

Supporting Information

Constructing porous MOF based on the assembly of layer framework and *p*-sulfonatocalix[4]arene nanocapsule with proton-conductive property

Guo-Li Zheng,^b Guo-Cheng Yang,^c Shu-Yan Song,^a Xue-Zhi Song^a and Hong-Jie Zhang^{*a}

^aState Key Laboratory of Application of Rare Earth Resources utilization, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, P. R. China.

^bKey Laboratory of Catalysis and Materials Science of the State Ethnic Affairs Commission & Ministry of Education, Hubei Province, South-Central University for Nationalities, Wuhan, 430074, PR China

^cSchool of Chemistry and Life Science, Changchun University of Technology, Changchun 130012, P. R. China

*Corresponding author. Fax: +86-431-85698041; Tel: +86-431-85262127.

E-mail address: hongjie@ciac.jl.cn (H.-J. Zhang)

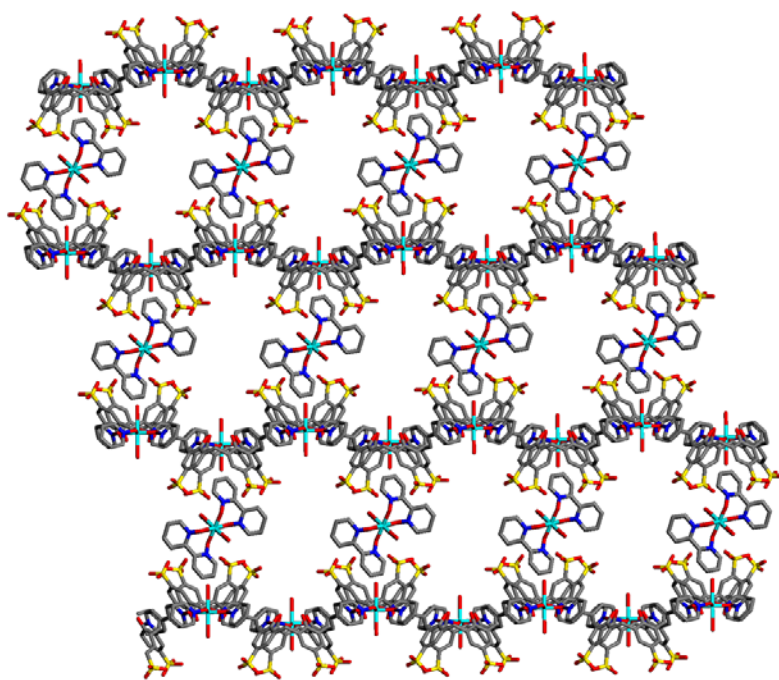


Fig S1 The Packing diagram down the *b* axis, showing the channel structure of compound **1**, the dissociative water molecules are omitted for clarity.

