Electronic Supplementary Material for CrystEngComm

ELECTRONIC SUPPLEMENTARY DATA

Syntheses, Structures and Sorption Properties of Two Framework-Isomeric Porous Copper-Coordination Polymers

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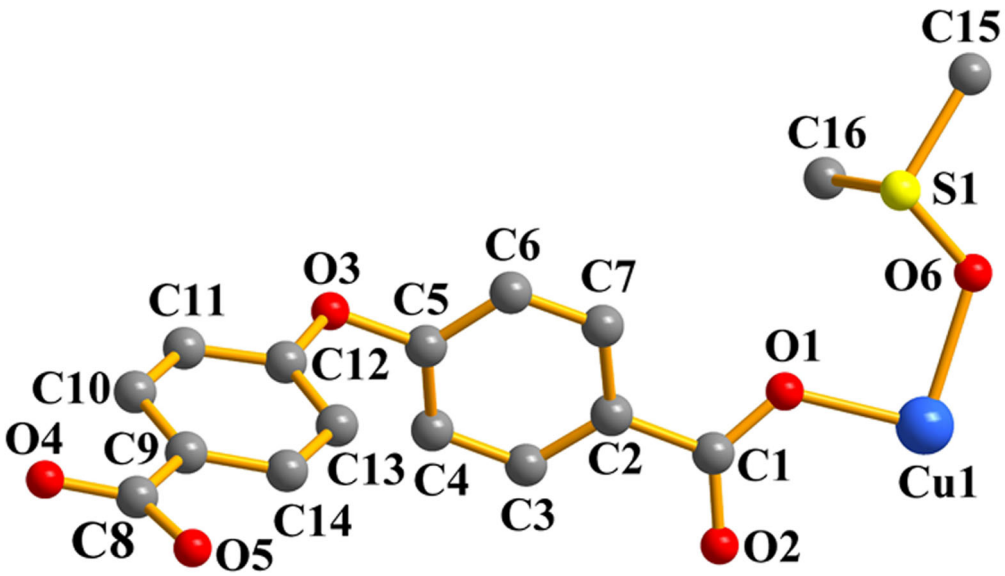


Fig. S1 The asymmetric unit of **MCF-21**.

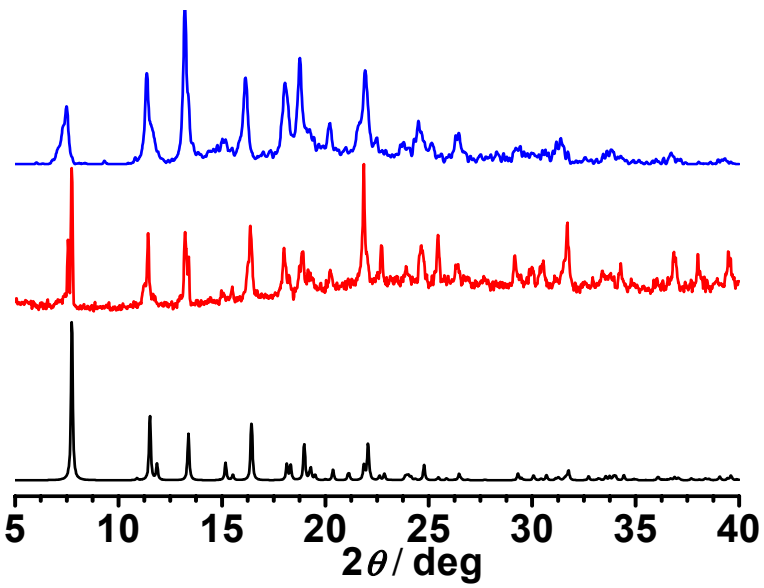


Fig. S2 PXRD patterns of simulated from the single-crystal data of **MCF-21** (black), as-prepared **MCF-21** (red) and desolvated **MCF-21'** (blue) obtained by heating **MCF-21** at 250 °C for 2 h under vacuum.

