Synthesis and Proton Conductivity of Two Novel Molybdate Polymers

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Table S1 Hydrogen bonds information of **1**.

D—H···A	D—H	H···A	D···A	D—H···A
O21—H21A···O28	0.850	2.121	149.72	2.888
O20—H20B···O17	0.844	1.976	168.30	2.808
C27—H27···O15	0.930	2.306	118.96	2.874
C27—H27···N1	0.930	2.528	112.67	3.011
C28—H28···O27	0.930	2.360	129.79	3.040
C36—H36···O28	0.930	2.238	135.18	2.971
C36—H36···N3	0.930	2.558	112.27	3.035
C35—H35···O5	0.930	2.533	146.74	3.349
C16—H16···O6	0.930	2.674	135.95	3.405
C16—H16···O22	0.930	2.608	111.88	3.078
C15—H15···O22	0.930	2.354	121.74	2.951
C15−H15···N6	0.930	2.603	112.00	3.075
C12—H12···O24	0.930	2.543	138.87	3.301
C12—H12···N6	0.930	2.521	111.67	2.992
C24—H24···O25	0.930	2.382	122.40	2.986

C24—H24···N2	0.930	2.593	111.39	3.057
C23—H23···O25	0.930	2.674	110.90	3.129
C3—H3···O17	0.930	2.448	145.01	3.254
C3—H3···N5	0.930	2.591	111.95	3.062
C4—H4···O14	0.930	2.546	123.11	3.151
O29—H29A···O24	0.845	2.244	140.64	2.947

Table S2 Hydrogen bonds information of **2**.

D—H···A	D—H	H···A	D···A	D—H···A
O15—H15A···O16	0.851	2.090	136.92	2.773
O15—H15B···O13	0.850	1.908	157.40	2.712
O16—H16A···O5	0.840	2.229	159.22	3.028
O16—H16B···O4	0.850	2.089	170.00	2.930
N1—H1···O15	0.980	1.755	163.10	2.708
N2—H2···O14	0.980	1.654	165.23	2.613
C1—H1A···O7	0.970	2.300	147.34	3.160
C1—H1B···O3	0.970	2.500	164.07	3.443
C1—H1B···O7	0.970	2.675	114.11	3.196
C2—H2A···O6	0.970	2.644	156.27	3.553
C2—H2A···O12	0.970	2.633	137.42	3.411
C2—H2B···O6	0.970	2.624	134.71	3.377
C3—H3A···O6	0.970	2.674	133.70	3.417
C3—H3B···O5	0.970	2.343	143.26	3.174
C4—H4A···O4	0.970	2.596	119.27	3.185
C4—H4B···O11	0.970	2.546	142.85	3.386
C5—H5···O10	0.970	2.546	121.11	3.159
C6—H6B···O10	0.970	2.487	140.63	3.294
C6—H6B···O11	0.970	2.577	142.53	3.398

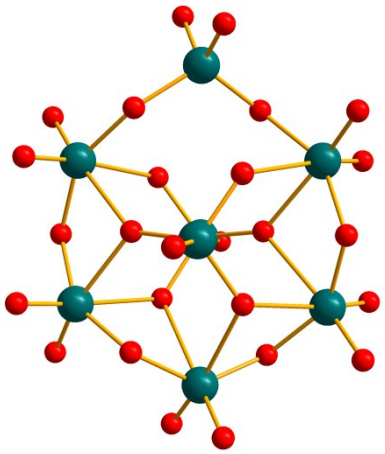

Fig. S1 The ball-and-stick representation of $[\tau\text{–}Mo_8O_{26}]^{4-}$; Color codes: Mo, dark green; O, red spheres.

