



Supporting Information

for

The role of sulfonate groups and hydrogen bonding in the proton conductivity of two coordination networks

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Supplementary data

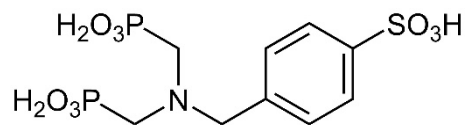


Figure S1: Linker molecule $(\text{H}_2\text{O}_3\text{PCH}_2)_2\text{-NCH}_2\text{-C}_6\text{H}_4\text{-SO}_3\text{H}$ (H_5L)

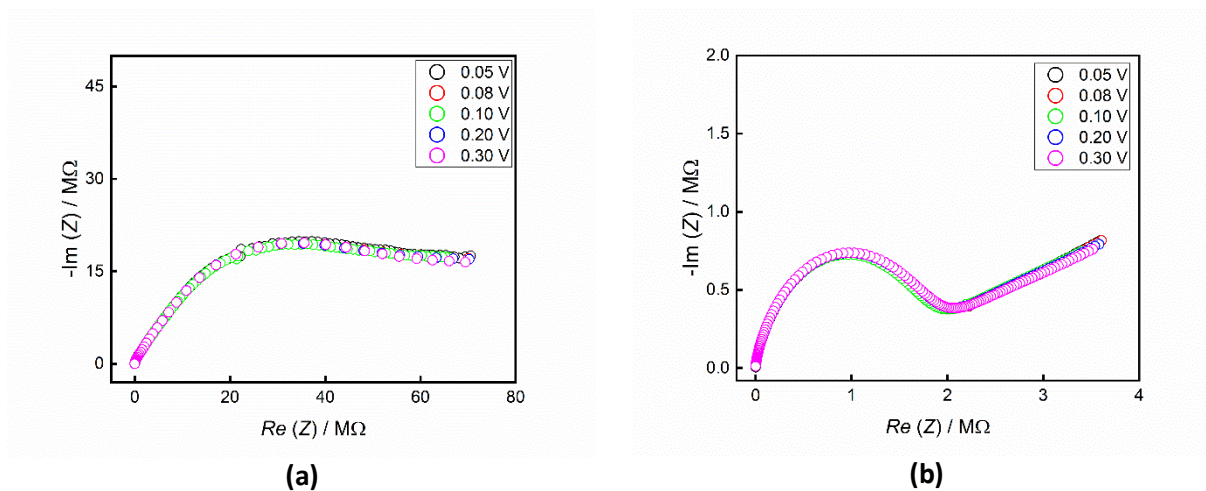


Figure S2: Exemplary Nyquist plots at various applied potentials for (a) $[\text{Mg}(\text{H}_2\text{O})_2(\text{H}_3\text{L})]\cdot\text{H}_2\text{O}$ (22 °C, 70% r.h.) and (b) $[\text{Pb}_2(\text{HL})]\cdot\text{H}_2\text{O}$ (22 °C, 90% r.h.).

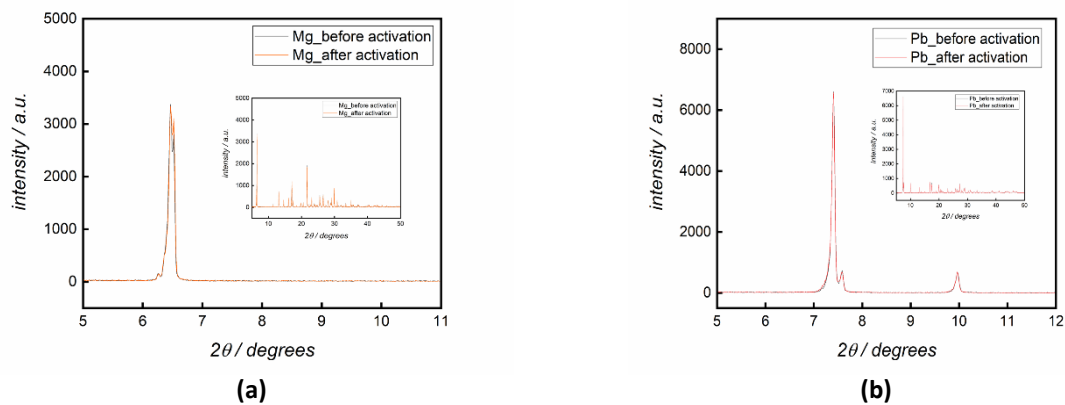


Figure S3: Powder XRD patterns of (a) $[\text{Mg}(\text{H}_2\text{O})_2(\text{H}_3\text{L})]\cdot\text{H}_2\text{O}$ and (b) $[\text{Pb}_2(\text{HL})]\cdot\text{H}_2\text{O}$. All measurements were performed at 25 °C and 90% relative humidity (r.h.). No significant change is observed after activation of the samples (i.e., exposure to 80 °C for 24 h).