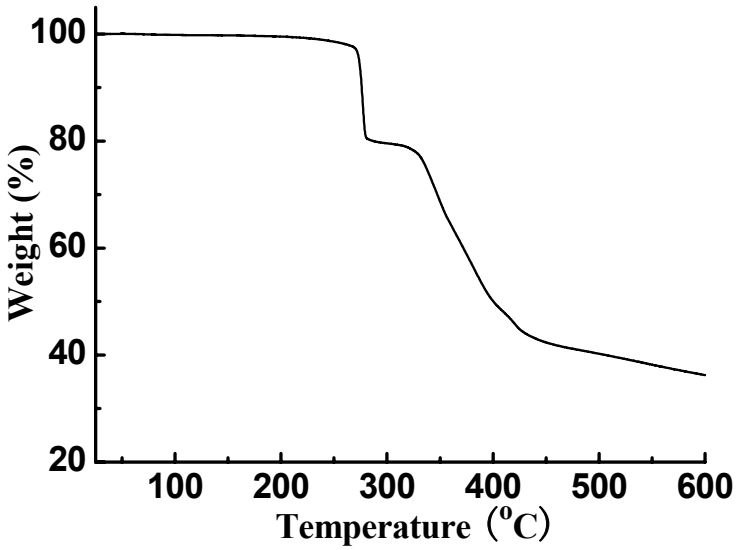


Fig. S3 TGA plot of **MCF-21** recorded under N_2 atmosphere.