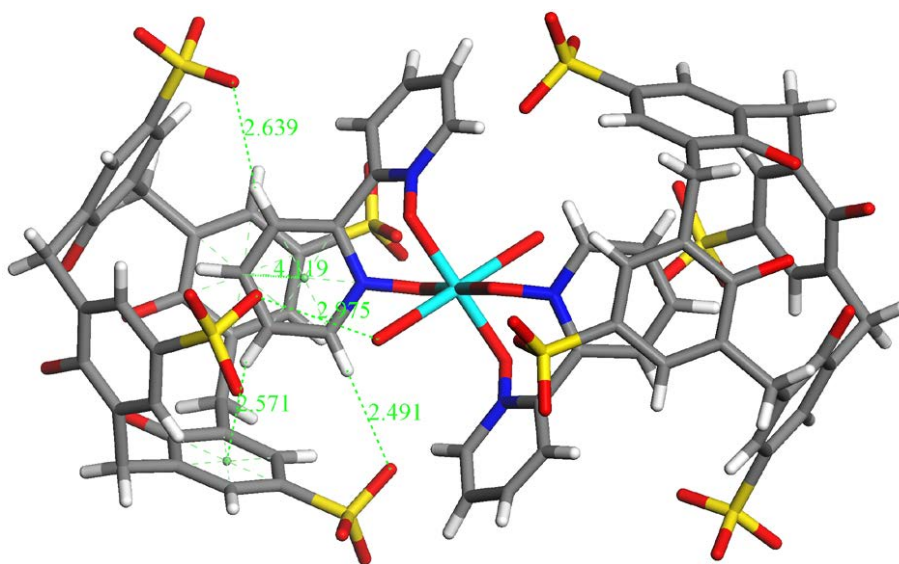


Fig S2 Structure of the supramolecular nanocapsule based on the *p*-sulfonatocalix[4]arenes and [Cu(bpdo)₂2H₂O]²⁺.

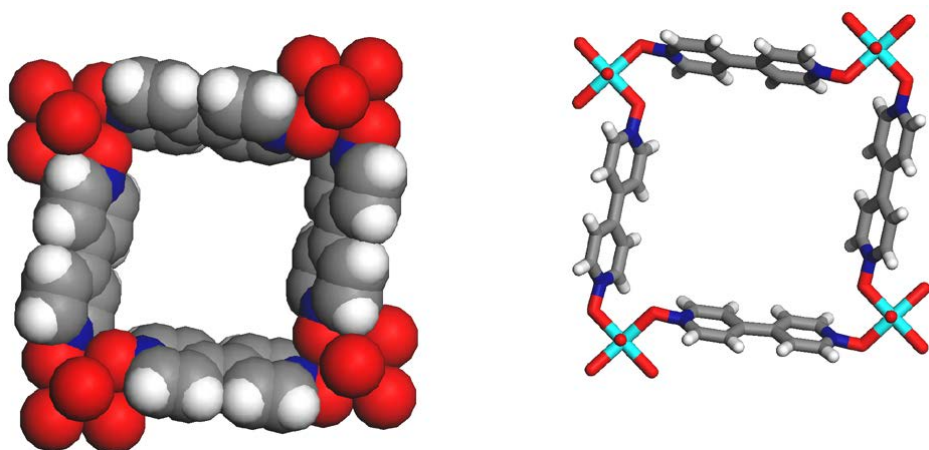


Fig S3 Structure of bowl shape frameworks based on the L and copper ions.

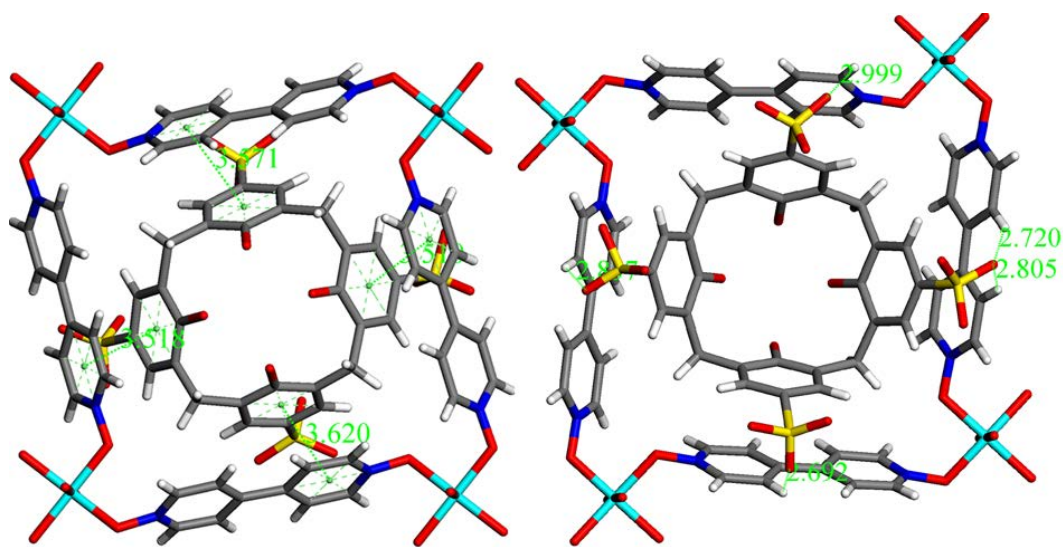


Fig S4 The weak interactions between the host bowl and the *p*-sulfonatocalix[4]arenes of capsules

