Electronic Supplementary Material (ESI) for Dalton Transactions.

Water stable oxalate-based coordination polymers with in situ generated cyclic dipeptides showing high proton conductivity

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Physical measurements:

IR spectra (KBr pellets) were recorded on a Nicolet Impact 410 FTIR spectrometer. Powder X-ray diffraction (XRD) data were obtained using a Shimazu XRD-6100 diffractometer with Cu-Kα radiation (λ = 1.5418 Å). 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. Magnetic measurement was performed on the Quantum Design SQUID MPMS XL-7 magnetometer in a magnetic field of 1000 Oe in the temperature range of 2-300 K. 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] Alternating current impedance measurements were carried out with a Solartron SI 1260 impedance/gain-phase analyzer over the frequency range from 0.1 Hz to 10 MHz with an applied voltage of 10 mV. The relative humidity was controlled by a STIK Corp. CIHI-150B incubator. The sample was pressed to form a cylindrical pellet of crystalline powder sample (~2 mm thickness ×5 mm ϕ) coated with C-pressed electrodes. Two silver electrodes were attached to both sides of pellet to form four end terminals (quasi-four-probe method).

Reference

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

Table S1. Hydrogen bond information for SCU-63

D-H···A[a]	d(D-H) (Å)	d(H···A) (Å)	d(D···A) (Å)	<(DHA) (deg)
N1-H1···O2#1	0.86	2.16	2.870(3)	139.2
N2-H2···O3	0.86	1.91	2.768(3)	174.8
N3-H3···O4	0.86	2.15	2.993(3)	166.4
N4-H4···O5#2	0.86	2.27	2.872(3)	127.0
N4-H4···O13#3	0.86	2.28	3.004(3)	142.4
N5-H5···O10	0.86	2.14	2.753(3)	127.9
N6-H6···O7#4	0.86	2.09	2.947(3)	175.8

[a] Symmetry transformations used to generate equivalent atoms: #1 -1+X,1+Y,+Z; #2 2-X,1-Y,1-Z; #3 1-X,1-Y,1-Z; #4 1-X,2-Y,1-Z.

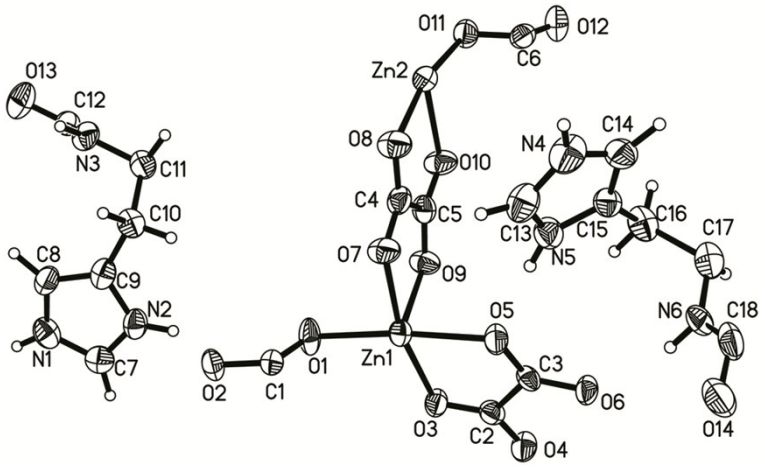

Fig. S1. ORTEP plot of the asymmetric unit of SCU-63, showing the labeling scheme and the 50% probability displacement ellipsoid.

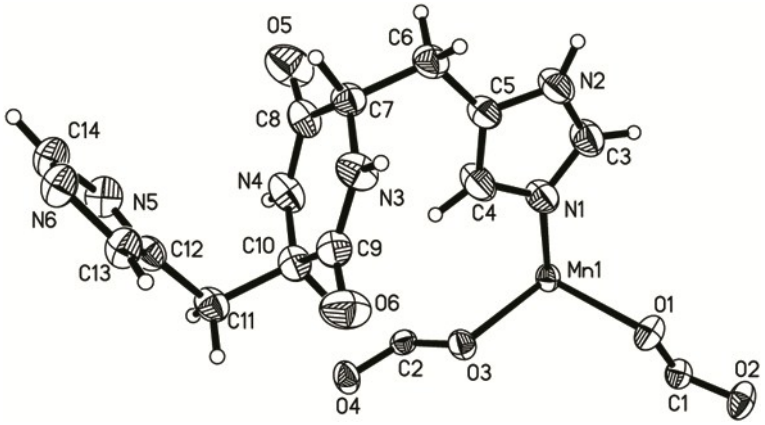

Fig. S2. ORTEP plot of the asymmetric unit of SCU-66, showing the labeling scheme and the 50% probability displacement ellipsoid.