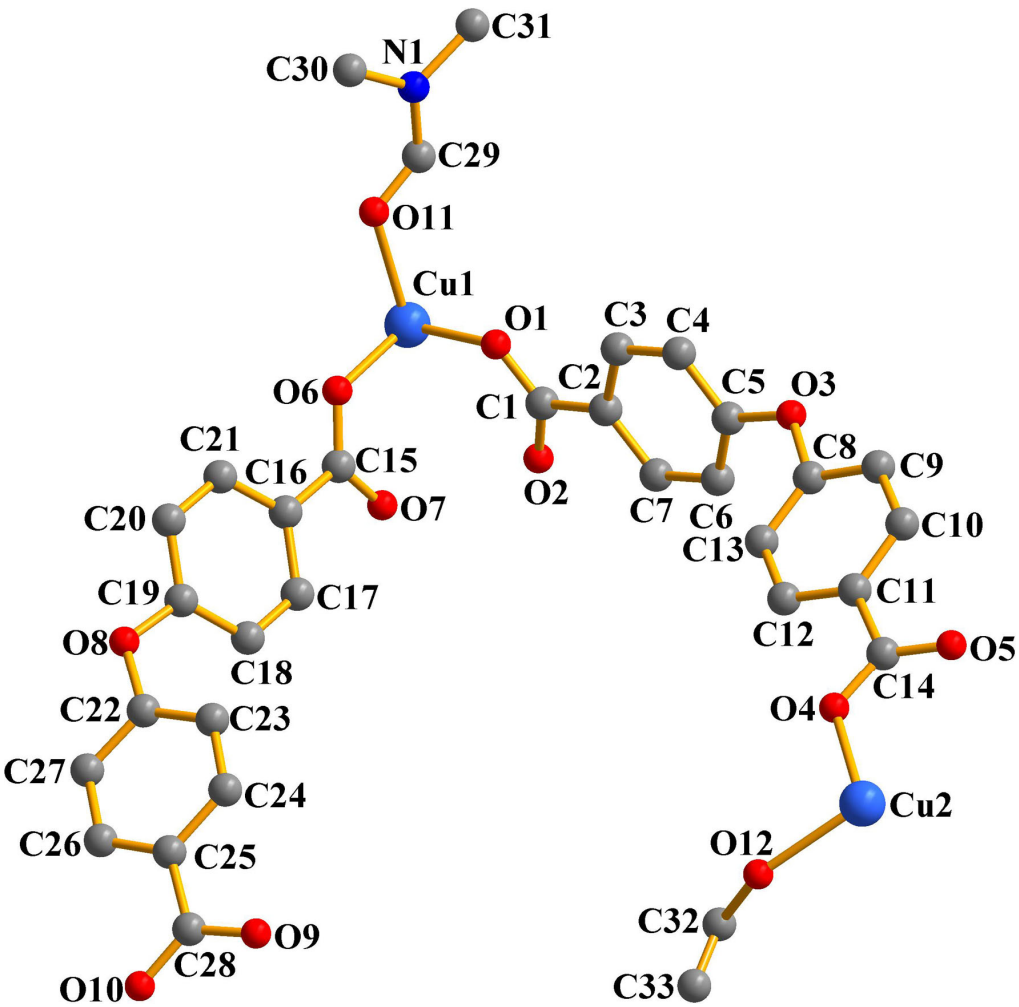


Fig. S4 The asymmetric unit of **MCF-22·guest**.

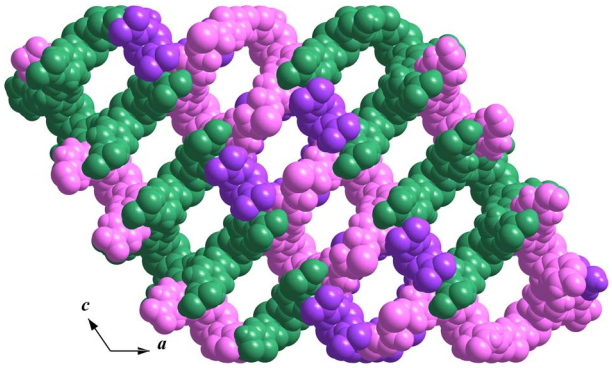


Fig. S5 The molecular packing in **MCF-22·guest** viewed along the *b*-axis.

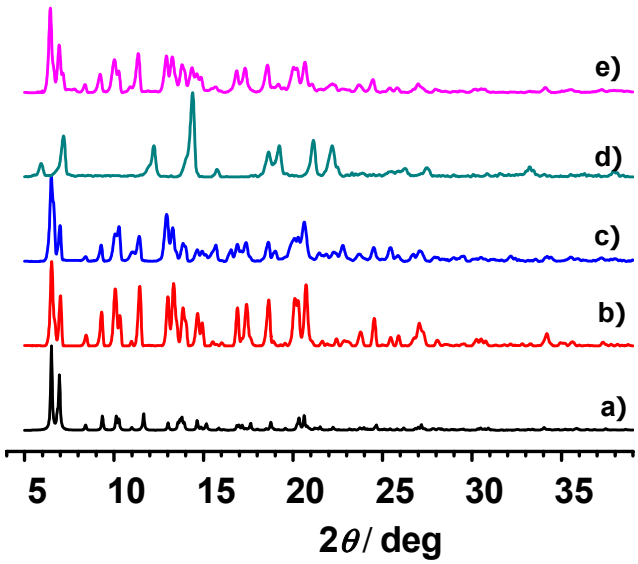


Fig. S6 PXRD patterns of (a) simulated from the single crystal data of **MCF-22·guest**; (b) as-prepared **MCF-22·guest**; (c) **MCF-22** obtained by heating **MCF-22·guest** to 100 °C for 5 h under vacuum; (d) **MCF-22'** obtained by heating **MCF-22·guest** to 180 °C for 4 h under vacuum as well as (e) regenerated **MCF-22** after treating **MCF-22'** in a dmf-ethanol-water mixture for 72 h.

