(8) Å	<i>α</i> = 90°	<i>b</i> = 9.764 Å	<i>β</i> = 90°	<i>c</i> = 20.5506(18) Å	<i>γ</i> = 90°
Volume	1959.1(2) Å ³					
Z, Calculated density	8, 2.763 mg/m ³					
Absorption coefficient	6.360 mm ⁻¹					
<i>F</i> (000)	1560					
Crystal size	0.21 × 0.20 × 0.18 mm					
Theta range for data collection	2.878 to 25.116°					
Limiting indices	-11 ≤ <i>h</i> ≤ 11, -6 ≤ <i>k</i> ≤ 11, -24 ≤ <i>l</i> ≤ 24					
Reflections collected / unique	10370 / 1743 [R(int) = 0.0989]					
Completeness to θ = 28.30	99.8 %					
Refinement method	Full-matrix least-squares on <i>F</i> ²					
Data / restraints / parameters	1743 / 0 / 137					
Goodness-of-fit on <i>F</i> ²	1.025					
Final <i>R</i> indices [<i>I</i> >2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0281, <i>wR</i> ₂ = 0.0790					
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0308, <i>wR</i> ₂ = 0.0807					
Largest diff. peak and hole	1.951 and -1.095 e. Å ⁻³					

Table S2 Selected bond lengths and bond angles for SmHEDP-H₂O

Bond	Bond Length (Å)	Bond	Bond Length (Å)
Sm(1)-O(2)	2.323(3)	Sm(1)-O(3)	2.339(3)
Sm(1)-O(1)	2.414(3)	Sm(1)-O(5)	2.460(3)
Sm(1)-O(4)#1	2.464(2)	Sm(1)-O(4)	2.485(2)
Sm(1)-O1w	2.647(3)	Sm(1)-O2w	2.508(3)
P(1)-O(1)	1.501(3)	P(1)-O(5)	1.501(3)
P(1)-O(7)	1.580(3)	P(1)-C(1)	1.834(4)
P(2)-O(2)	1.509(3)	P(2)-O(3)	1.512(3)
P(2)-O(4)	1.539(3)	P(2)-C(1)	1.843(4)
O(6)-C(1)	1.467(4)	C(1)-C(2)	1.515(5)
Bond Angle	Value (°)	Bond Angle	Value (°)
O(2)-Sm(1)-O(3)	87.31(9)	O(2)-Sm(1)-O(1)	86.18(9)
O(3)-Sm(1)-O(1)	76.43(9)	O(2)-Sm(1)-O(5)	74.86(9)
O(3)-Sm(1)-O(5)	140.25(9)	O(1)-Sm(1)-O(5)	67.33(9)
O(2)-Sm(1)-O(4)	152.64(10)	O(3)-Sm(1)-O(4)	108.06(9)
O(1)-Sm(1)-O(4)	76.09(8)	O(5)-Sm(1)-O(4)	79.09(9)
O(2)-Sm(1)-O(4)	112.18(9)	O(3)-Sm(1)-O(4)	145.34(9)
O(1)-Sm(1)-O(4)	130.91(9)	O(5)-Sm(1)-O(4)	74.15(9)
O(4)-Sm(1)-O(4)	67.57(10)	O(2)-Sm(1)-O(2w)	134.09(9)
O(3)-Sm(1)-O(2w)	69.43(9)	O(1)-Sm(1)-O(2w)	123.09(9)
O(5)-Sm(1)-O(2w)	145.66(8)	O(4)-Sm(1)-O(2w)	73.24(9)
O(4)-Sm(1)-O(2w)	76.71(9)	O(2)-Sm(1)-O(1w)	67.03(9)
O(3)-Sm(1)-O(1w)	72.29(9)	O(1)-Sm(1)-O(1w)	139.19(9)
O(5)-Sm(1)-O(1w)	128.11(9)	O(4)-Sm(1)-O(1w)	138.57(9)
O(4)#1-Sm(1)-O(1w)	88.77(9)	O(2w)-Sm(1)-O(1w)	68.32(9)
O(1)-P(1)-O(5)	115.07(16)	O(1)-P(1)-O(7)	106.15(15)
O(5)-P(1)-O(7)	109.79(15)	O(1)-P(1)-C(1)	109.89(15)
O(5)-P(1)-C(1)	109.05(15)	O(7)-P(1)-C(1)	106.54(17)
O(2)-P(2)-O(3)	115.23(16)	O(2)-P(2)-O(4)	112.30(15)
O(3)-P(2)-O(4)	110.21(14)	O(2)-P(2)-C(1)	104.21(16)
O(3)-P(2)-C(1)	108.30(17)	O(4)-P(2)-C(1)	105.92(16)
P(1)-O(1)-Sm(1)	139.78(15)	P(2)-O(2)-Sm(1)	151.26(17)
P(2)-O(3)-Sm(1)	144.80(16)	P(2)-O(4)-Sm(1)	122.95(13)
O(6)-C(1)-P(2)	107.6(2)	O(6)-C(1)-C(2)	107.2(3)
O(6)-C(1)-P(1)	109.1(2)	C(2)-C(1)-P(2)	107.6(2)
P(2)-C(1)-P(1)	108.2(2)	C(2)-C(1)-P(1)	112.3(3)

