

Electronic Supplementary Information for *Chemical Communications*

Design and construction of an organic crystal with a novel interpenetrated n-Borromean linked topology

Yong-Biao Men,^a Junliang Sun,^{*b} Zhi-Tang Huang^a and Qi-Yu Zheng^{*a}

^a *Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Molecular Recognition and Function, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China.*

^b *Structural Chemistry and Berzelii Centre EXSELENT on Porous Materials, Stockholm University, SE-106 91 Stockholm, Sweden.*

Electronic Supplementary Information

- 1. Experimental Section**
- 2. Figure S1-S4**

1. Experimental section

Preparation of [2TCA•3dpyb].

A mixture of 1,3,5-tris(4-carboxy-phenyl)adamantane (TCA) (15 mg, 0.03 mmol) and 1,4-di(pyridin-4-yl)benzene (dpyb) (10.4 mg, 0.045 mmol) was dissolved in THF/MeOH (v/v=1:2, 15 mL). The solution was filtered and left to stand at room temperature. Upon slow evaporation of the solvents, block colorless crystals single crystals suitable for X-ray diffraction were produced over a period of two weeks.

2. Figure S1-S4

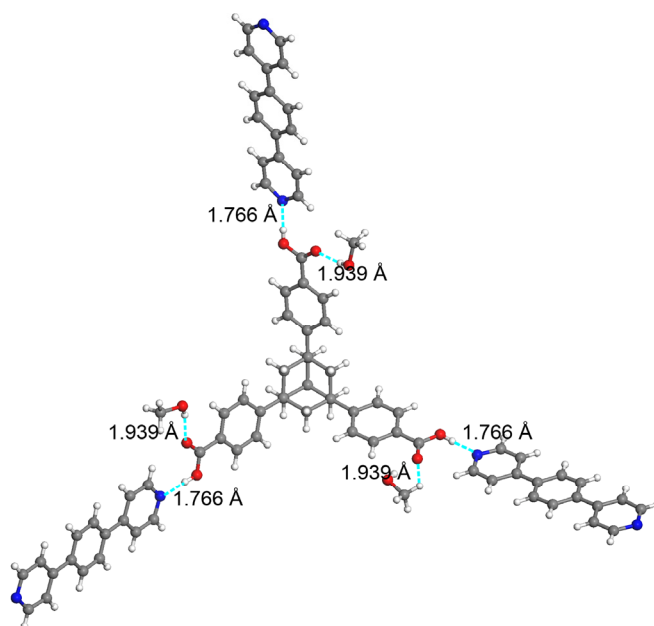


Fig. S1 Ball and stick view of the hydrogen bonds of TCA with dpyb and methanol in **[2TCA•3dpyb]**. Red: O; blue: N; gray: C; white: H.