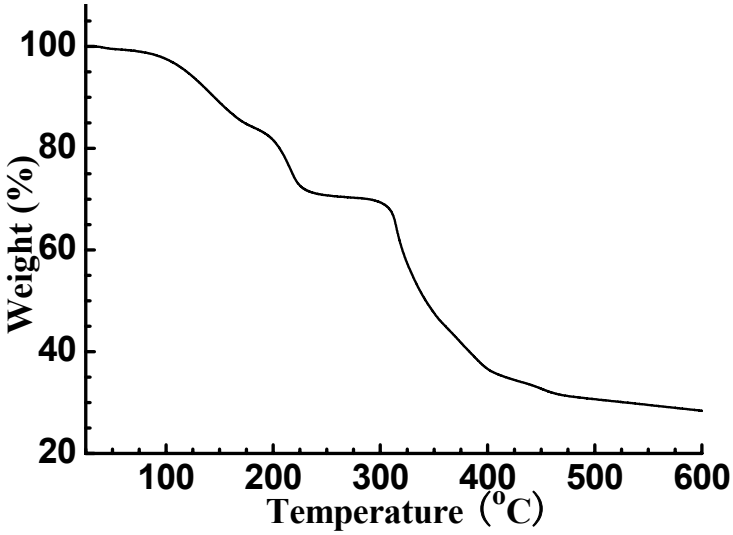


Fig. S7 TGA plot of **MCF-22·guest** recorded under N_2 atmosphere.

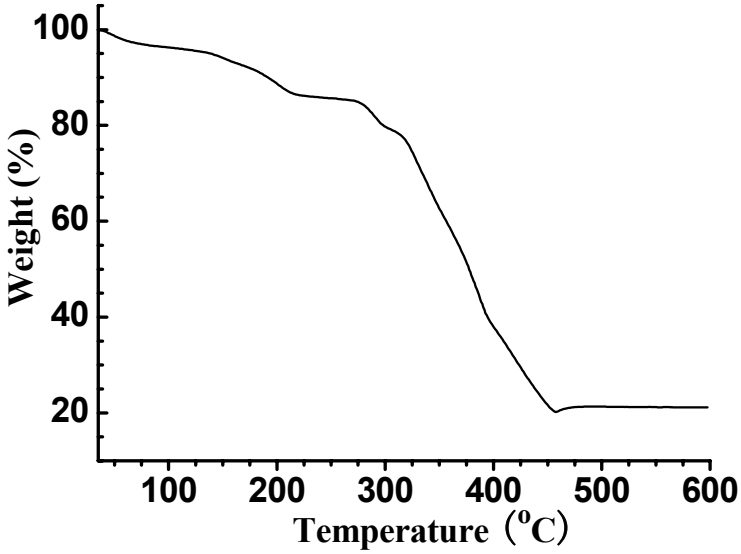


Fig. S8 TGA plot of **MCF-22** recorded under N_2 atmosphere.

