

Bent Tritopic Carboxylates for Coordination Networks: Clues to the Origin of Self-penetration

Jin-Xiang Chen,* Hai-Qing Zhao, Huan-Huan Li, Sheng-Li Huang, Ni-Ni Ding, Wen-Hua Chen,

David J. Young, Wen-Hua Zhang,* and T. S. Andy Hor*

Figure S1. Packing diagram of 2 looking along the <i>a</i> axis showing extensive hydrogen bonding among the one-dimensional chains.....	2
Figure S2. Packing diagram of 3 showing the open cavity been threaded by the disordered free Cbdcp ligands.	2
Figure S3. Network entanglement formed by Cu1 and its ligands in complex 4.....	3
Figure S4. TG analysis plots of complexes 4 (a) and 1–3 (b).....	3
Figure S5. Simulated and assynthesized PXRD patterns of complexes 1–3, showing phase purity of the samples.....	4
Figure S6. PXRD patterns of complex 4, showing agreement among the simulated, as-synthesized and activated samples.	5
A brief comment on the PXRD data of complexes 1–4.	5

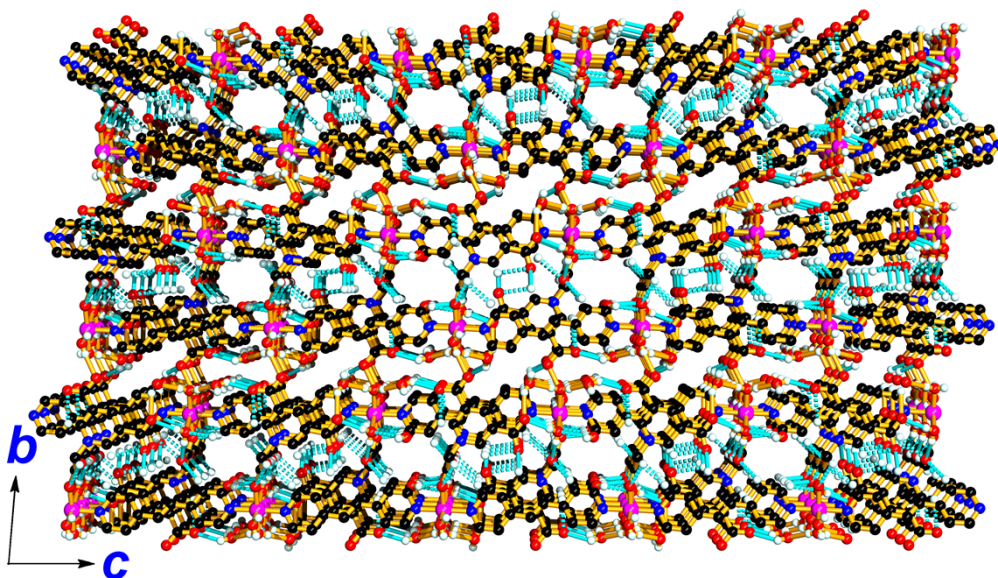


Figure S1. Packing diagram of **2** looking along the *a* axis showing extensive hydrogen bonding among the one-dimensional chains.

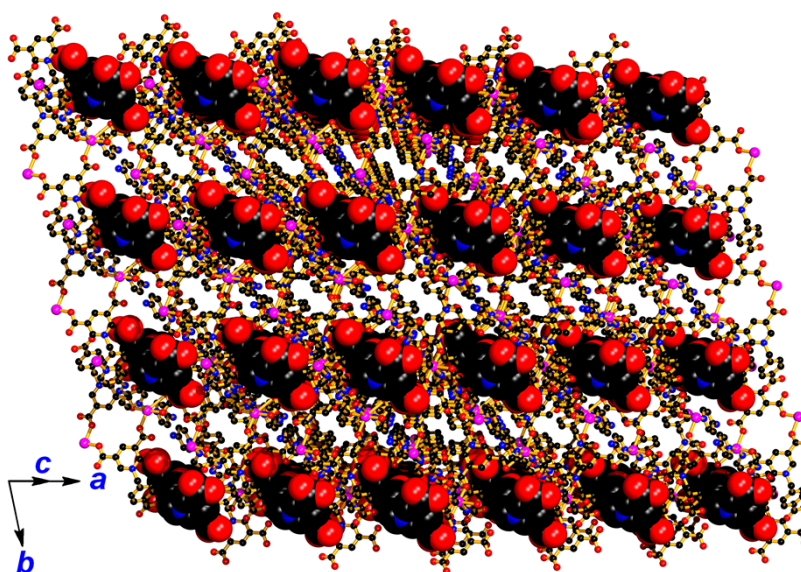


Figure S2. Packing diagram of **3** showing the open cavity been threaded by the disordered free Cbdcp ligands.