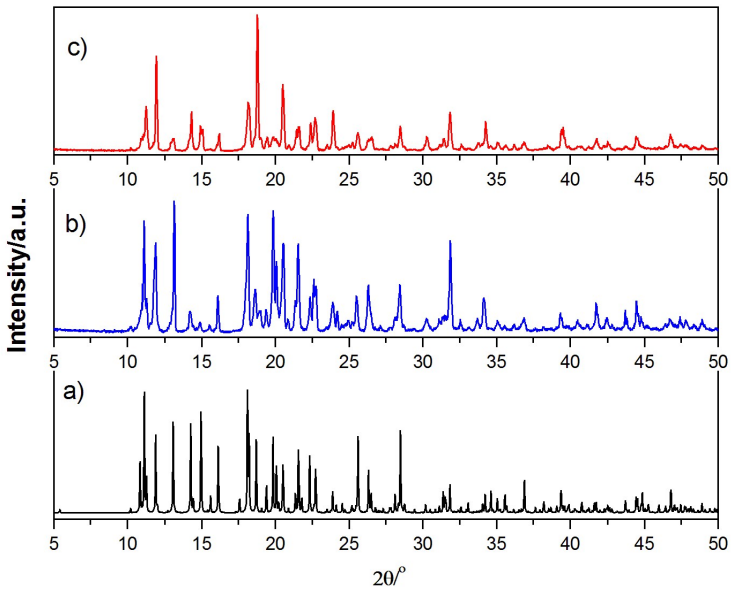

Fig. S3. Experimental and simulated powder XRD patterns of SCU-63: (a) Simulated; (b) as-synthesized; (c) after impedance measurements.

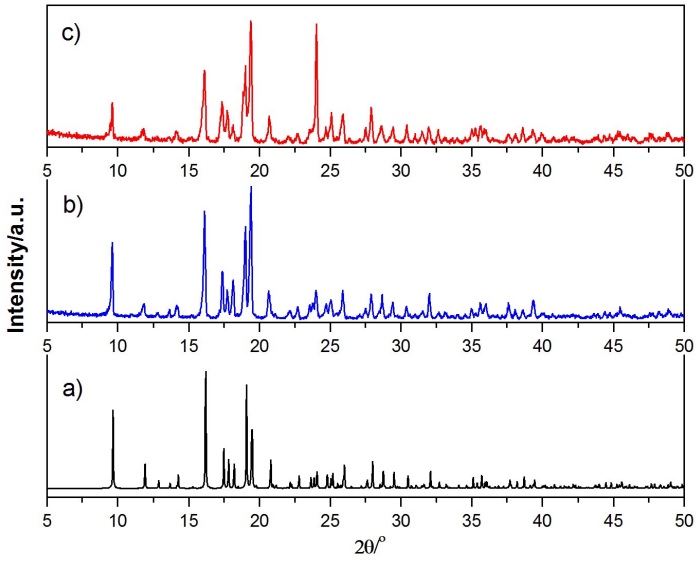

Fig. S4. Experimental and simulated powder XRD patterns of SCU-66 : (a) Simulated; (b) as-synthesized; (c) after impedance measurements.

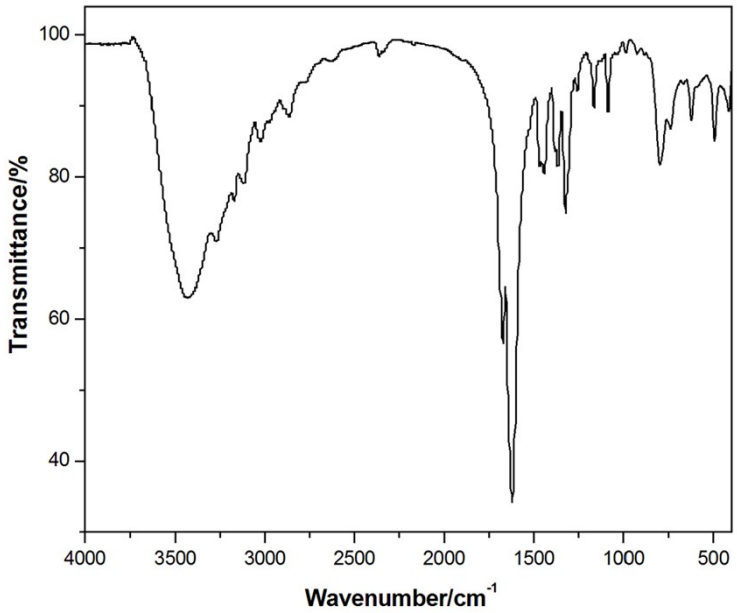

Fig. S5. IR spectrum of SCU-63.

