

Supplementary Material (ESI) for CrystEngComm

**A novel 1D independent metal-organic nanotube based on
cyclotrimeratrylene ligand**

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I. Structure diagrams of CTV-Cu

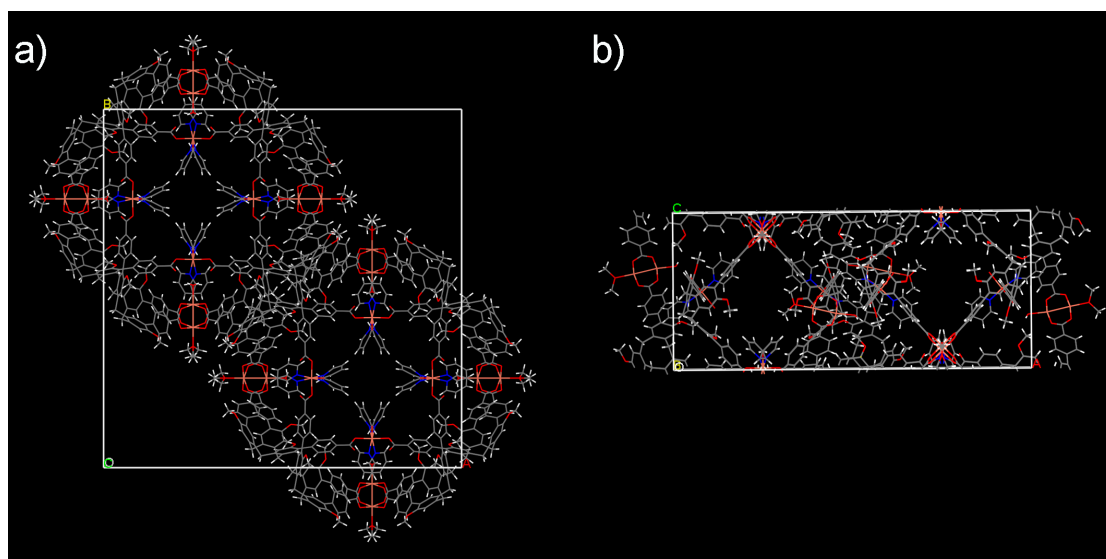


Fig. S1 The unit cell of CTV-Cu, a) see along the *c* axis. b) see along the *b* axis. (Cu orange; O, red; C, gray; N, blue; H, white).

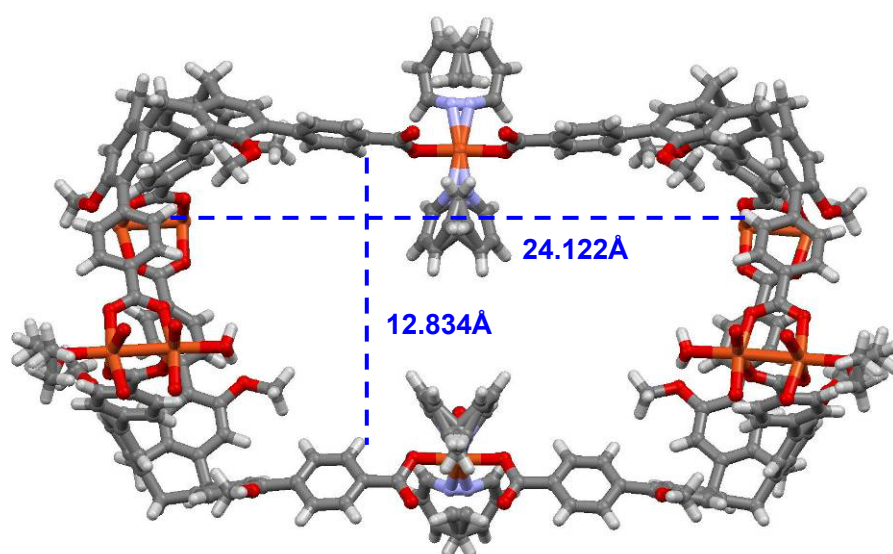


Fig. S2 The single cuboid cavity of CTV-Cu, see along the *c* axis. (Cu orange; O, red; C, gray; N, blue; H, pale). The cuboid unit has a cavity of 24.1×12.8 Å (atom to atom distance).