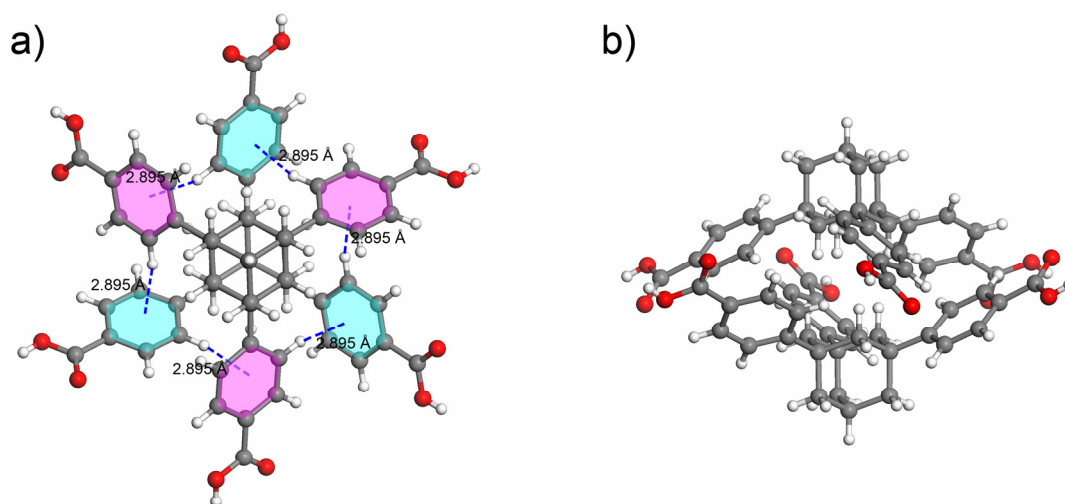


Fig. S2 Ball and stick view of the six-fold phenyl embrace and C—H... π interactions of TCA dimer in **[2TCA•3dpyb]**. Red: O; blue: N; gray: C; white: H. a) top view; b) side view.

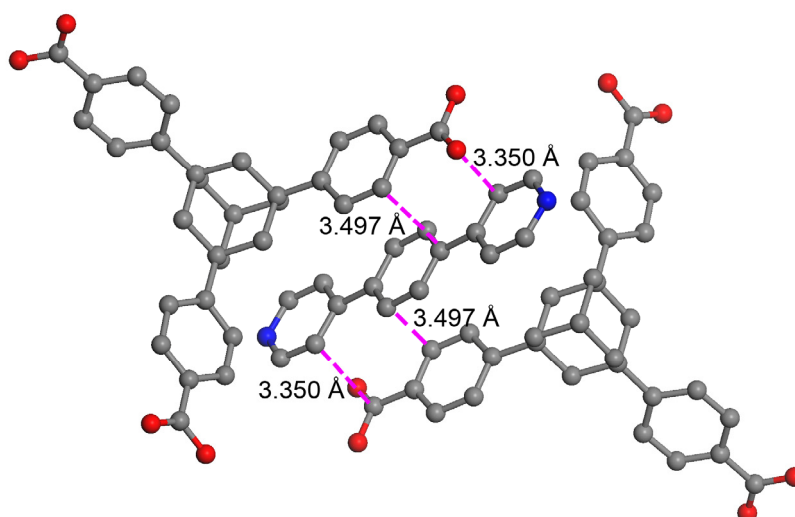


Fig. S3 Ball and stick view of $\pi \cdots \pi$ interactions of TCA-dpyb-TCA edges in [2TCA•3dpyb]. Red: O; blue: N; gray: C. The hydrogen atoms are omitted for clarity.

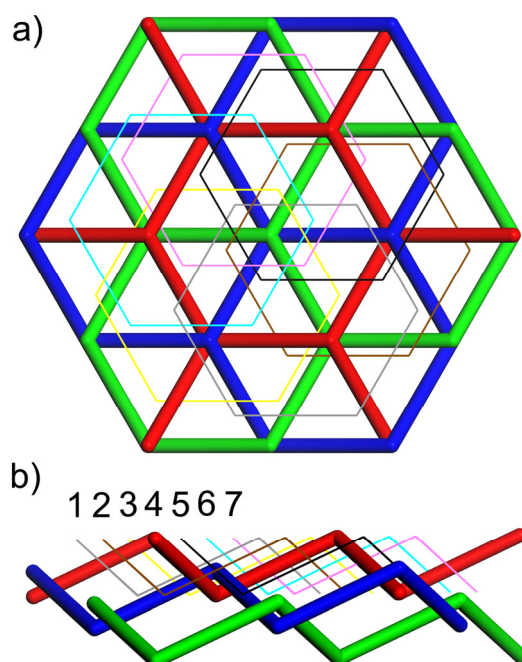


Fig. S4 Different topological view of the 7-fold interpenetrated 2D→3D extended Borromean-linked networks in [2TCA•3dpyb]. a) Top view. b) Side View. Three honeycomb nets in a Borromean weave are shown as red, blue and green with thick stick. The hexagonal rings of other six n-Borromean networks are shown as different colours with thin stick.