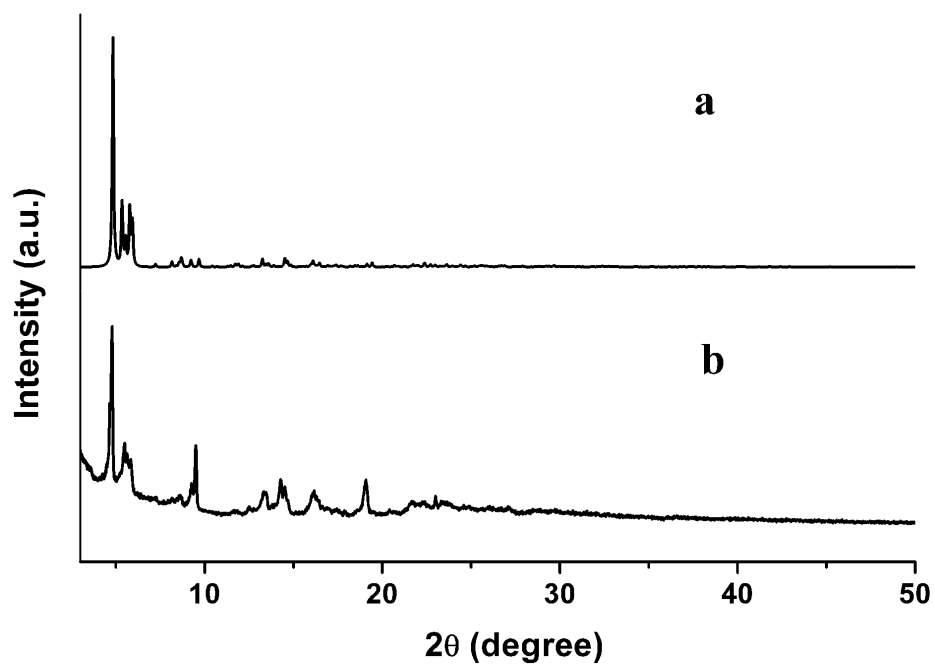


Fig S5 (a) Simulated from single crystal data; (b) Powder XRD patterns of compound 1.

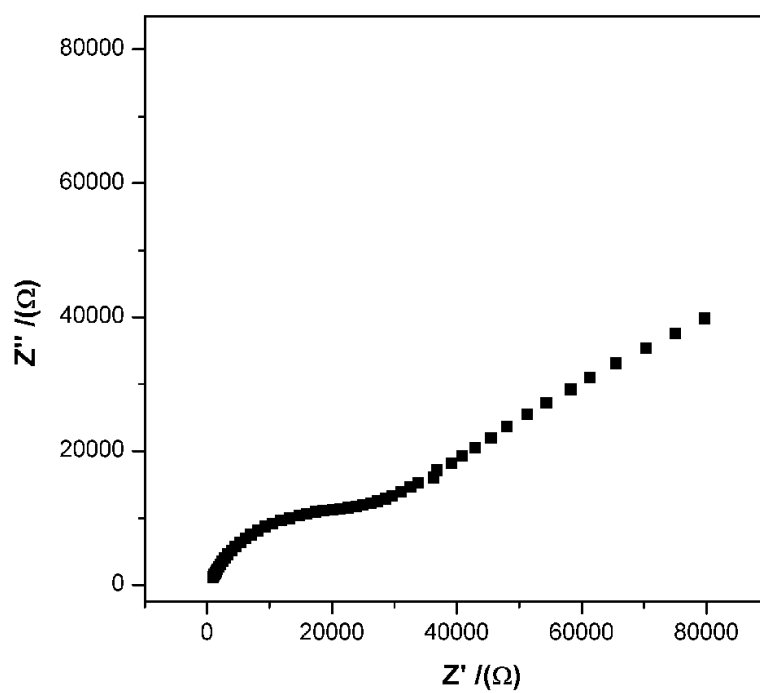


Fig S6 Nyquist plot of compound 1.

