Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Proton conduction via lattice water molecules in oxalato-bridged lanthanide porous coordination polymers

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TableS1. Summary of cell parameters for **1** and **2** obtained by Le Bail refinements. PXRD data for **1** and **2** were collected at room temperature.

Cell parameters	**1**	**2**
Space group	monoclinic	hexagonal
a / Å	11.390	30.567
b / Å	9.632	30.567
c / Å	10.503	7.171
α / °	90.000	90.000
β / °	114.585	90.000
γ / °	90.000	120.000
V / Å^3	1047.83	5802.99
R_p / %	5.05	4.24
R_e / %	5.24	3.90
R_{wp} / %	6.40	5.46
S	1.2225	1.4002

Table S2. Summary of fitting parameters for **1** and **2** obtained by the Jonscher's power law.

Compound **1**	T / K	σ_0 / S cm^{-1}	A / S cm^{-1} S^n	n
	368	3.41×10^{-7}	7.22×10^{-16}	1.66
	362	2.99×10^{-7}	9.59×10^{-16}	1.65
	352	2.29×10^{-7}	2.39×10^{-15}	1.59
	343	1.66×10^{-7}	6.33×10^{-15}	1.54
Compound **2**	T / K	σ_0 / S cm^{-1}	A / S cm^{-1} S^n	n
	363	1.80×10^{-6}	2.83×10^{-14}	1.33
	353	1.68×10^{-6}	4.46×10^{-14}	1.31
	343	1.25×10^{-6}	1.12×10^{-13}	1.27
	322	5.29×10^{-7}	4.64×10^{-14}	1.37

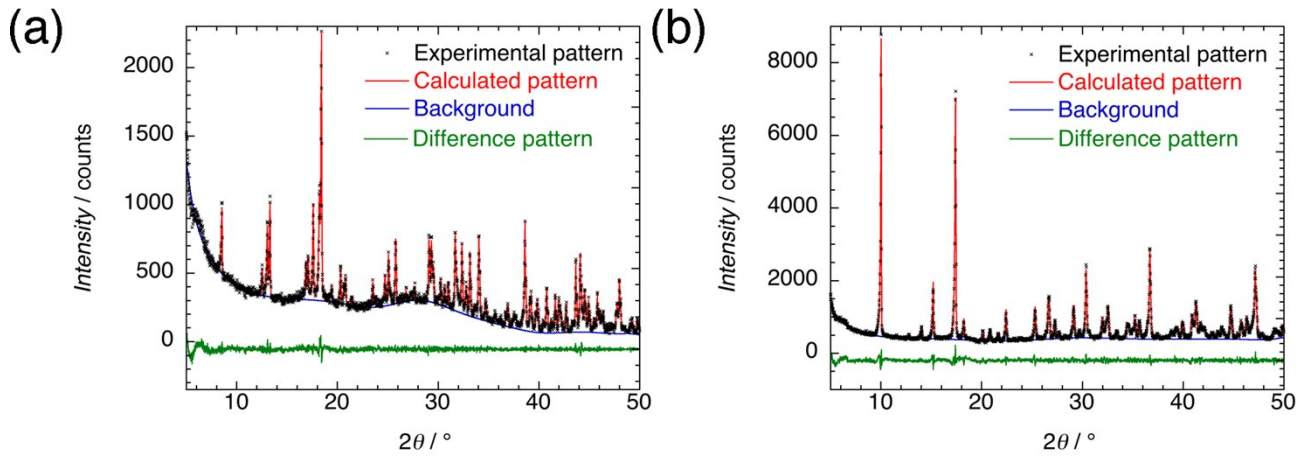

Fig. S1. Le Bail refinements of the PXRD patterns of (a) **1** and (b) **2**. The calculated patterns (solid red lines) agree with the experimental data (crosses) as evidenced by the difference pattern (solid green line) Solid blue lines are background. PXRD data for **1** and **2** were collected at room temperature.

