Electronic Supplementary Information

Atom orientation in the SBU induced conformational isomerism in the hydroxamate-based In-MOFs

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Contents

1. The table of selected bond lengths and bond angles, and hydrogen bonds

Table S1 Selected bond lengths (Å) and angles (°) for **1**-**3**.

1		**2**		**3**	
In1-O1	2.164(3)	In1-O1	2.145(6)	In1-O1	2.242(14)
In1-O2	2.171(3)	In1-O2	2.194(6)	In1-O3	2.28(3)
In1-O4^{i}	2.167(3)	In1-O3^{i}	2.144(6)	In1-O2	2.267(4)
In1-O5	2.117(3)	In1-O4^{i}	2.164(6)	In1-N2	2.405(6)
In1-O3^{i}	2.149(3)	In1-O5	2.159(6)	N2-C6	1.336(9)
In1-O6	2.172(3)	In1-O6	2.193(6)	N2-C7	1.327(9)
In1···In1^{ii}	11.178(3)	In1···In1^{ii}	11.276(6)	N1-C1	1.447(18)
In1···In1^{iii}	11.424(3)	In1···In1^{iii}	11.478(6)	N1-O1	1.361(17)
O5-In1-O2	91.81(14)	O5-In1-O4^{i}	101.5(2)	O1^{i}-In1-O1	127.8(10)
O3^{i}-In1-O2	90.75(12)	O1-In1-O5	161.4(2)	O1-In1-O3	141.8(9)
O5-In1-O4^{i}	102.15(14)	O2-In1-O1	75.5(2)	O1-In1-O3^{i}	73.0(11)
O3^{i}-In1-O4^{i}	75.68(10)	O2-In1-O4^{i}	163.3(2)	O1-In1-O2	74.3(4)
O2-In1-O4^{i}	160.50(13)	O5-In1-O3^{i}	85.7(2)	O3-In1-O2^{i}	74.0(8)
O5-In1-O1	159.70(13)	O6-In1-O2	94.9(2)	O3-In1-O2	143.9(8)
O1-In1-O6	90.23(11)	O3^{i}-In1-O6	157.1(2)	O1^{i}-In1-N2	71.6(5)
O4^{i}-In1-O1	93.38(11)	O3^{i}-In1-O1	110.4(2)	O3^{i}-In1-N2	74.8(10)
O2-In1-O1	76.69(11)	O5-In1-O6	74.3(2)	O2^{i}-In1-N2	136.26(19)
O5-In1-O6	76.37(12)	O2-In1-O6	94.9(2)	O1-In1-N2	141.8(4)
O3^{i}-In1-O6	160.11(12)	O3^{i}-In1-O4^{i}	76.8(2)	O3-In1-N2	70.4(8)

Symmetry codes: **1**: i) *x*-1, *y*-1, *z*; ii) 1+*x*, 1+*y*, *z*; iii) 1-*x*, -*y*, -*z*. **2**: i) *x*, *y*+1, *z*; ii) *x*, *y*-1, *z*; iii) 1-*x*, 1-*y*, 1-*z*. **3**: i) 1-*x*, *y*, 1.5-*z*.

Table S2 The Hydrogen-bond geometry (Å, °) in **1** and **2**.

MOF	D–H···A	d(D–H)	d(H···A)	d(D···A)	∠D–H···A
1	N1-H1A···O3^{i}	0.90	2.20	3.047(3)	158
	N2-H2A···O1^{ii}	0.90	2.09	2.831(3)	140
	N3-H3A···O7^{iii}	0.90	1.91	2.716(3)	148
	C11-H11···O7^{iii}	0.93	2.40	3.213(3)	146
	C15-H15B···O1W	0.96	2.26	3.031(2)	136
	O1W-H1WA···O5^{iv}	0.85	1.89	2.737(2)	174
	O1W-H1WB···O6	0.85	2.34	3.185(3)	175
2	N1-H1···O1W^{i}	0.86	1.93	2.763(2)	163
	N2-H2···O5^{ii}	0.86	2.05	2.832(3)	151
	N3-H3B···O1^{iii}	0.86	2.04	2.758(3)	140
	C4-H4···O2W^{i}	0.93	2.41	3.314(2)	166
	O1W-H1WA···N3	0.85	2.62	3.235(3)	131