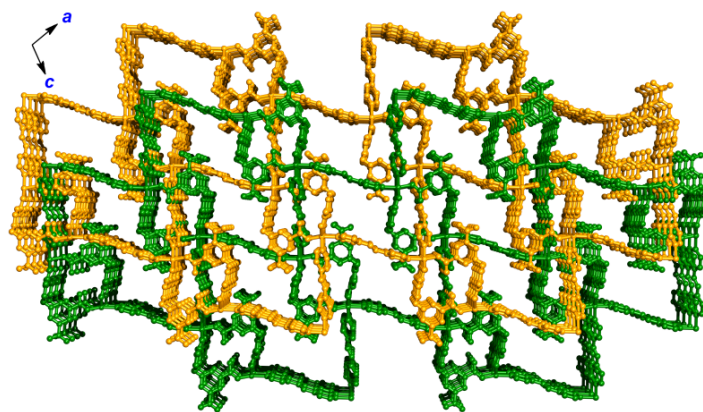
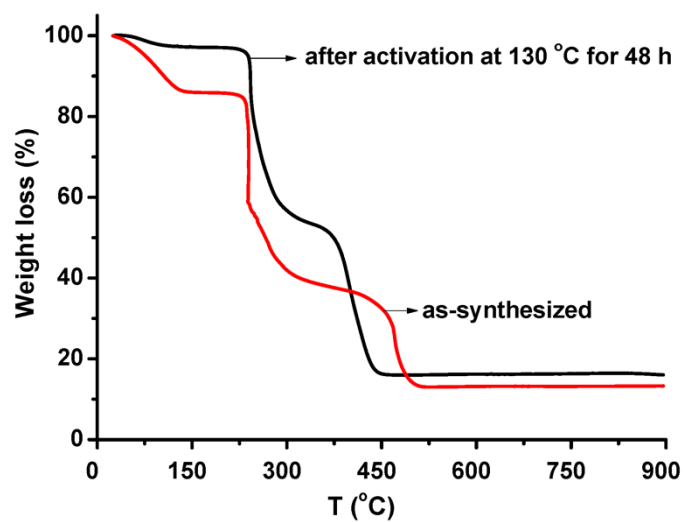
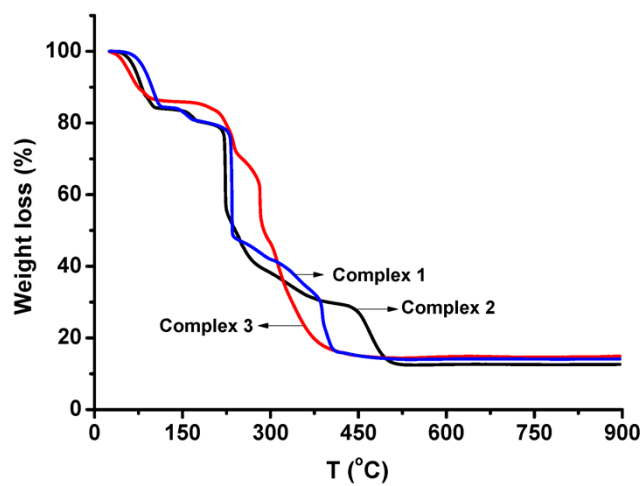


Figure S3. Network entanglement formed by Cu1 and its ligands in complex 4.



(a)



(b)

Figure S4. TG analysis plots of complexes 4 (a) and 1–3 (b).