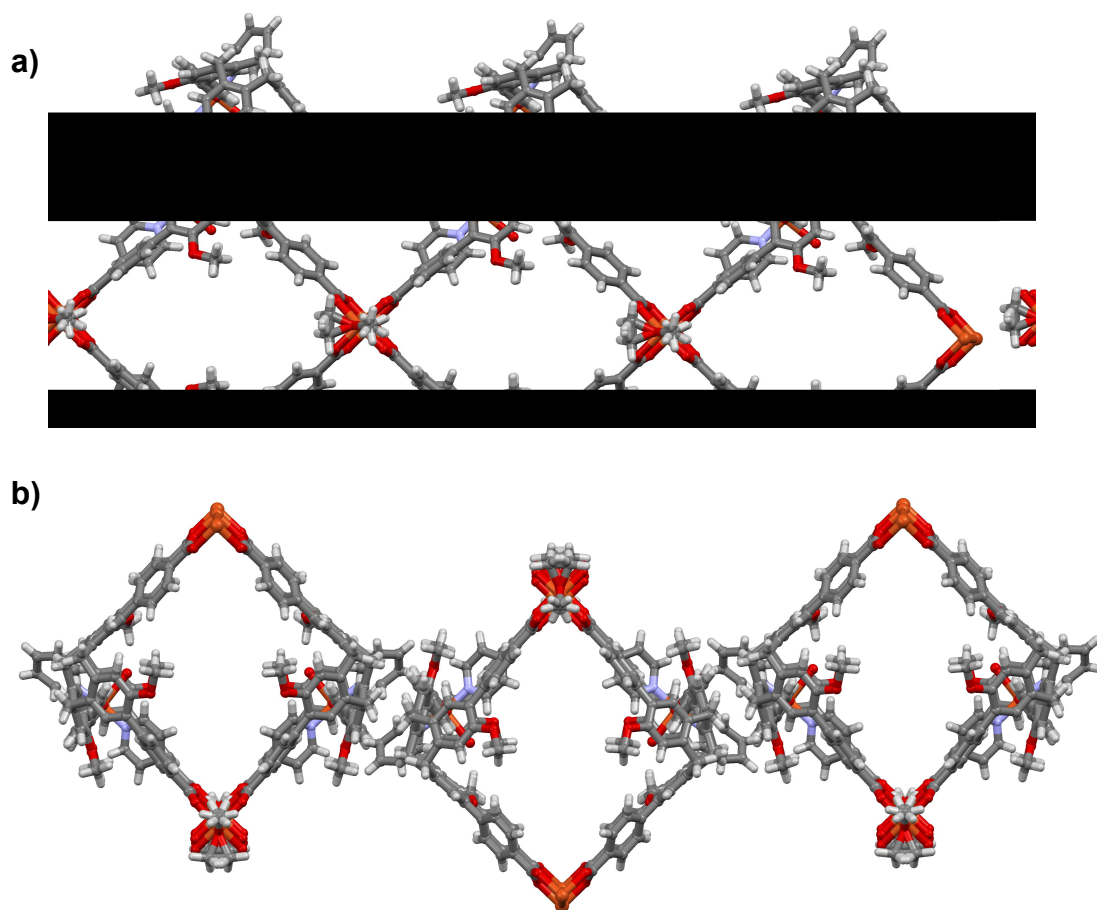


Fig. S3 Crystal structure of **CTV-Cu**, a) CTV ligands are linked by square bicopper clusters, see from the *a* axis; b) layered structure, see from the *b* axis, there is no covalent bonds nor coordination interactions between those voids. (Cu orange; O, red; C, gray; N, blue; H, pale).