T / K	1000/K	R / Ω	$\sigma = 1/RS$
298	3.3557	5.16E+04	5.42E-07
308	3.2468	3.08E+04	9.08E-07
318	3.1447	1.11E+04	2.51E-06
328	3.0488	7158	3.90E-06
338	2.9586	3529	7.92E-06
348	2.8736	1864	1.50E-05
358	2.7933	907	3.08E-05

Table S1 Proton Conductivity at different temperatures under 95% RH for compound 1.

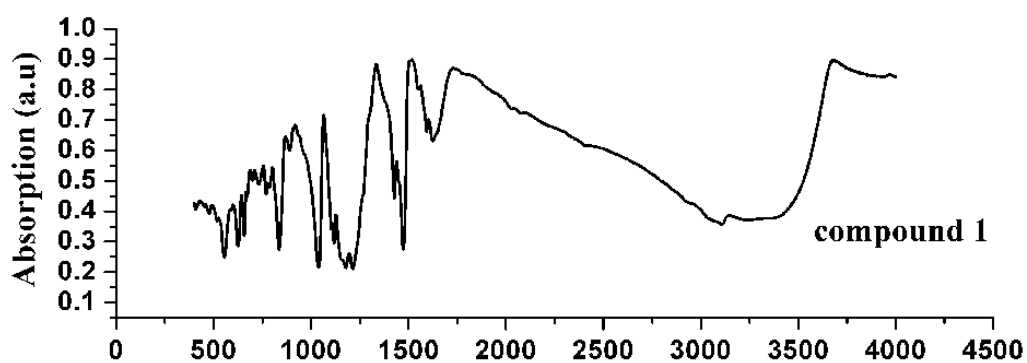


Fig S7 The infrared spectra of compounds 1.

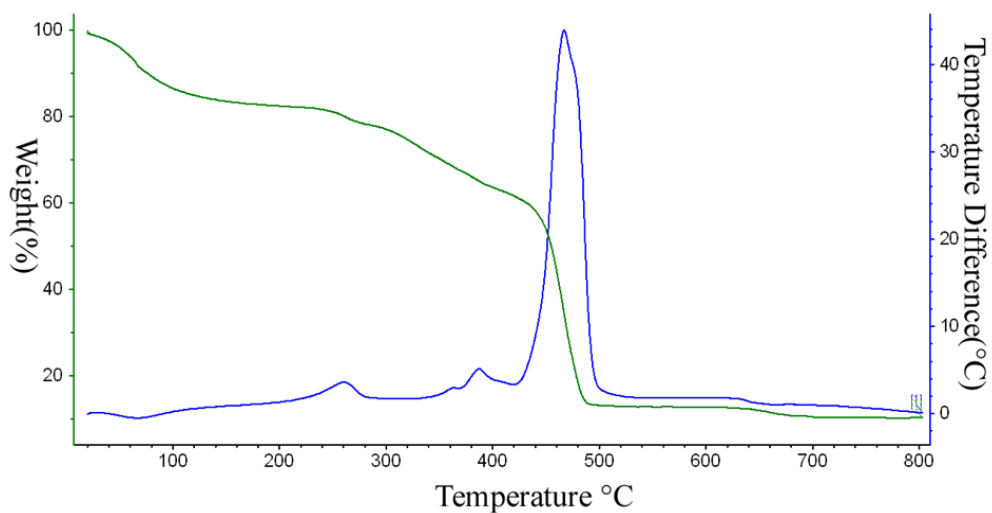


Fig S8 TGA of compound **1**.

The crystal structure of compound **1** contains both dissociative and coordinated water molecules. The observed mass loss (15.1%) while heating up to 120 °C is attributed to the loss of dissociative or coordinated water molecules.