O1W-H1WB···O2	0.85	2.20	2.964(3)	151
O2W-H2WA···O3^{iv}	0.85	2.32	2.933(2)	130
O2W-H2WB···O5^{v}	0.85	2.53	3.042(4)	120
O3W-H3WA···O2W	0.85	2.03	2.877(3)	171
O3W-H3WB···O1W	0.85	1.86	2.671(3)	159
O4W-H4WB···O3W	0.85	2.65	3.214(2)	125
O5W-H5WB···O4W	0.85	2.30	3.050(5)	148

Symmetry codes: **1**: i) *x*, *y*-1, *z*; ii) *x*, 1+*y*, *z*; iii) -*x*, 1-*y*, -*z*; iv) 1+*x*, *y*, *z*. **2**: i) *x*-1, *y*, *z*; ii) 1-*x*, 1-*y*, -*z*; iii) *x*+1, *y*, *z*; iv) 1-*x*, -*y*, -*z*; v) *x*, *y*-1, *z*.

Table S3 The Hydrogen-bond geometry (Å, °) in MOF **3**.

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠D–H···A
N1–H1···O1^{i}	0.86	1.83	2.539(4)	138
N3–H3B···O4	0.89	1.90	2.787(4)	171
C7–H7···O2	0.93	2.44	3.005(4)	119
C4–H4···O4^{ii}	0.93	2.20	2.983(4)	141

Symmetry codes: i) 1.5-*x*, 1.5-*y*, 2-*z*; ii) *x*+0.5, *y*+0.5, *z*.

2. Photographs of crystals for 1-3

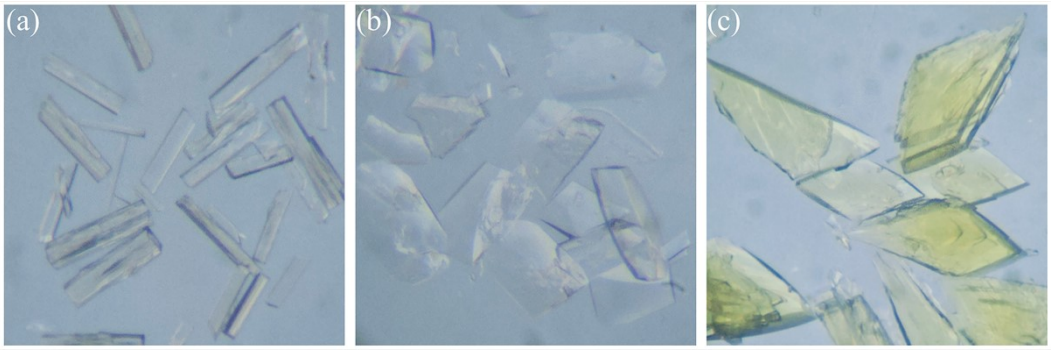

Fig. S1 Optical images of crystals for MOFs **1** (a), **2** (b) and **3** (c).