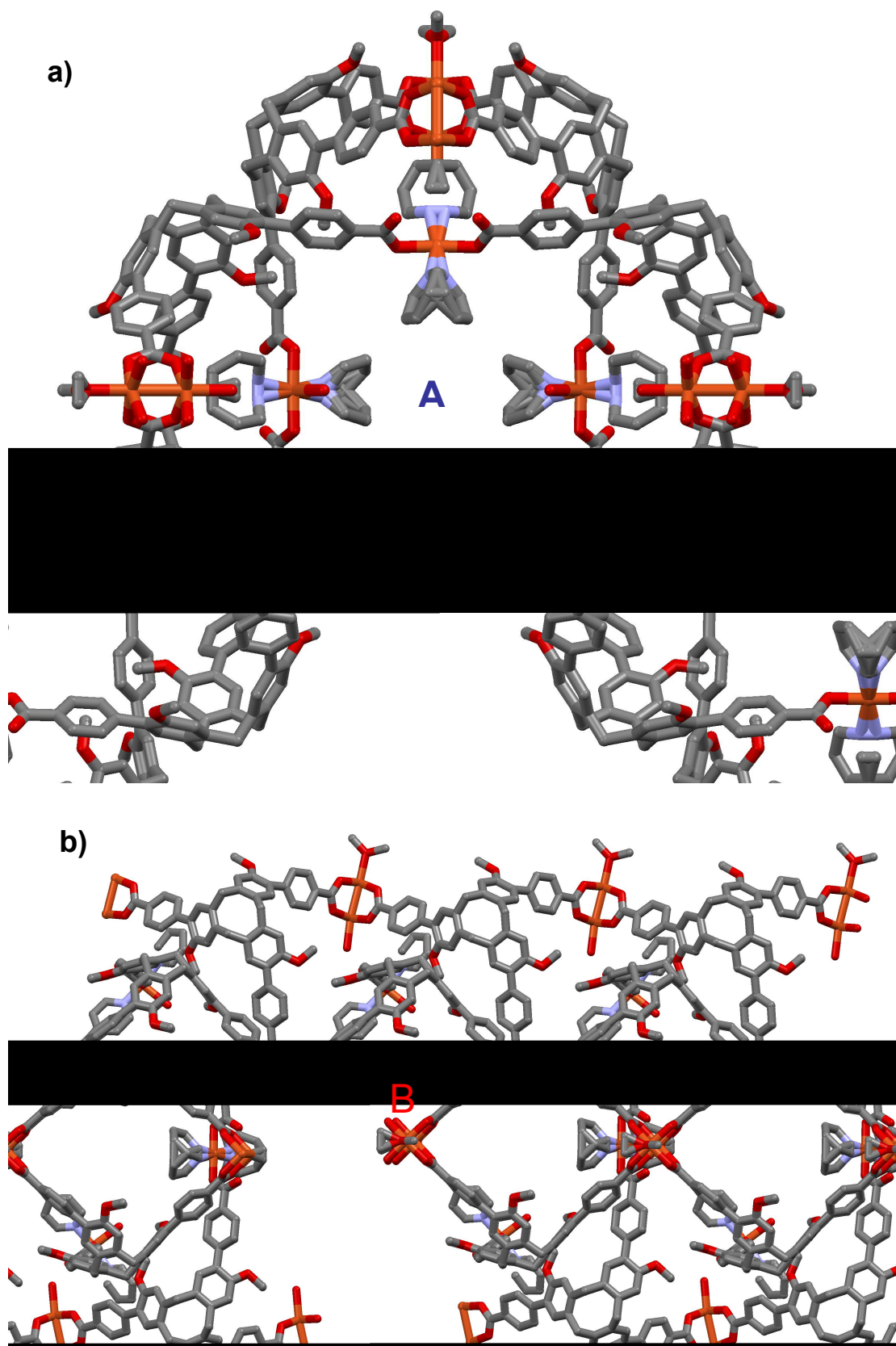


Fig. S4 Pores structures of CTV-Cu, a) Pore A is surrounded by CTV ligands and Cu₃, see from the *c* axis; b) structure of pore B, see from the *a* axis (Cu orange; O, red; C, gray; N, blue; all hydrogen atoms are omitted for clarity).

V. Thermal gravimetric analysis (TGA)

The green block shaped crystals were washed with DEF (3×2 ml) and a little amount of ethanol (2×0.3 ml), dried in air overnight. A crystalline sample (4.105 mg) was heated at a constant rate $10\text{ }^{\circ}\text{C}/\text{min}$ in air from $16\text{ }^{\circ}\text{C}$ to $550\text{ }^{\circ}\text{C}$. As shown in **Fig. S5**, the guest molecules are steadily lost below $250\text{ }^{\circ}\text{C}$, which is ~~34~~36% weight loss, corresponding to the liberation of 9 DEF and 8 water molecules.