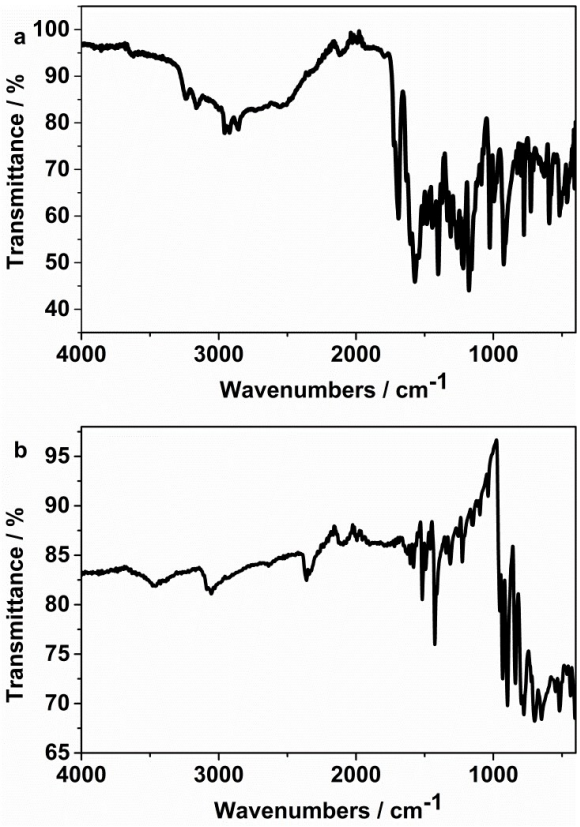

Fig. S2 **(a)** The FT-IR spectra of **1** from 4000-400 cm^{-1}; (b) The FT-IR spectra of **2** from 4000-400 cm^{-1}

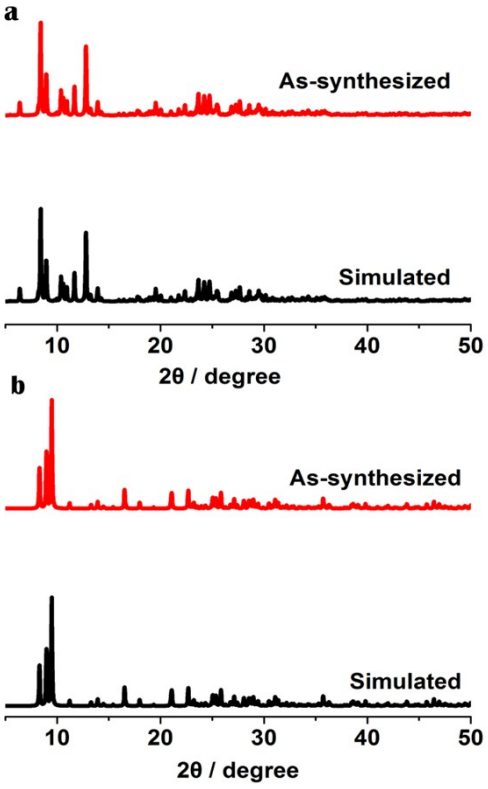

Fig. S3 (a) Powder X-ray diffraction patterns of simulated **1** and as-synthesized; (b) Powder X-ray diffraction patterns of simulated **2** and as-synthesized.

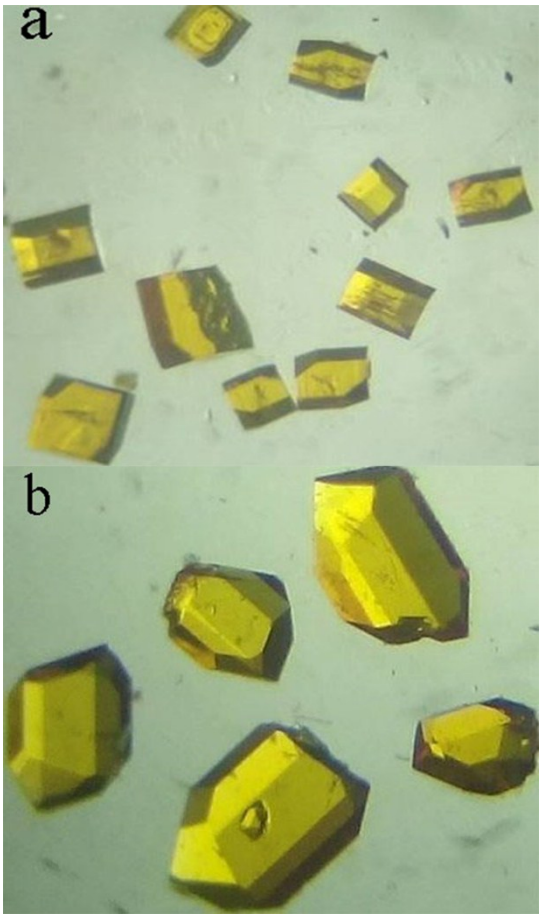

Fig. S4 (a) Crystal Photograph for **1** under optical microscope; (b) Crystal Photograph for **2** under optical microscope.