3. The asymmetric units of 1 and 2

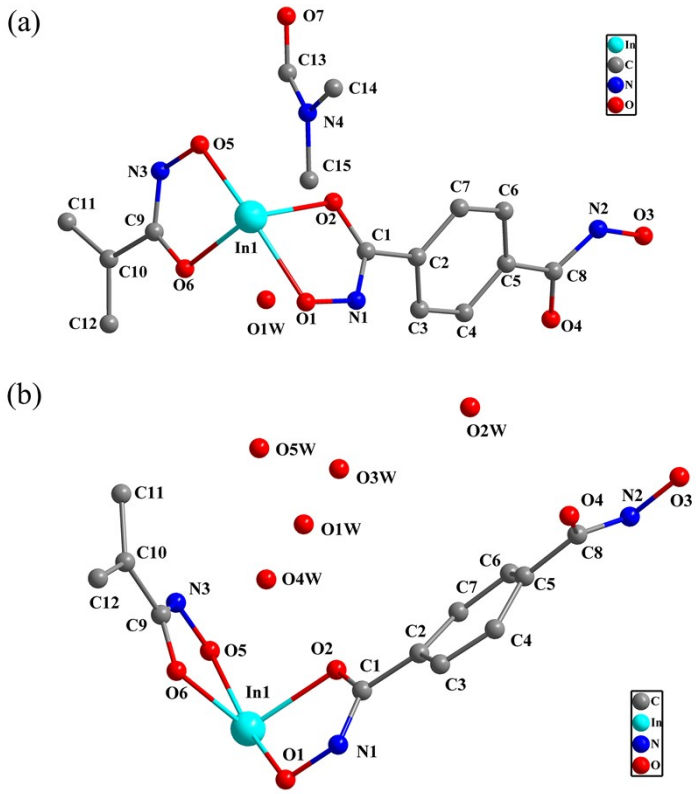

Fig. S2 The asymmetric units of **1** (a) and **2** (b) (Hydrogen atoms have been omitted for clarity).

4. The hydrogen-bond interactions of 1 and 2

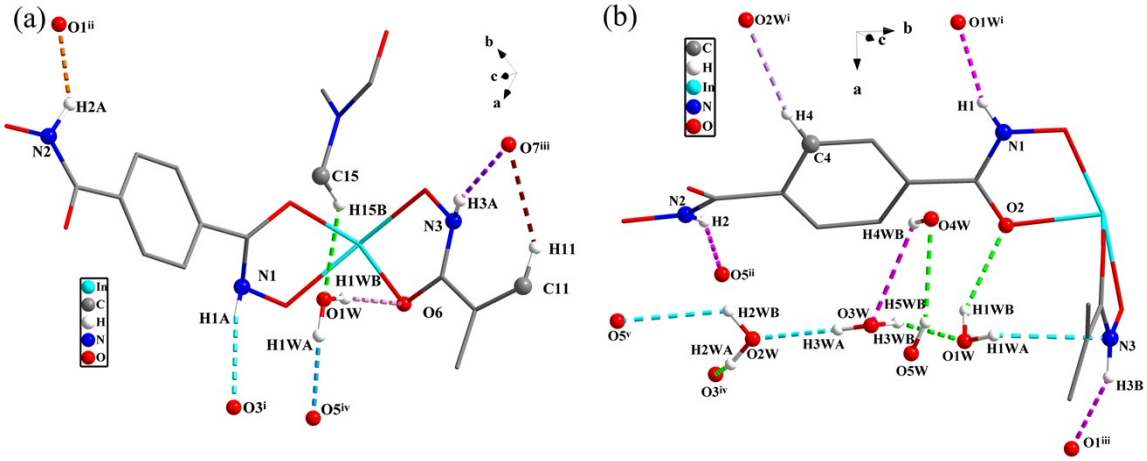

Fig. S3 Hydrogen-bond interactions in **1** (a) and **2** (b).

5. The structural stacking diagrams of 1 and 2

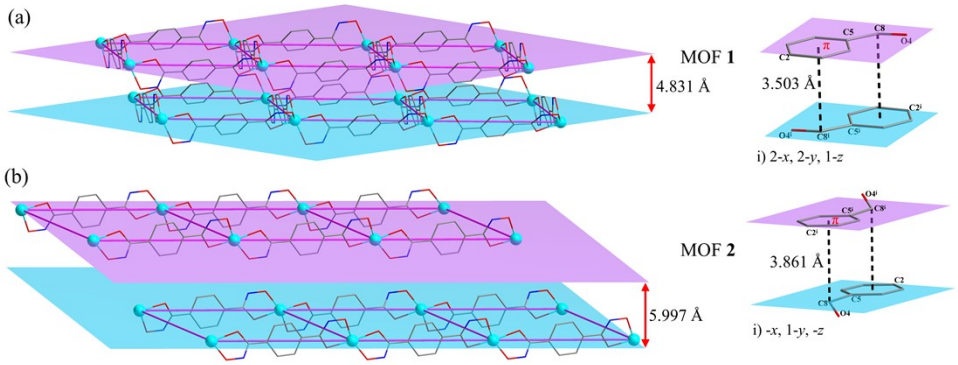

Fig. S4 The structural stacking diagrams in **1** (a) and **2** (b).