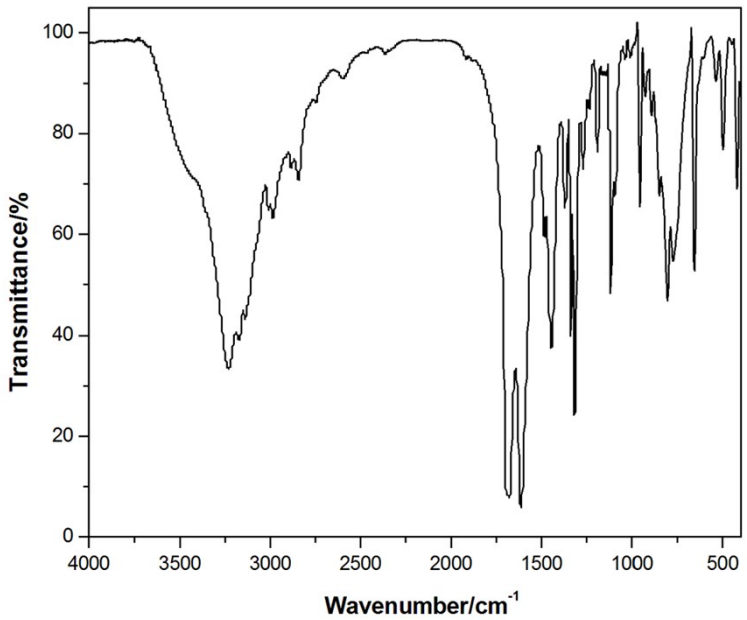

Fig. S6. IR spectrum of SCU-66.

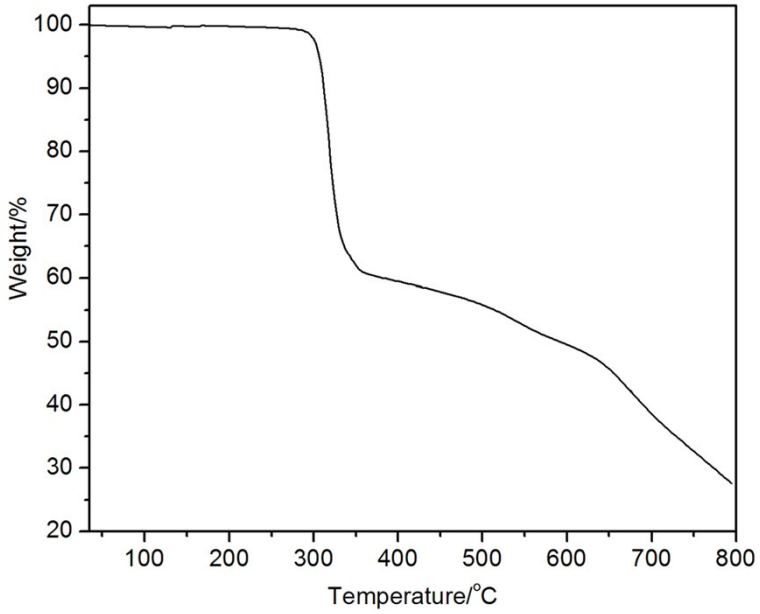

Fig. S7. TGA curve of SCU-63.