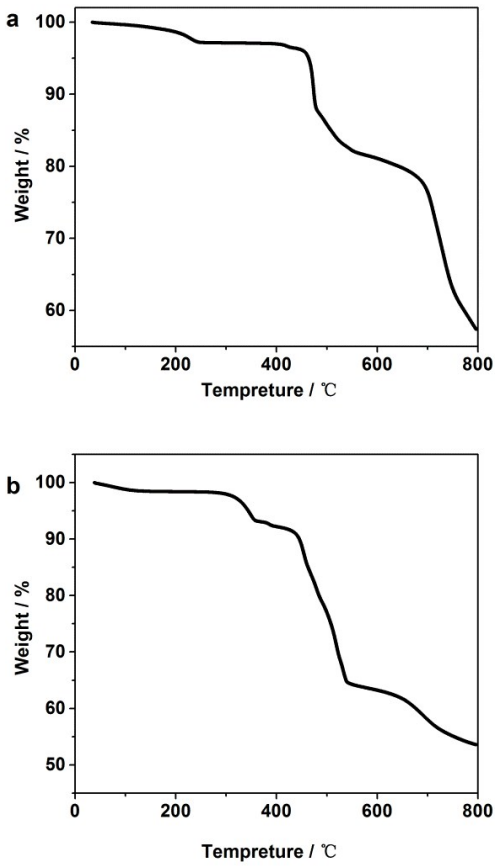

Fig. S5 (a) The thermogravimetric (TG) curves of **1**; (b) The thermogravimetric (TG) curves of **2** measured from 30 to 800 ℃ under N_2 atmosphere with the heating rate of 10 ℃/min.

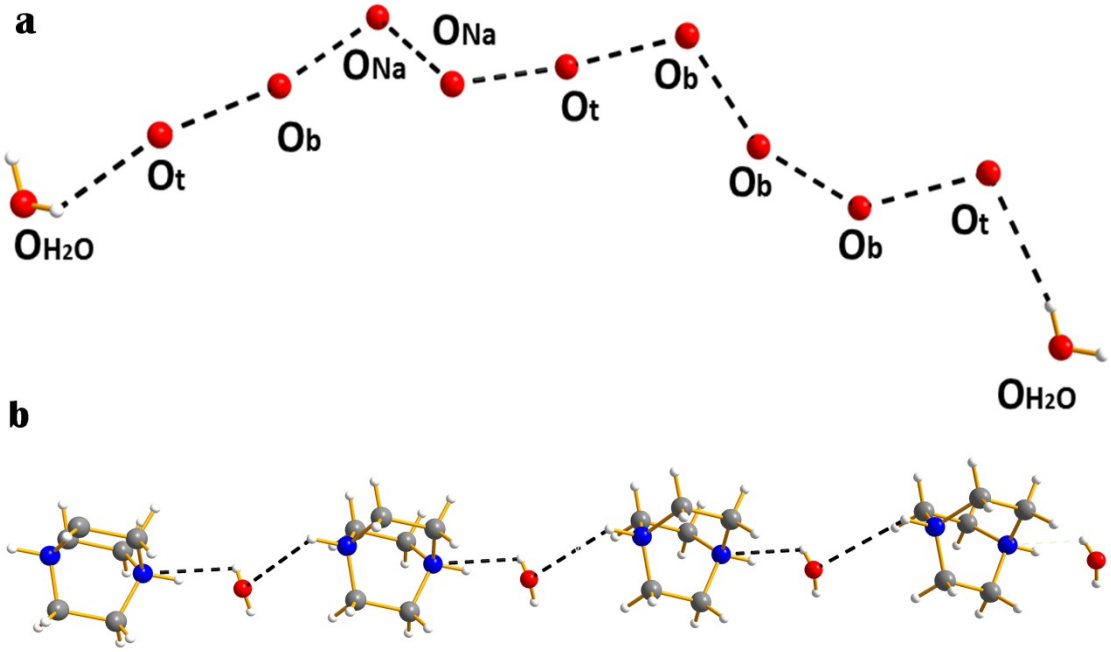

Fig. S6 (a) Simplified schematic representation of chains along 1D channels for **1**;(b) Simplified schematic representation of chains along 1D channels for **2**.

