

Supplemental Material for:

## Three 3D octamolybdate-based hybrids with 1D–3D

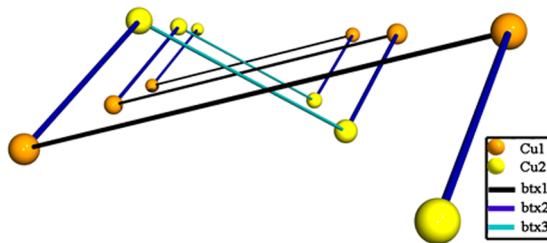
### Cu<sup>I</sup>/Cu<sup>II</sup>-bis(triazole) motifs: influence of the amount of Et<sub>3</sub>N

Chun-Jing Zhang,<sup>a</sup> Hai-Jun Pang,<sup>b</sup> Qun Tang,<sup>a</sup> Hui-Yuan Wang<sup>a</sup> and Ya-Guang Chen<sup>\*a</sup>

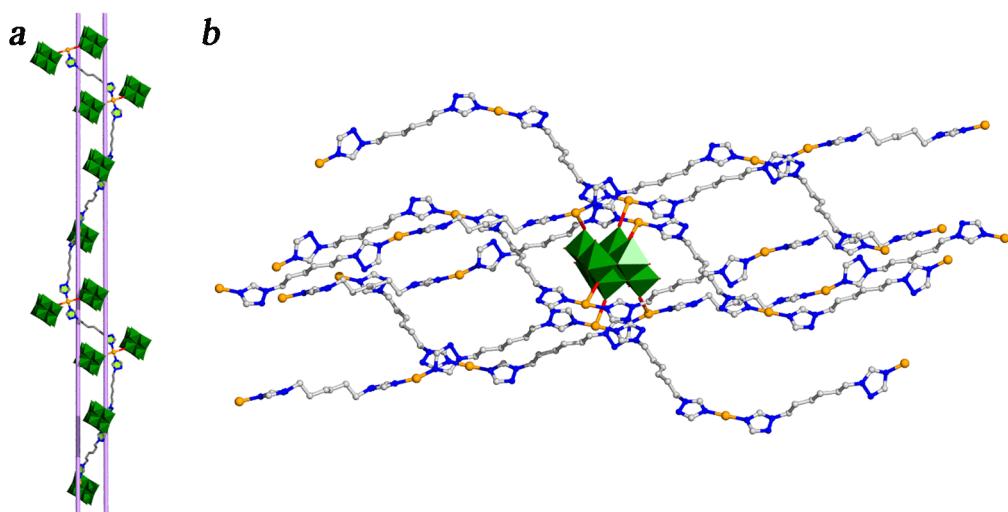
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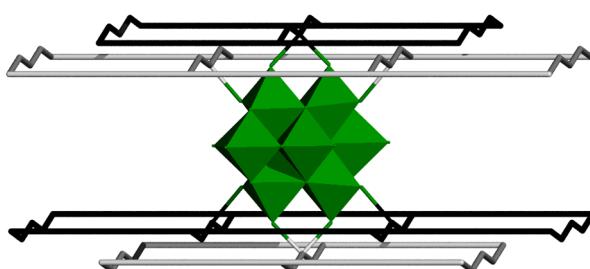
**Fig. S1** Perspective view of the meso-helical structure of **1**.



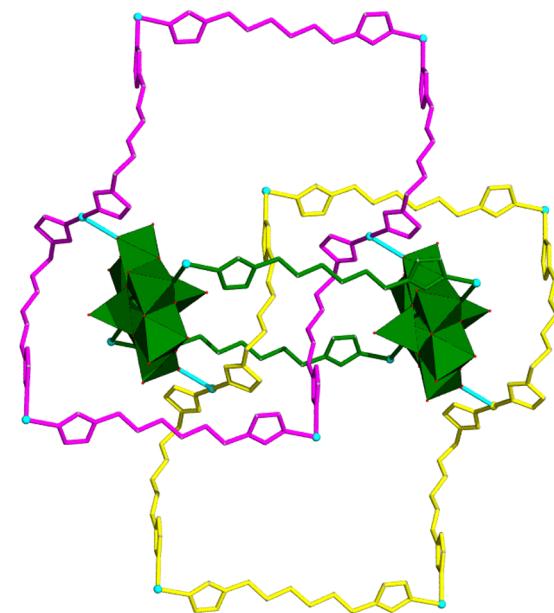
**Fig. S2** (a) View of the connectivity of meso-helix chain and  $\beta$ -Mo<sub>8</sub> anions. (b) Each  $\beta$ -Mo<sub>8</sub> anion is surrounded by six meso-helix chains with different orientation.