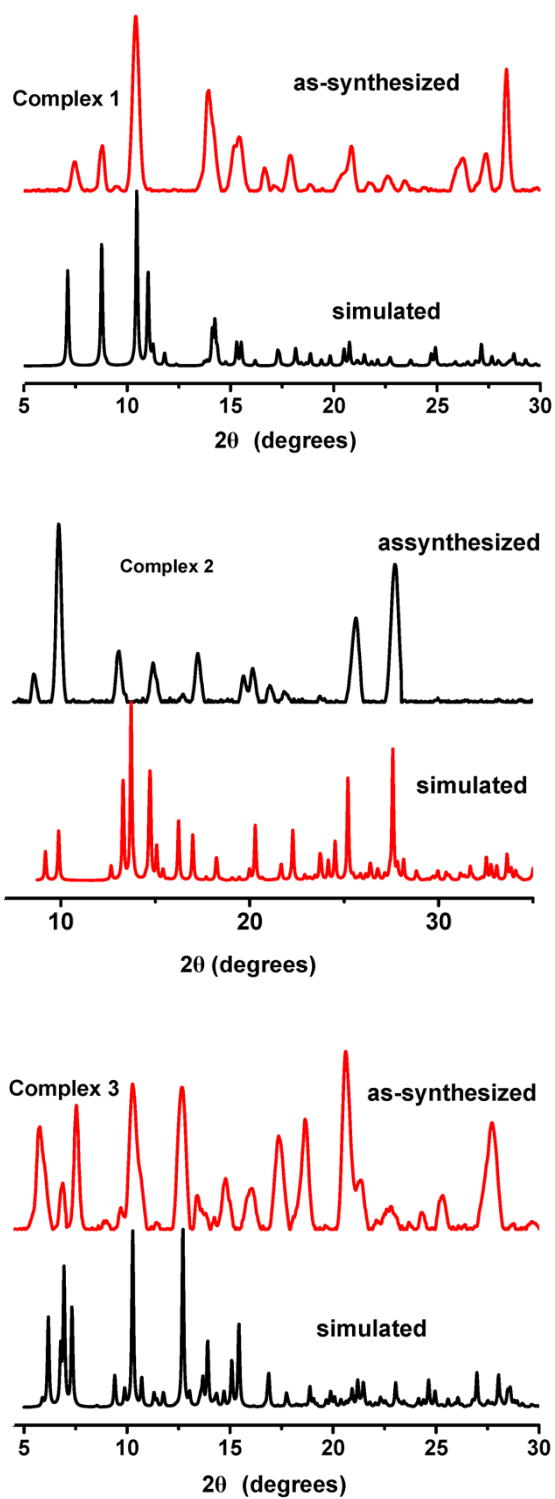


Figure S5. Simulated and assynthesized PXRD patterns of complexes 1–3, showing phase purity of the samples.

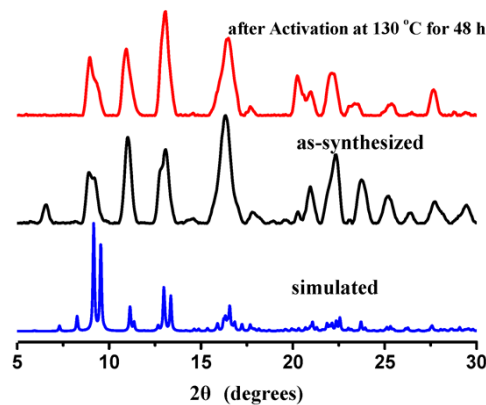


Figure S6. PXRD patterns of complex 4, showing agreement among the simulated, as-synthesized and activated samples.

A brief comment on the PXRD data of complexes 1–4.

The relatively high intensity at high theta angles for complexes 1–4 is caused by Bruker D8 GADDS micro-diffractometer used in the Institute (Institute of Materials Research and Engineering). In principle, the ideal measurement range (2θ) is from 18-161° for Bruker D8 GADDS XRD model with the detector-to-sample distance (D) of 30 cm. While the scan range is less than 18°, the detector area is partially shielded by sample stage due to the ω rotation. The intensity accumulation in that range ($2\theta < 18^\circ$) is thus accordingly weaker. After integrating the low and high angle data followed by normalization, the intensity at higher angle appears relatively enhanced.