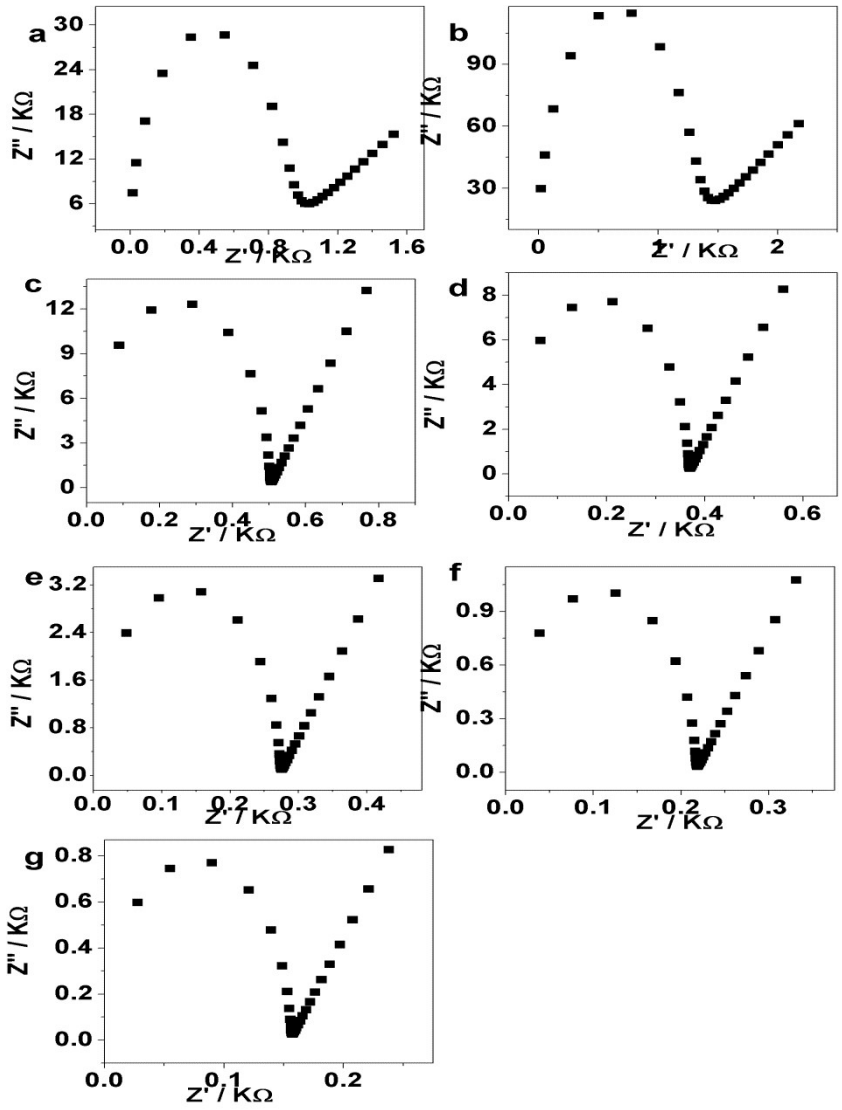

Fig. S7 Nyquist plots of **1** at 97% RH with various temperatures (a) 25 °C, (b) 35°C, (c) 45 °C, (d) 55°C, (e) 65 °C, (f) 75 °C, (g) 85°C