6. The asymmetric unit of 3

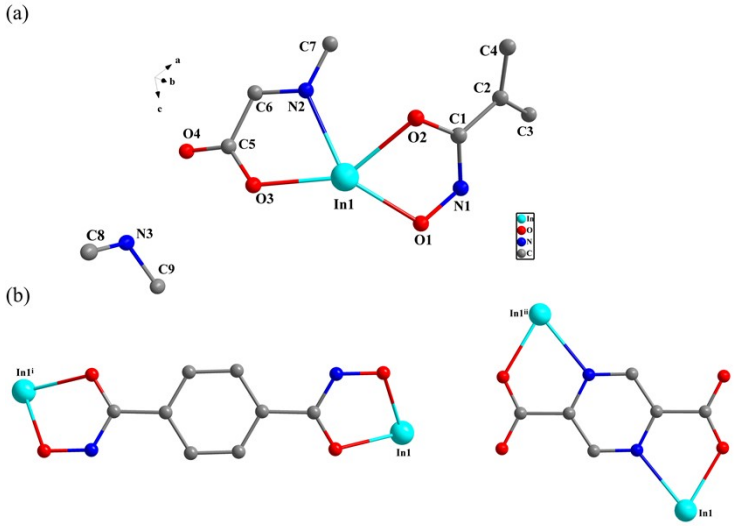

Fig. S5 (a) The asymmetric unit of **3**; (b) the coordination modes of L^{2-} and $pzdc^{2-}$ ligands (Hydrogen atoms have been omitted for clarity).

7. The hydrogen-bond interactions of 3

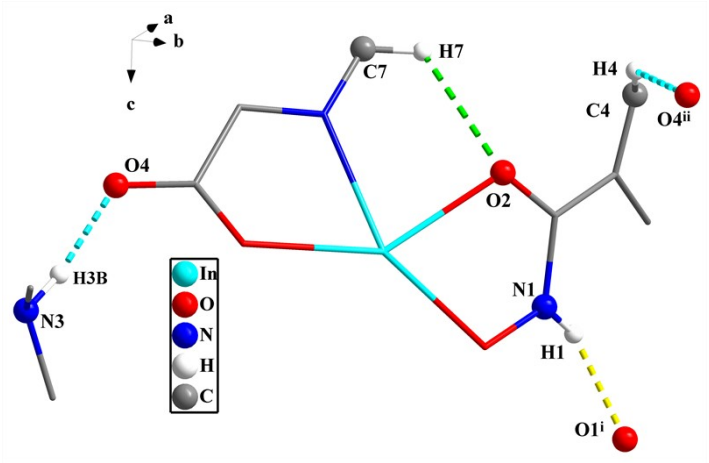

Fig. S6 Hydrogen-bond interactions in MOF **3**.