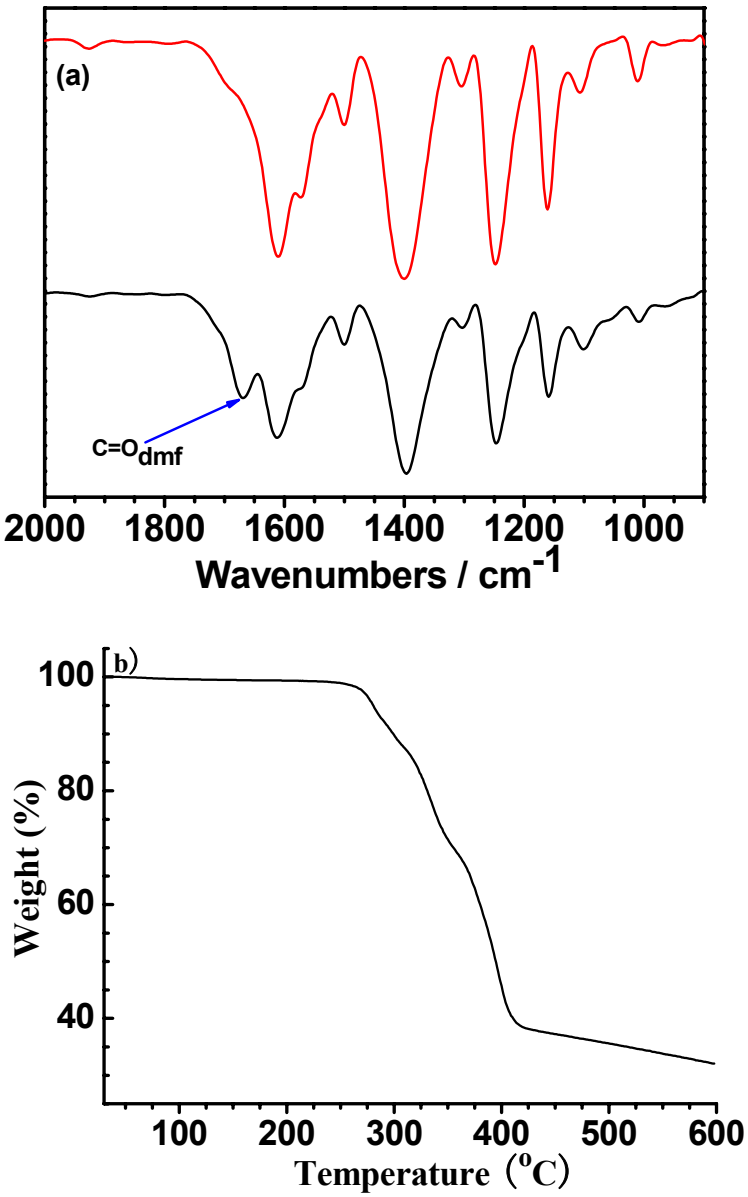


Fig. S9 IR spectrum of **MCF-22·guest** (black) and **MCF-22'** (red) (a) and TGA plot of **MCF-22'** recorded under an N_2 atmosphere (b).

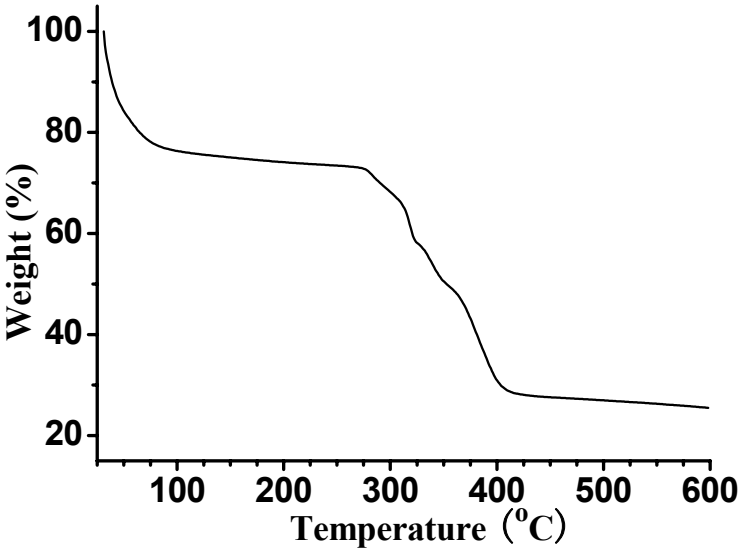
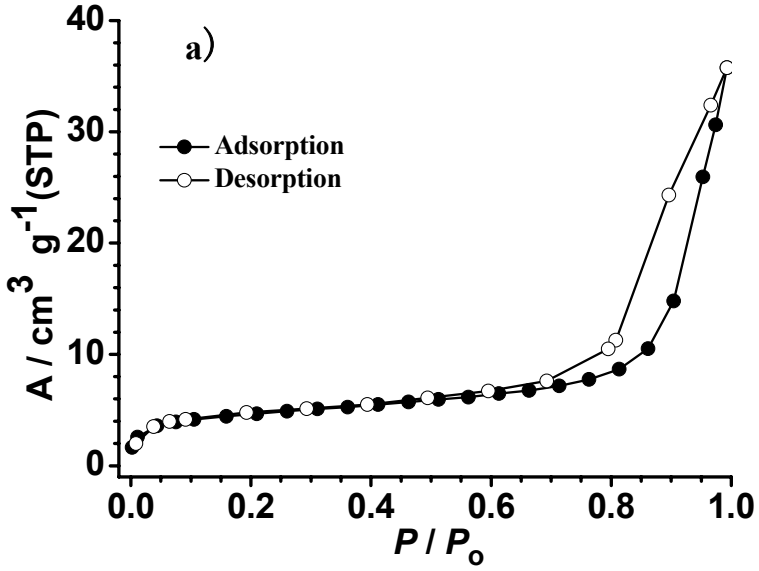