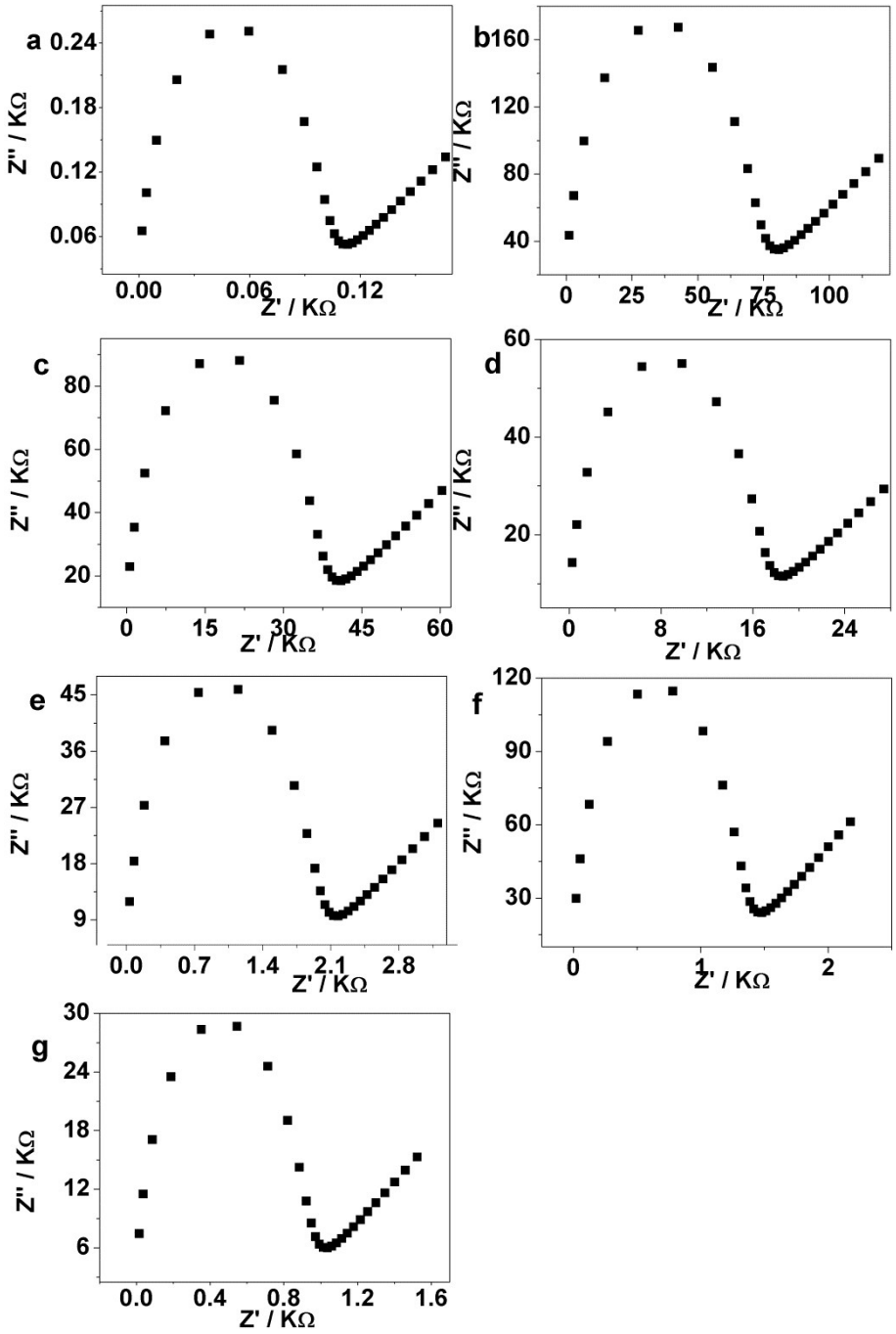

Fig. S8 Nyquist plots of **1** at 25 °C RH with various RH (a) 45%, (b) 55%, (c) 65%, (d) 75%, (e) 85%, (f) 95%, (g) 97%.