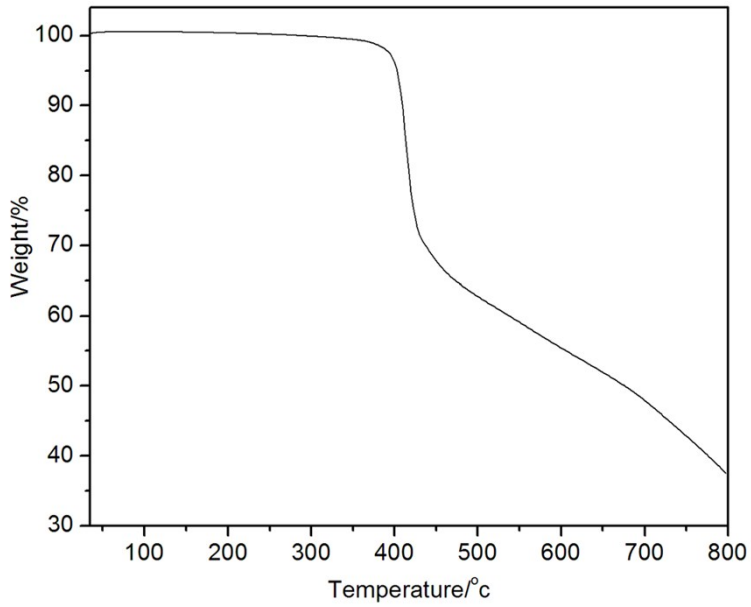

Fig. S8. TGA curve of SCU-66.

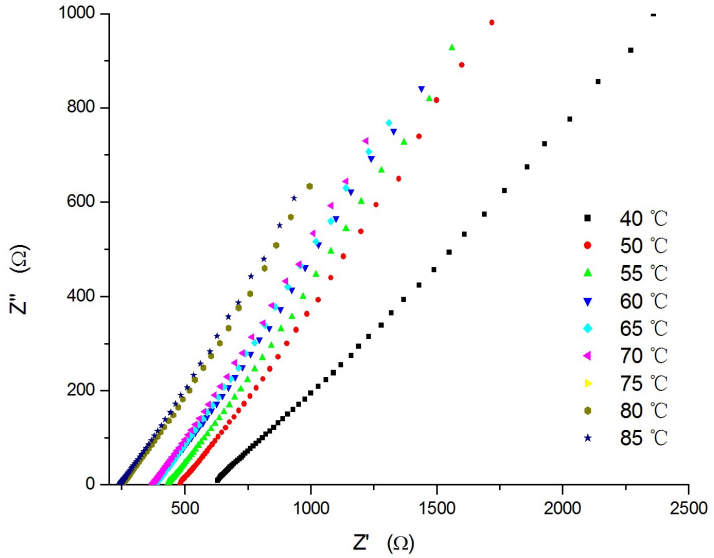

Fig. S9. Nyquist plot of SCU-63 at different temperature under 98% relative humidity. The conductivity is 1.7×10^{-3} S·cm^{-1} (40 °C), 2.2×10^{-3} S·cm^{-1} (50 °C), 2.5×10^{-3} S·cm^{-1} (55 °C), 2.7×10^{-3} S·cm^{-1} (60 °C), 2.8×10^{-3} S·cm^{-1} (65 °C), 3.1×10^{-3} S·cm^{-1} (70 °C), 3.4×10^{-3} S·cm^{-1} (75 °C), 3.8×10^{-3} S·cm^{-1} (80 °C), and 4.2×10^{-3} S·cm^{-1} (85 °C) for SCU-63.

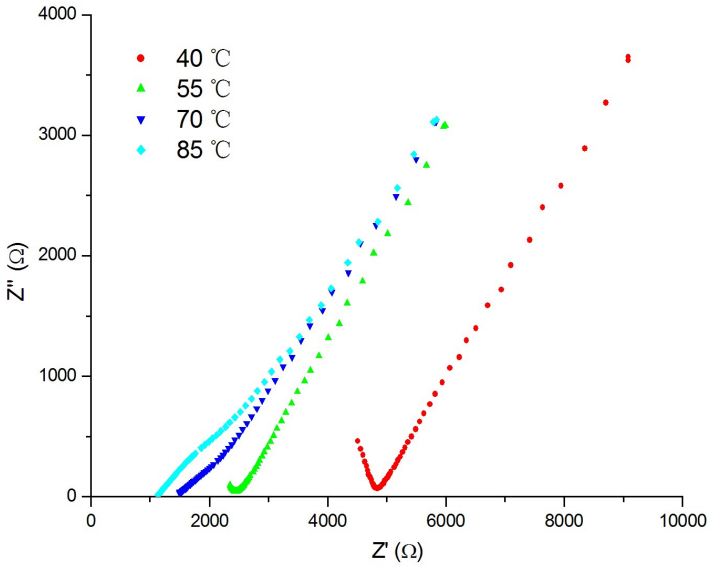

Fig. S10. Nyquist plot of SCU-66 at different temperature under 98% relative humidity. The conductivity is 3.1×10^{-4} S·cm^{-1} (40 °C), 6.2×10^{-4} S·cm^{-1} (55 °C), 9.9×10^{-4} S·cm^{-1} (70 °C), and 1.3×10^{-3} S·cm^{-1} (85 °C) for SCU-66.