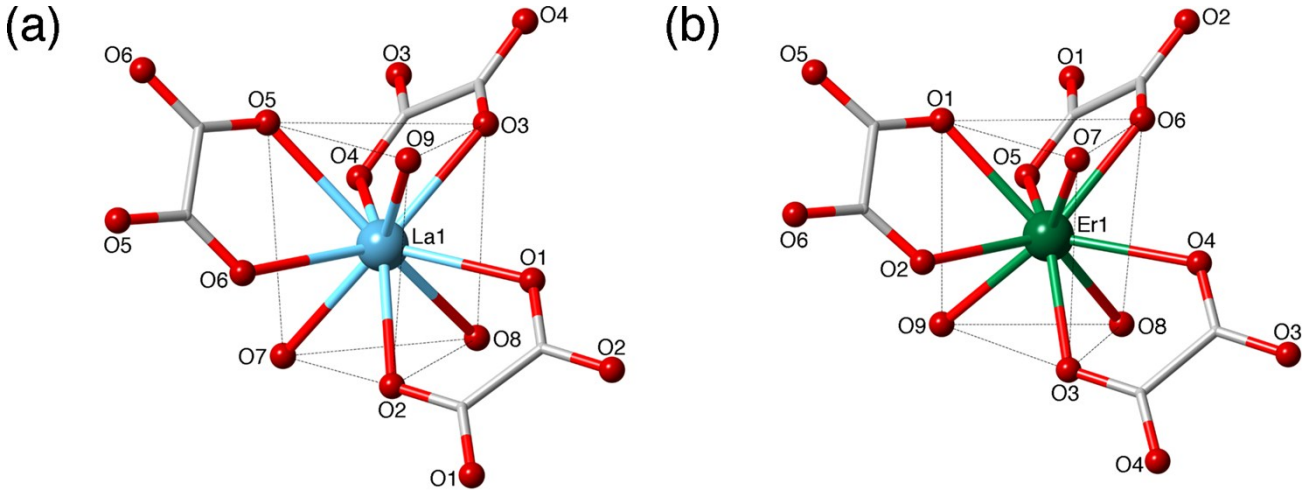

Fig. S2. Tricapped trigonal prismatic metal coordination environments in (a) **1** and (b) **2**. Light blue, green, gray and red balls and sticks represent La, Er, C, and O atoms, respectively. The H atoms are omitted for clarity.