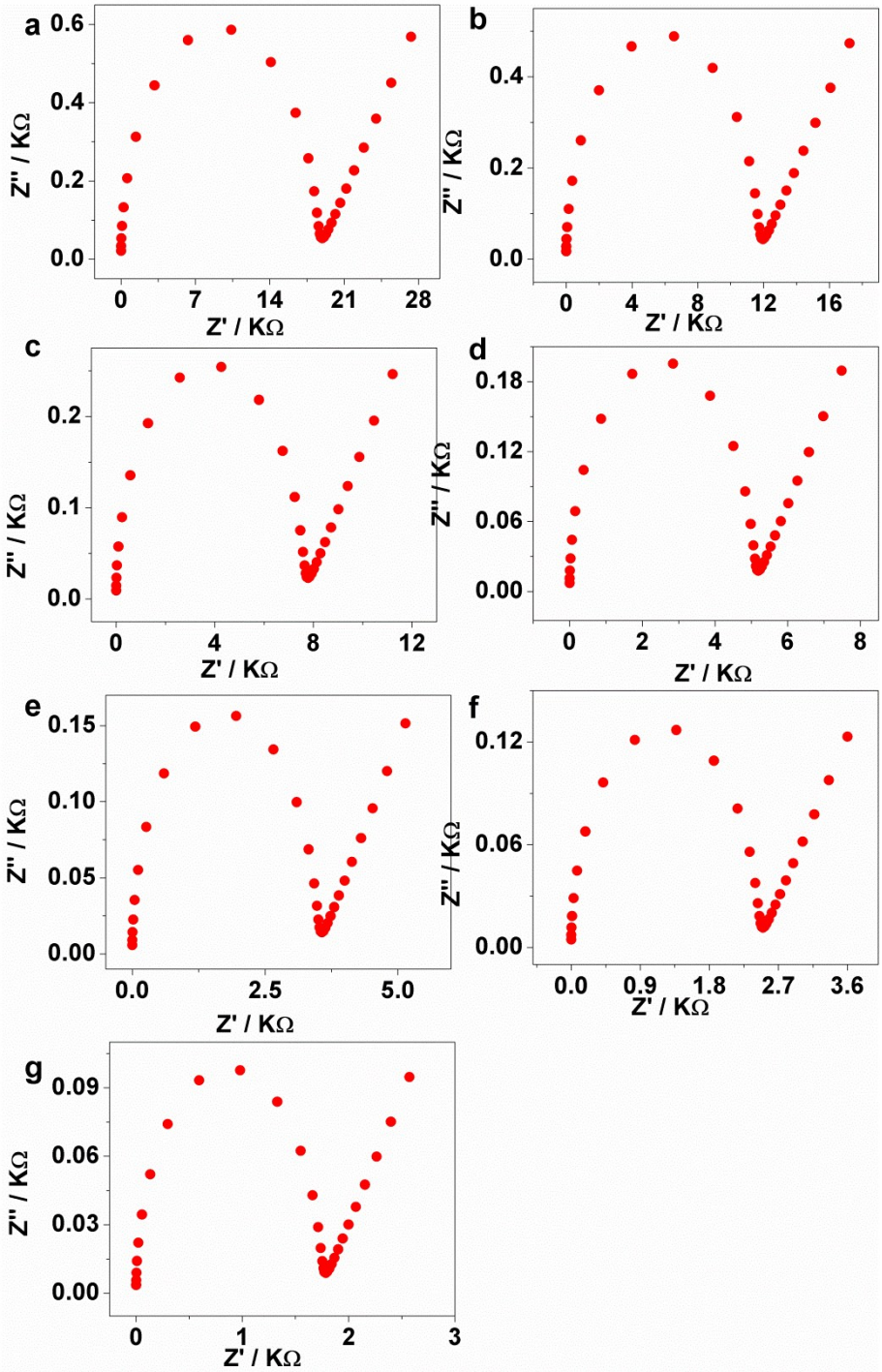

Fig. S9 Nyquist plots of **2** at 97% RH with various temperatures (a) 25 °C, (b) 35°C, (c) 45 °C, (d) 55°C, (e) 65 °C, (f) 75 °C, (g) 85°C