8. The FT-IR spectra of 1-3

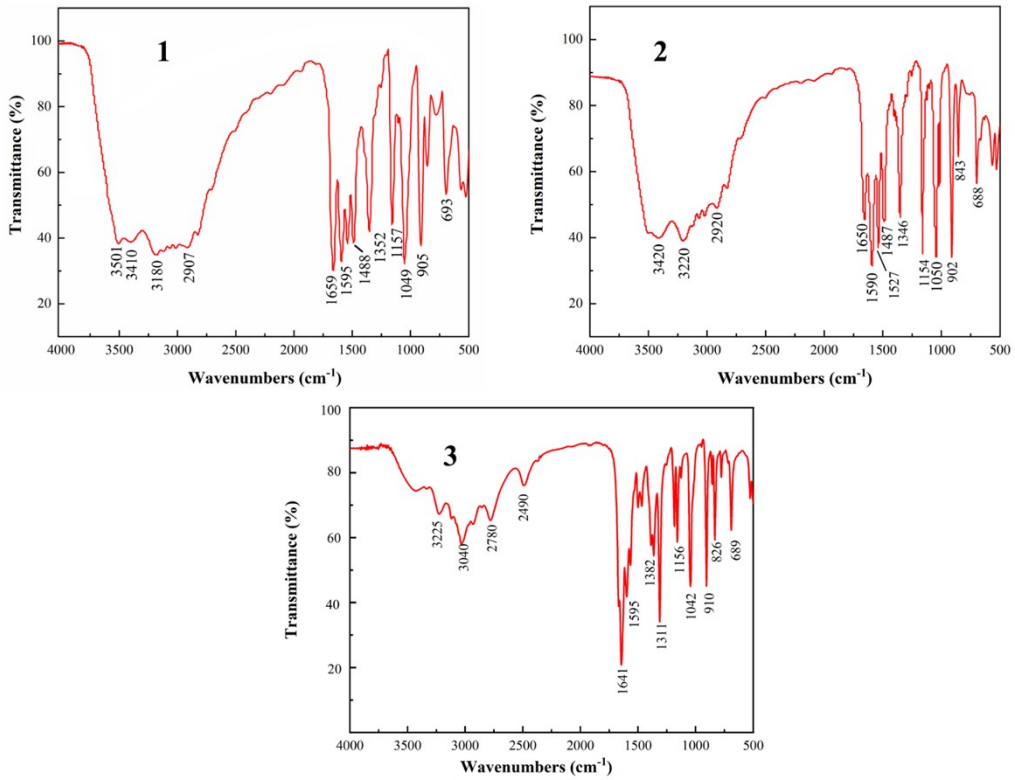

Fig. S7 The IR spectra of MOFs **1-3**.

9. The PXRD patterns of 1-3

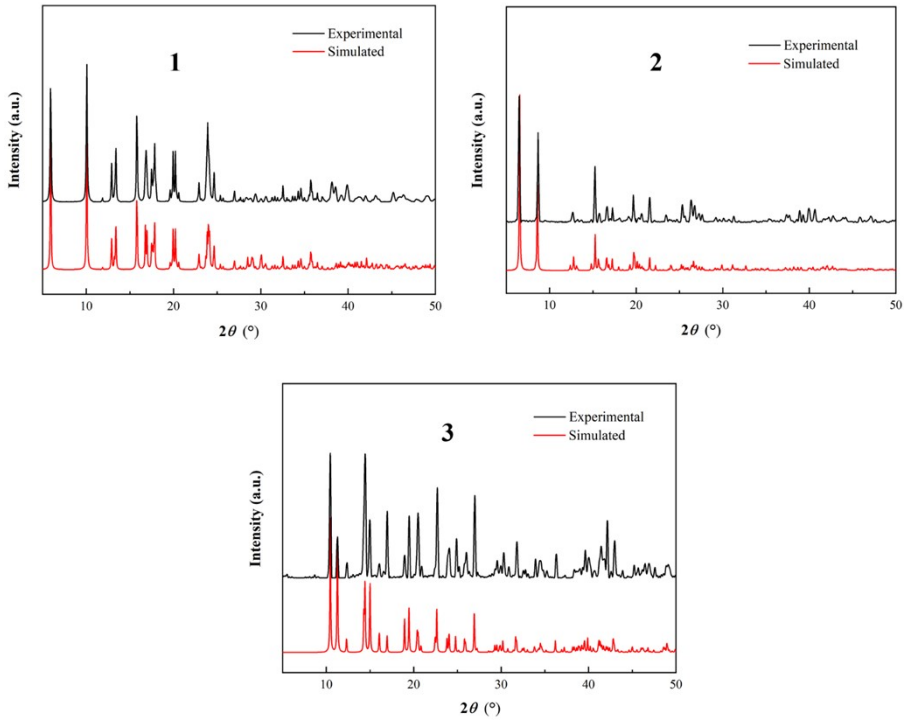

Fig. S8 The PXRD patterns of MOFs **1-3**.