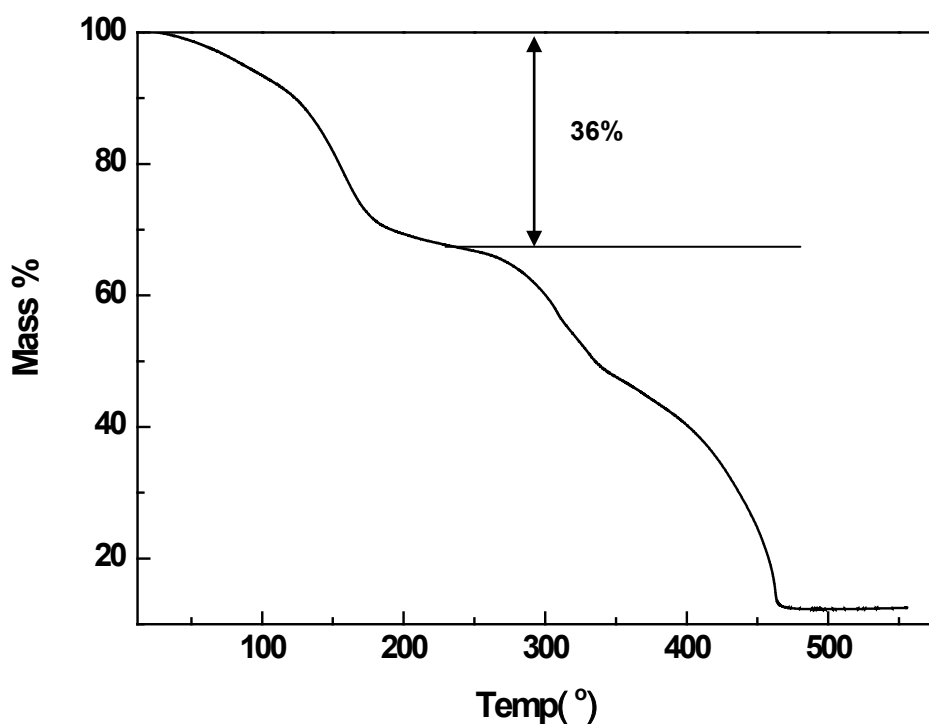


Fig. S5 TGA measurement of CTV-Cu.

VII. ^1H -NMR spectra

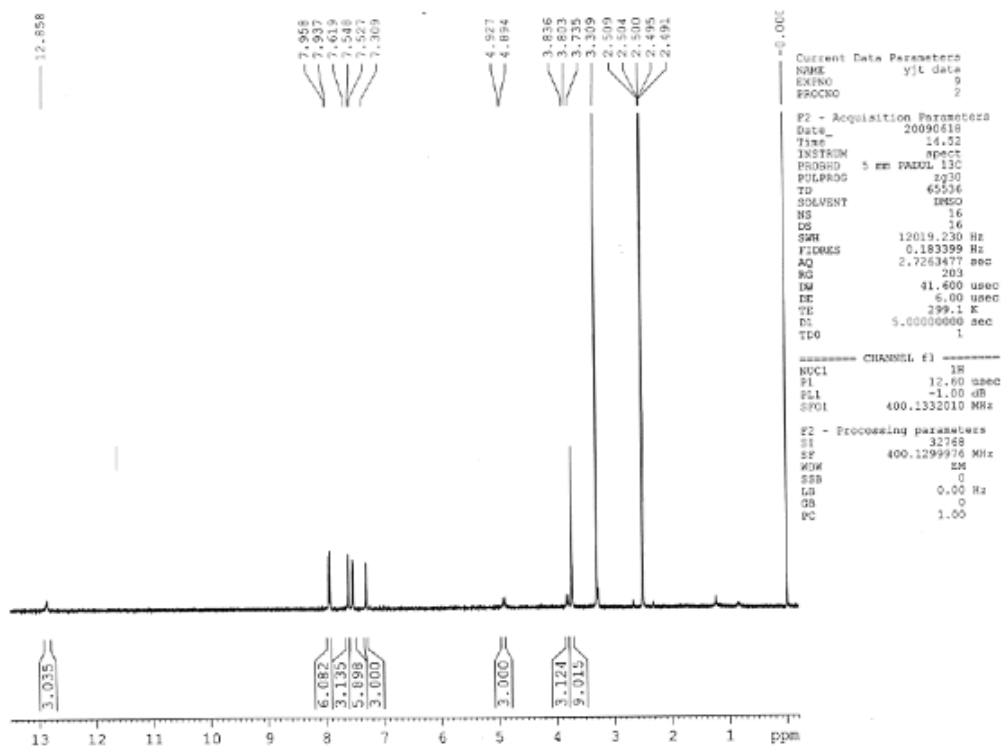


Figure S6 ^1H -NMR spectrum of H_3L in $\text{DMSO-}d_6$.