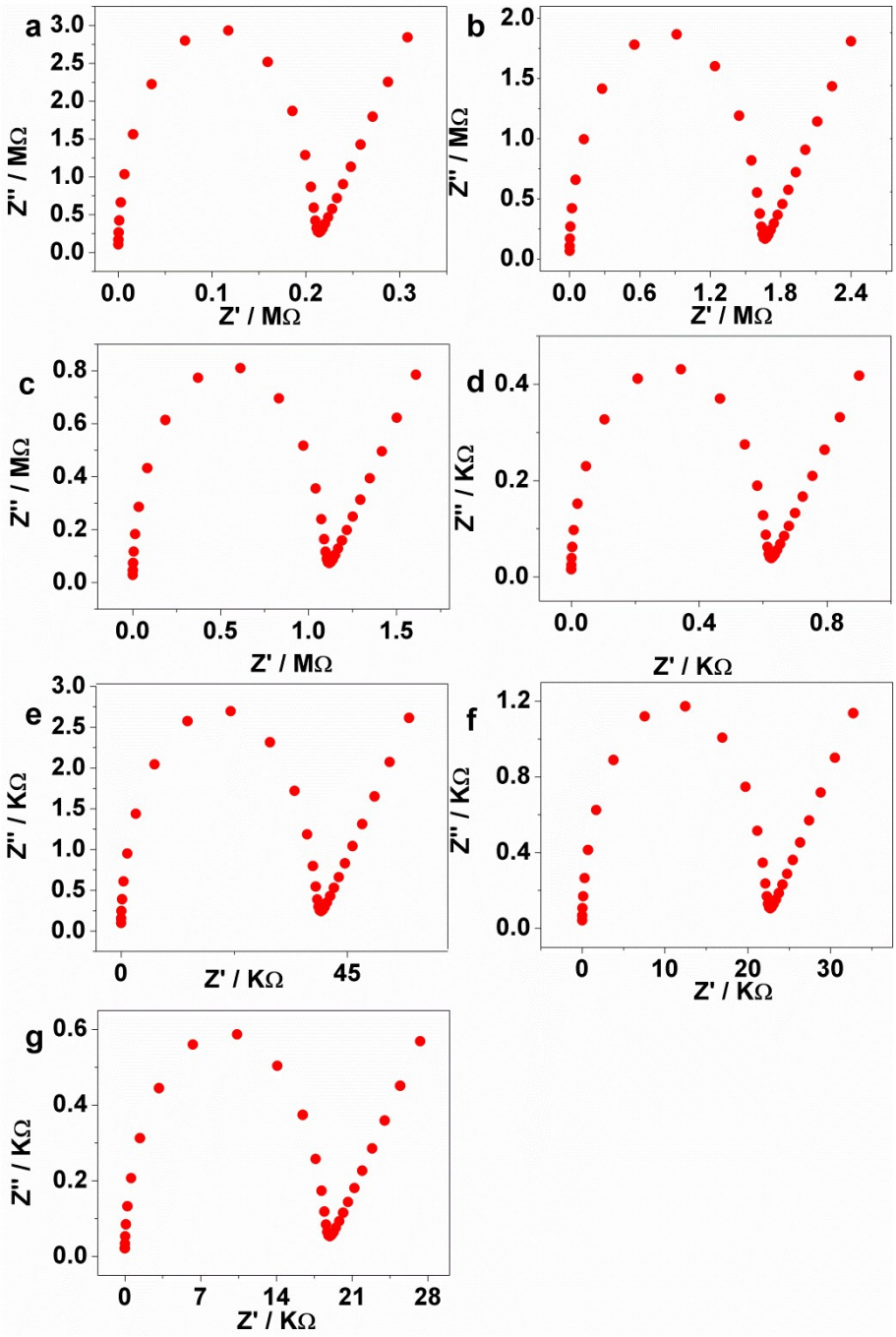

Fig. S10 Nyquist plots of **2** at 25 °C RH with various RH (a) 45%, (b) 55%, (c) 65%, (d) 75%, (e) 85%, (f) 95%, (g) 97%.

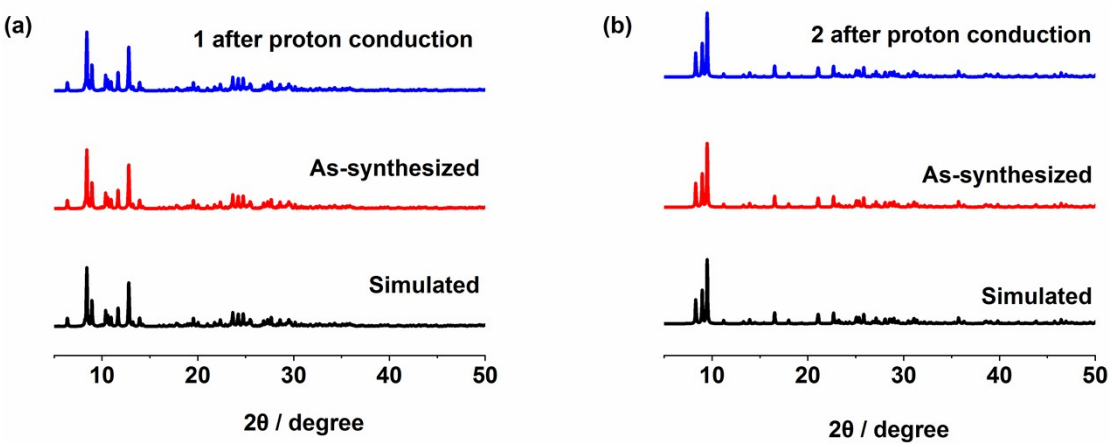

Fig. S11 (a) Powder X-ray diffraction patterns of **1** afer proton conduction test; (b) Powder X-ray diffraction patterns of **2** afer proton conduction test.