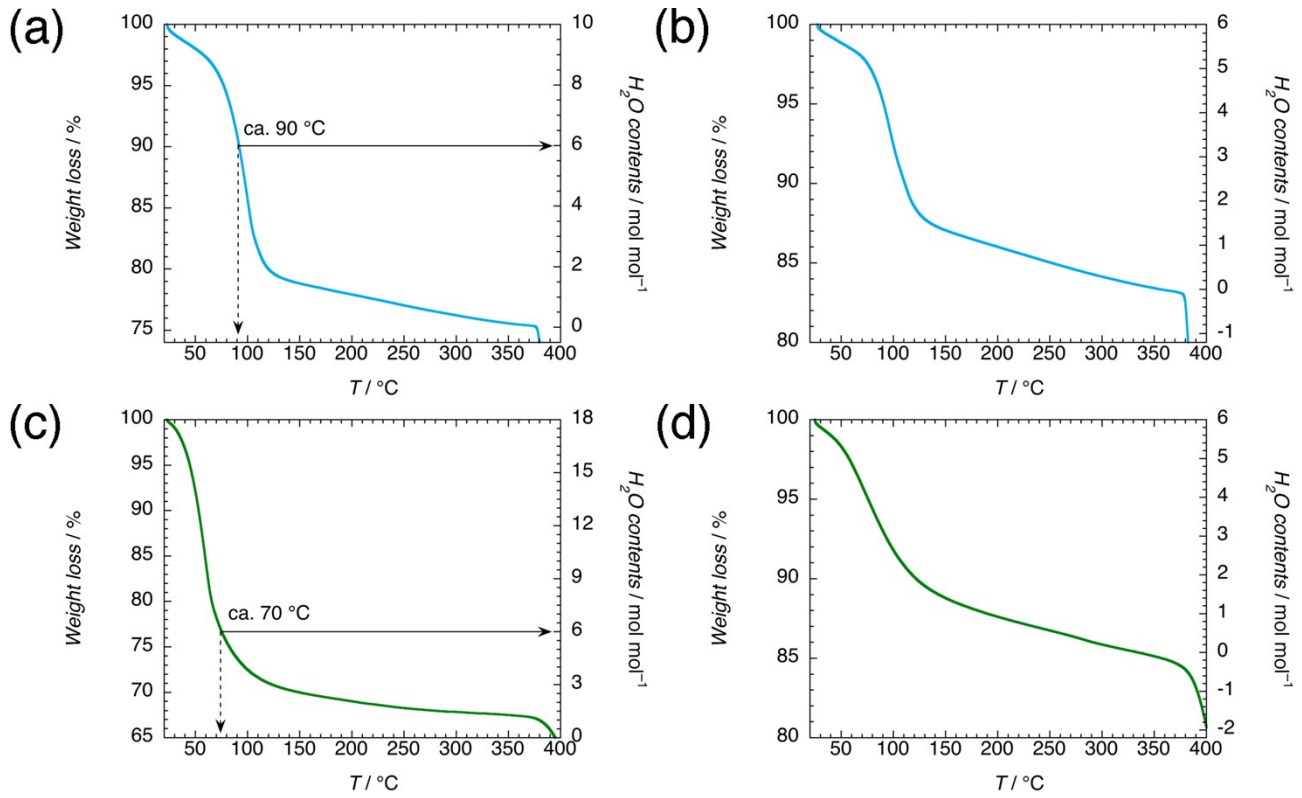

Fig. S3. TG curves of (a) **1**, (c) **2**, (b) **1'** activated at 90 °C for 1 day and (d) **2'** activated at 70 °C for 1 day.

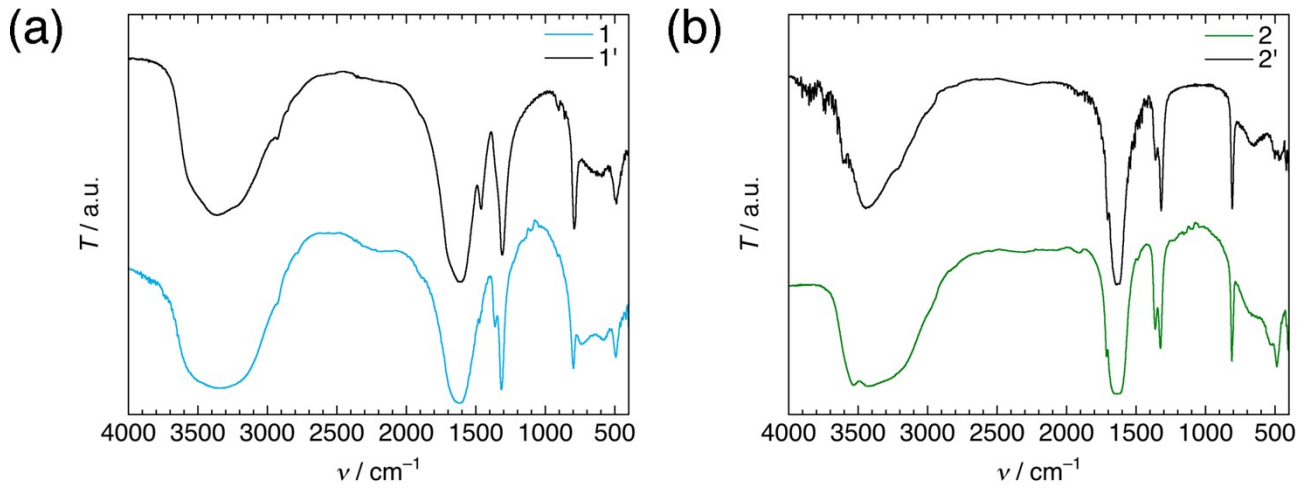

Fig. S4. FT-IR spectra of (a) **1** (light blue) and **1'** (black) and (b) **2** (green) and **2'** (black).