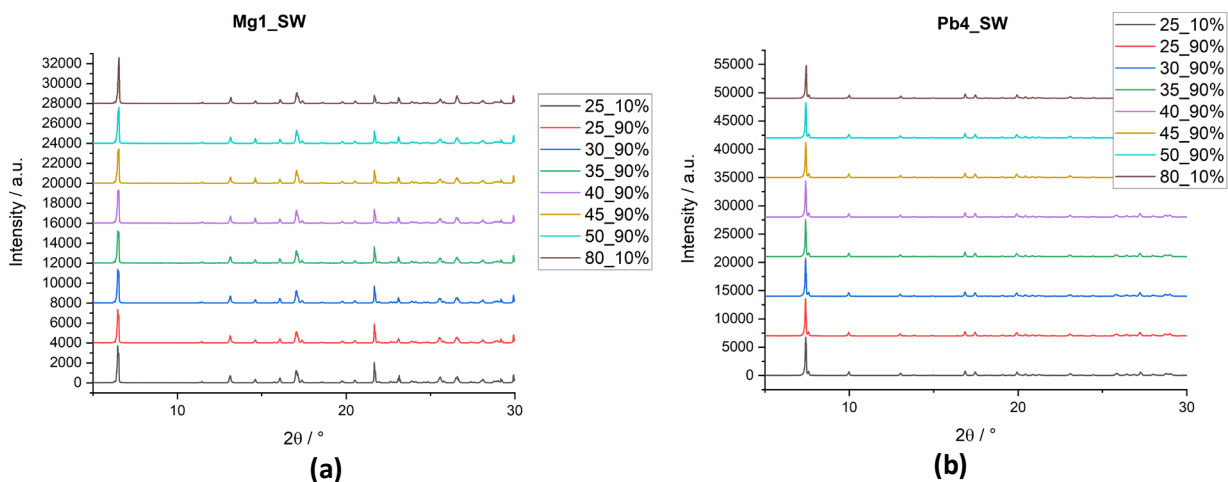


Figure S: Powder XRD patterns of (a) $[\text{Mg}(\text{H}_2\text{O})_2(\text{H}_3\text{L})]\cdot\text{H}_2\text{O}$ and (b) $[\text{Pb}_2(\text{HL})]\cdot\text{H}_2\text{O}$ at variable temperature and humidity.

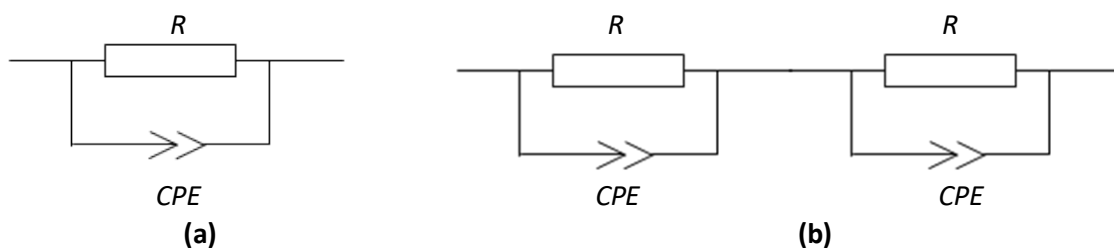


Figure S5: Equivalent circuit models used: (a) Activated $[\text{Mg}(\text{H}_2\text{O})_2(\text{H}_3\text{L})]\cdot\text{H}_2\text{O}$ and for activated/non-activated $[\text{Pb}_2(\text{HL})]\cdot\text{H}_2\text{O}$, (b) non-activated $[\text{Mg}(\text{H}_2\text{O})_2(\text{H}_3\text{L})]\cdot\text{H}_2\text{O}$.

Table S1: Some proton-conducting coordination networks containing sulfonate groups [1,2]

sample name	conditions	σ (S/cm)	E_A (eV)
$\{[\text{Zn}(\text{bpeH})(5\text{-sip})(\text{H}_2\text{O})]\cdot(\text{H}_2\text{O})\}_n$	65 °C, 95% r.h.	2.5×10^{-6}	0.54
$\{[\text{Cu}(\text{pyz})(5\text{-Hsip})(\text{H}_2\text{O})_2]\cdot(\text{H}_2\text{O})_2\}_n$	65 °C, 95% r.h.	3.5×10^{-5}	0.35
$\{[\text{Cu}(\text{bpee})_{0.5}(5\text{-sip})(\text{H}_2\text{O})_2]\cdot(\text{H}_2\text{O})_4(\text{bpeeH}_2)_{0.5}\}_n$	65 °C, 95% r.h.	9.9×10^{-8}	0.40
$\{[\text{Cu}(\text{bpy})(5\text{-Hsip})(\text{H}_2\text{O})]\cdot(\text{H}_2\text{O})_2\}_n$	65 °C, 95% r.h.	5.8×10^{-6}	0.43
$\{[\text{Cu}(\text{bpy})_2(5\text{-H}_2\text{sip})_2]\cdot(\text{H}_2\text{O})_6\}_n$	65 °C, 95% r.h.	1.4×10^{-6}	0.45
$\{[\text{Cu}_2(\text{sba})_2(\text{bpg})_2(\text{H}_2\text{O})_3]\cdot 5\text{H}_2\text{O}\}_n$	80 °C, 95% r.h.	9.4×10^{-3}	0.64
$\text{Cu}_4(5\text{-sip})_2(\text{OH})_2(\text{DMF})_2$	95 °C, 95% r.h.	7.4×10^{-4}	1.32
UiO-66(SO ₃ H) ₂	80 °C, 90% r.h.	8.4×10^{-2}	0.32
MIL-101-SO ₃ H	70 °C, 90% r.h.	4.3×10^{-5}	0.27

References

1. Liu, R.; Wang, D.-Y.; Shi, J.-R.; Li, G. *Coord. Chem. Rev.* **2021**, *431*, 213747. doi:10.1016/j.ccr.2020.213747
2. Lim, D.-W.; Kitagawa, H. *Chem. Rev.* **2020**, *120*, 8416. doi:10.1021/acs.chemrev.9b00842