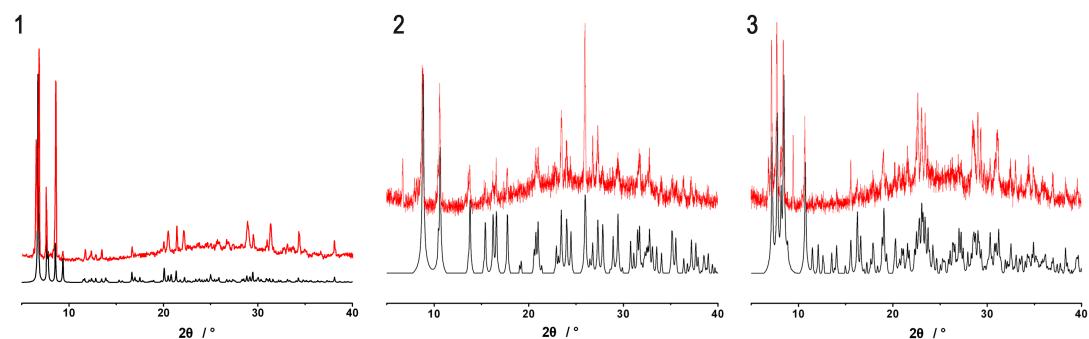
**Fig. S3** Each  $\beta$ -Mo<sub>8</sub> anion is surrounded by four 2D grid sheets.



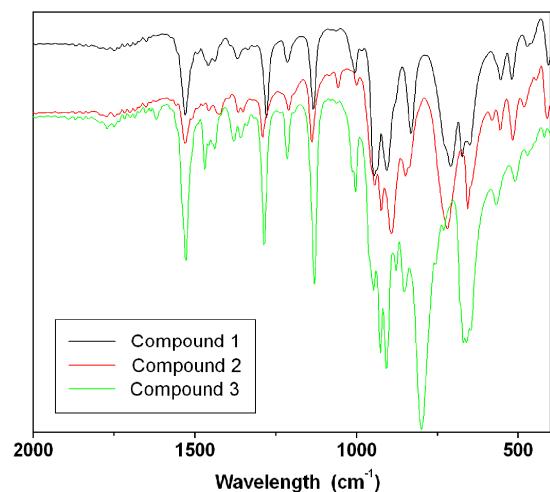
**Fig. S4** A detail of the self-threading feature in **3**.



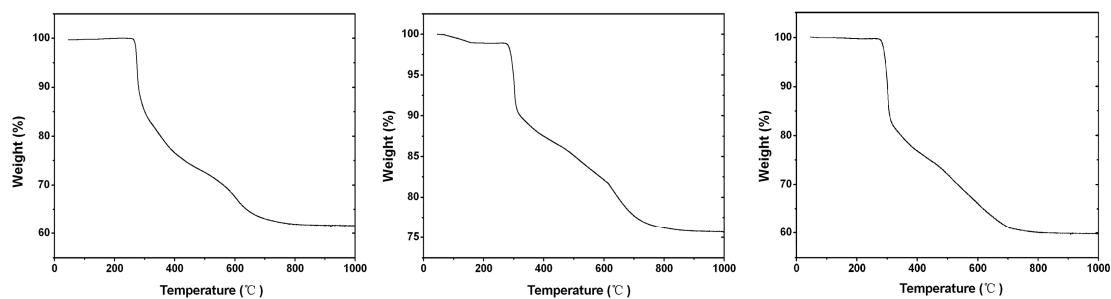
**Fig. S5** The simulative (black) and experimental (red) PXRD patterns of compounds **1–3**.



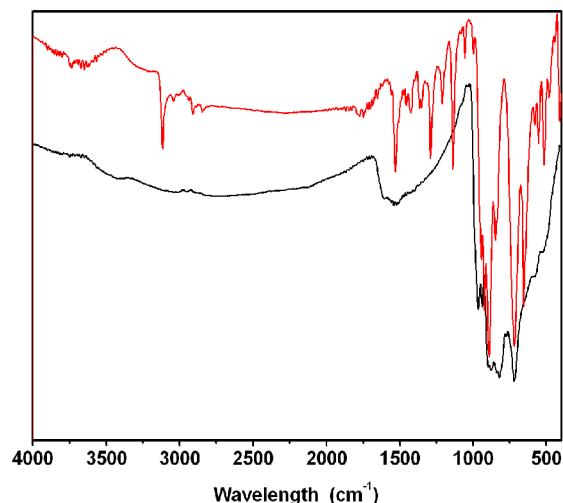
**Fig. S6** The IR spectra of compounds **1–3**.



**Fig. S7** The TG curves of compounds **1–3**.



**Fig. S8** The IR spectra of compound **2** before (red) and after heated (black).



**Fig. S8** Emission spectrum of bttx ligand in the solid state.