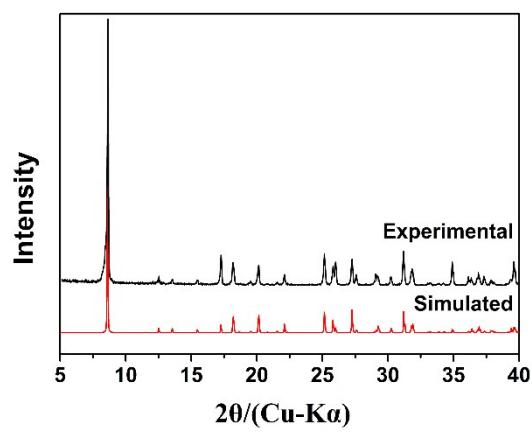


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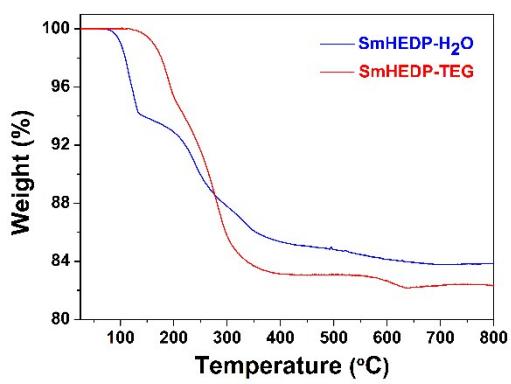


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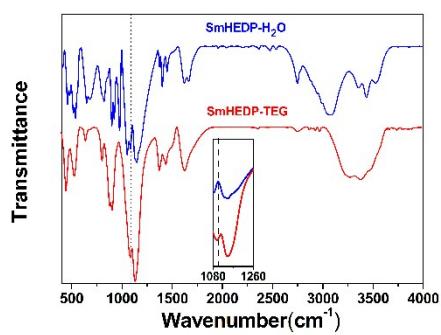


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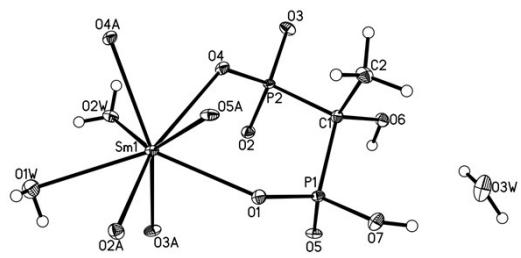


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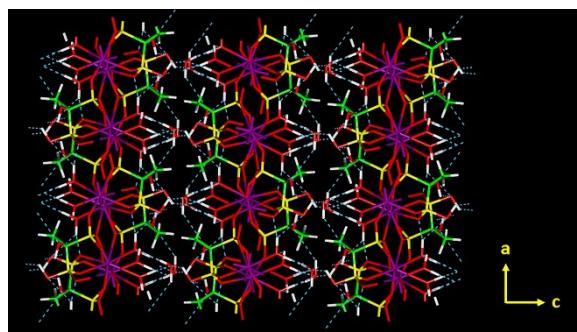


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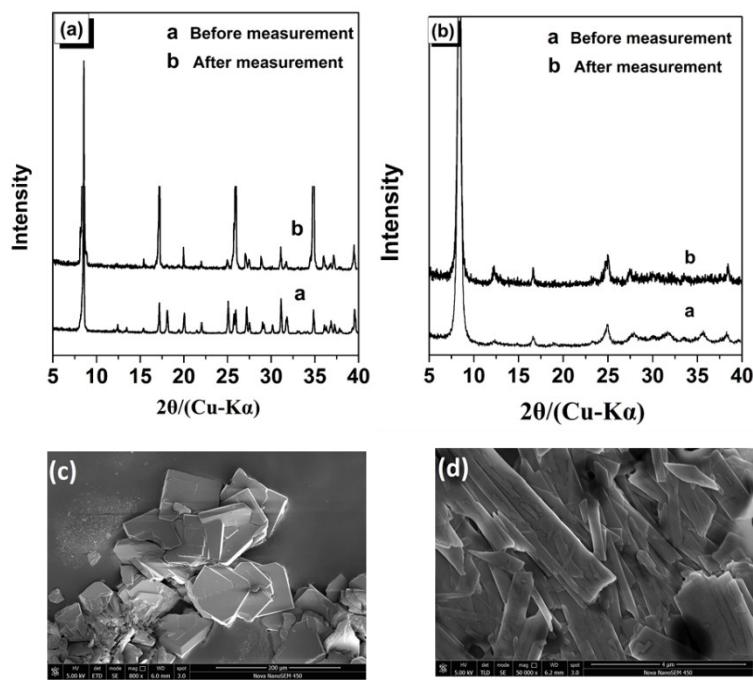


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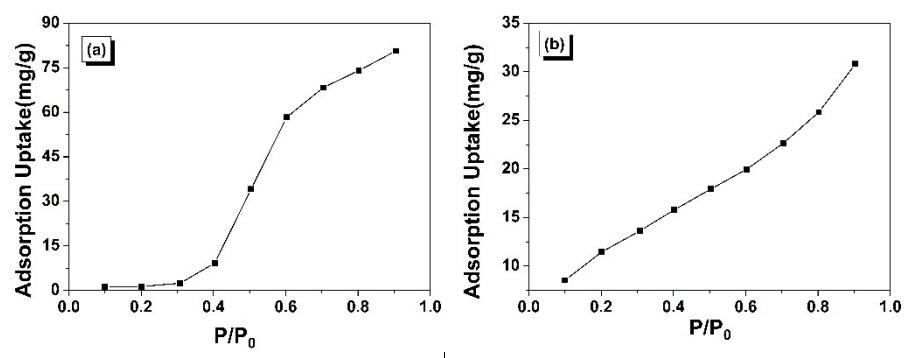


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