10. The thermogravimetric analysis curves of 1-3

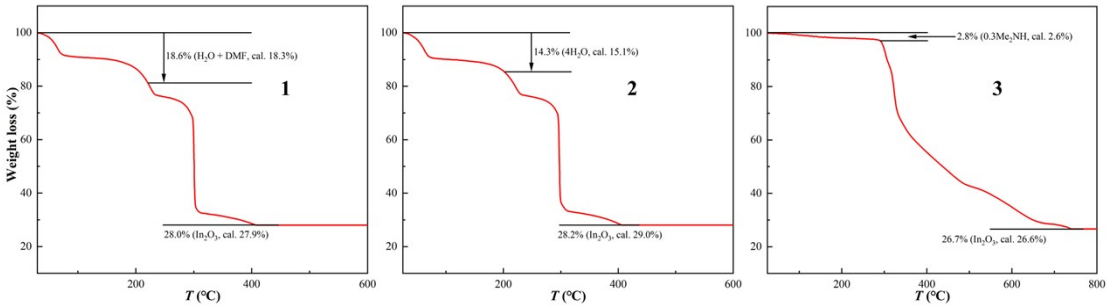

Fig. S9 Thermogravimetric analysis curves of MOFs **1-3**.

11. The water and chemical stabilities of 1 and 2

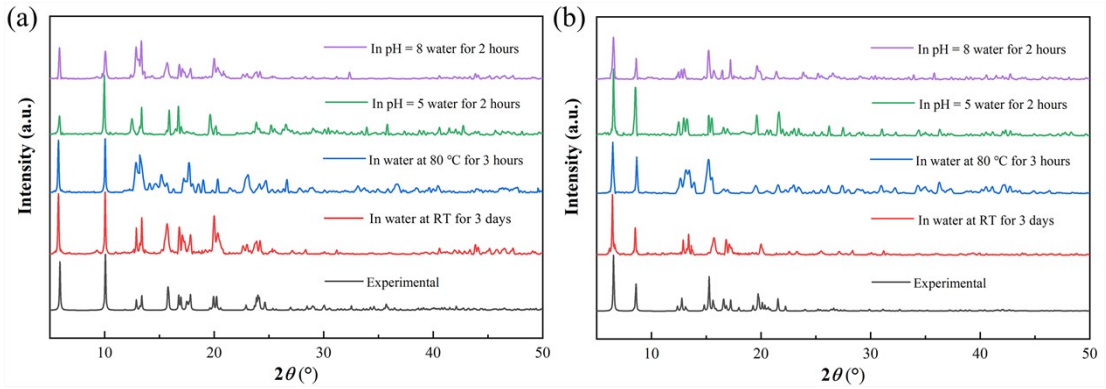

Fig. S10 Water and chemical stabilities of **1** (a) and **2** (b).