Fig. S10 TGA plot of methanol solvated **MCF-22'** recorded under an N_2 atmosphere.



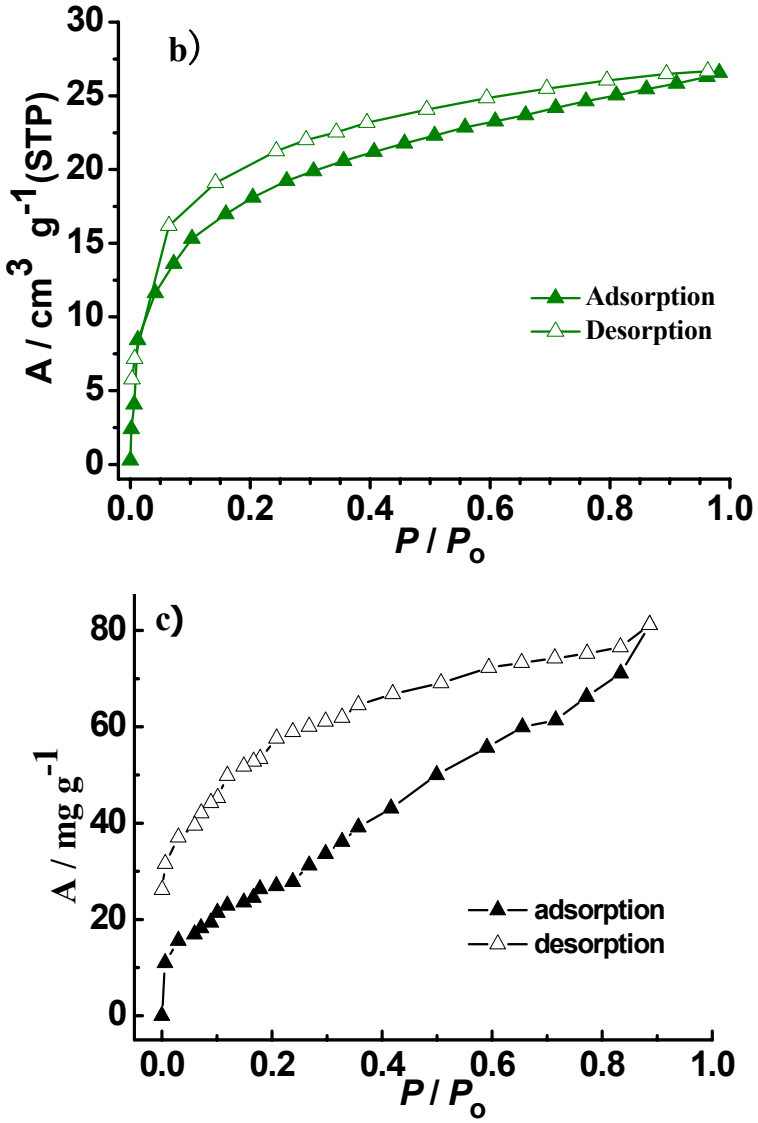


Fig. S11 Sorption isotherms of N_2 (a) at 77 K, CO_2 (b) at 195 K and methanol (c) at 298 K for **MCF-21'**.