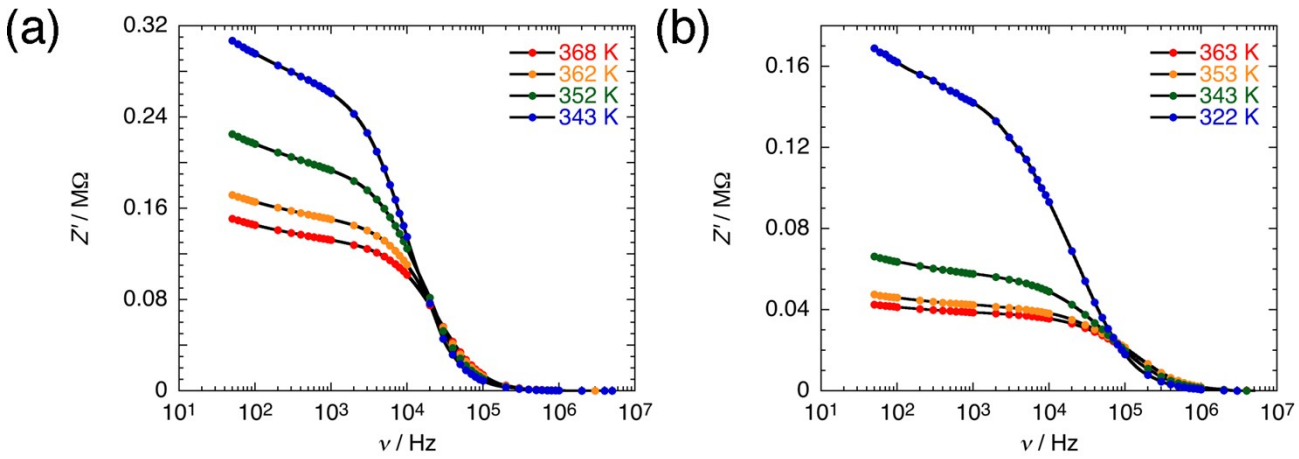

Fig. S5. Frequency-dependence of *Z'* for (a) **1** and (b) **2** in the frequency range of 50 Hz–5 MHz at given temperatures. Solid black lines serve as guides for the eye.

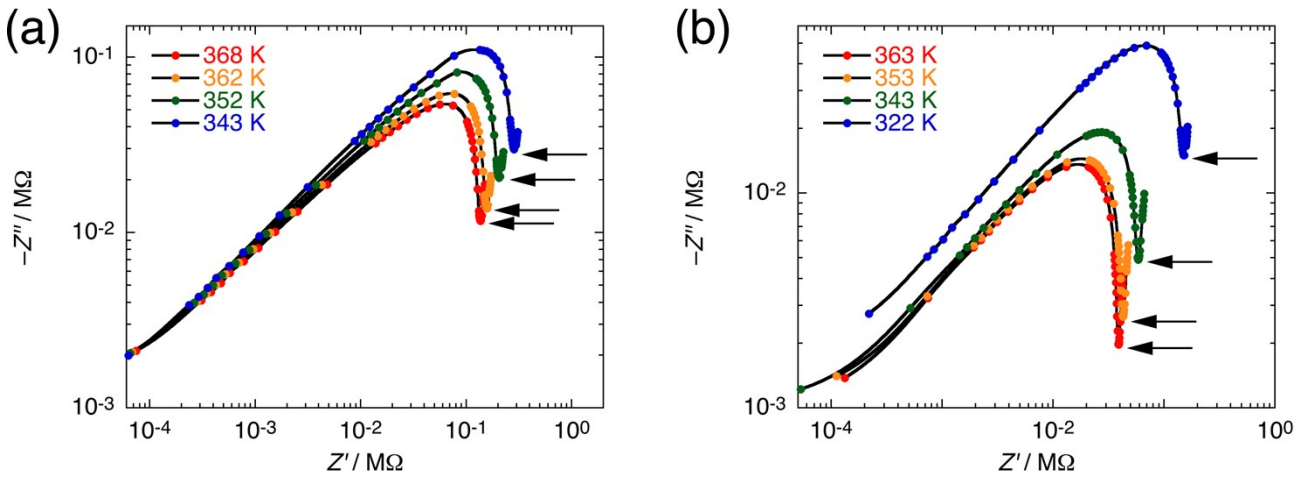

Fig. S6. Nyquist plots for (a) **1** and (b) **2** with a double logarithmic scale in the ν range of 50 Hz–5 MHz at a given *T*. Solid black lines serve as guides for the eye. The resistance (*R*) can be estimated as *Z'* where the high ν semi-circle and low ν line intersect on the Nyquist plot (black arrows). The conductivity (σ) was calculated by using the formula $\sigma = (1/R)/(L/A)$, where *R* is the resistance, *L* the thickness of the electrolyte between the electrodes, and *A* the cross-sectional contact area of the electrodes.