12. The organic solvent stabilities of 1-3

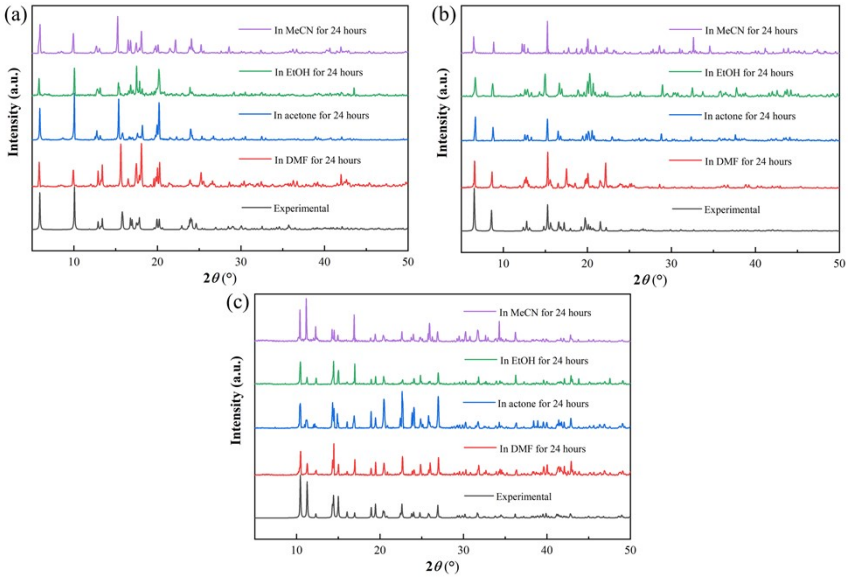

Fig. S11 The stabilities of **1-3** in some common organic solvents.

13. Proton conductivity of 3

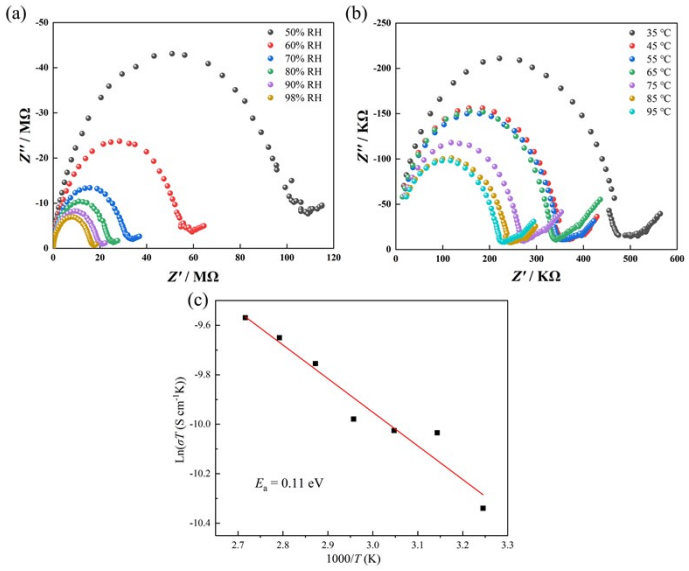

Fig. S12 (a) AC impedance spectra at variable RH (50-98%) at 25℃. (b) The variable temperature impedance spectra from 35 to 95 °C at 98% RH. (c) Arrhenius plot at 98% RH.

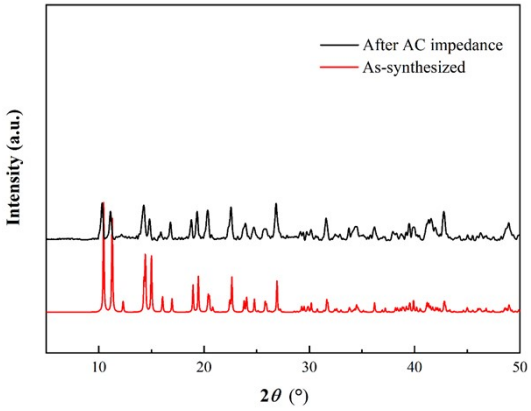

Fig. S13 PXRD patterns of as-synthesized **3** and after AC impedance measurements.

Table S4 Proton conductivities of **3** at RT and various RH.

RH (%)	σ (S cm^{-1})
50	8.93×10^{-8}
60	1.64×10^{-7}
70	2.91×10^{-7}
80	3.84×10^{-7}
90	1.04×10^{-6}
98	1.26×10^{-6}

Table S5 Proton conductivities of **3** at 98% RH and different temperature.

T (°C)	σ (S cm^{-1})
35	2.35×10^{-6}
45	3.20×10^{-6}
55	3.23×10^{-6}
65	3.39×10^{-6}
75	4.24×10^{-6}
85	4.70×10^{-6}
95	5.10×10^{-6}