

Supplementary Material

for

Zn(II) Metal–Organic Frameworks with a Long Spacer Ligand and a Tricarboxylate Coligand

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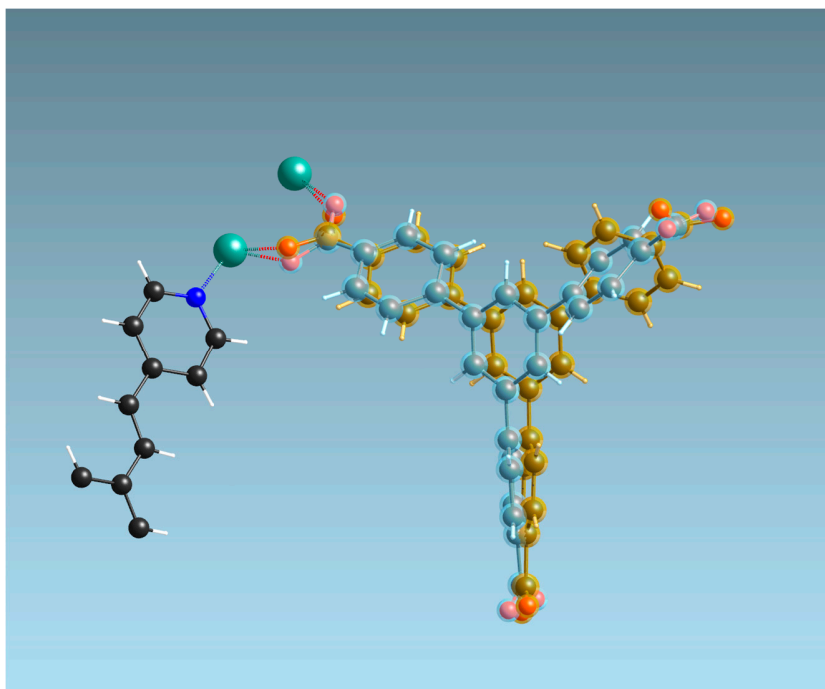


Figure S1. Crystal structure of **2** showing whole btb molecules disordered in two position (blue: yellow=53:47).

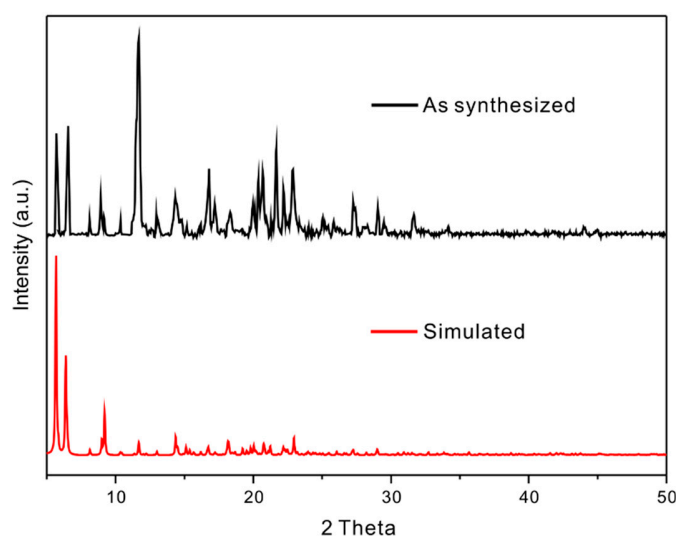


Figure S2. PXRD patterns for **1**: (top) as synthesized and (bottom) simulated from the single crystal X-ray data. The discrepancies in the intensities may be due to preferred orientations of the powder or partial removal of solvents during grinding.

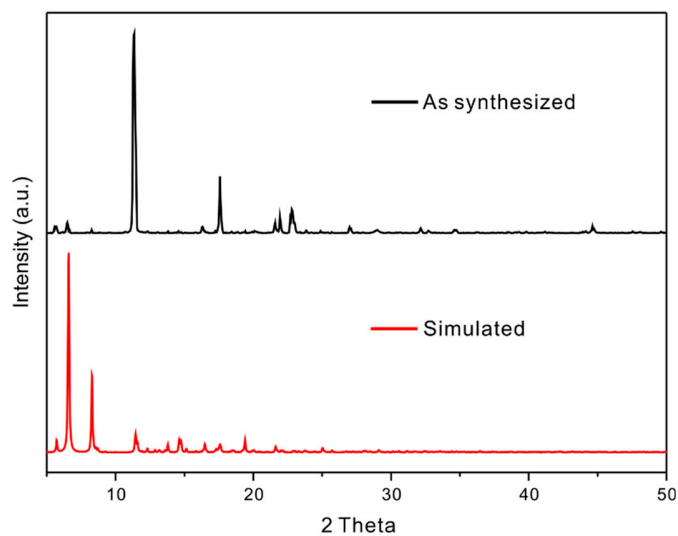


Figure S3. PXRD patterns for **2**: (top) as synthesized and (bottom) simulated from the single crystal X-ray data. The discrepancies in the intensities may be due to preferred orientations of the powder or partial removal of solvents during grinding. The simple patterns and intensity variations for the synthesized sample compared to the simulated one are mainly due to the flexible nature of the product [S1-S3].

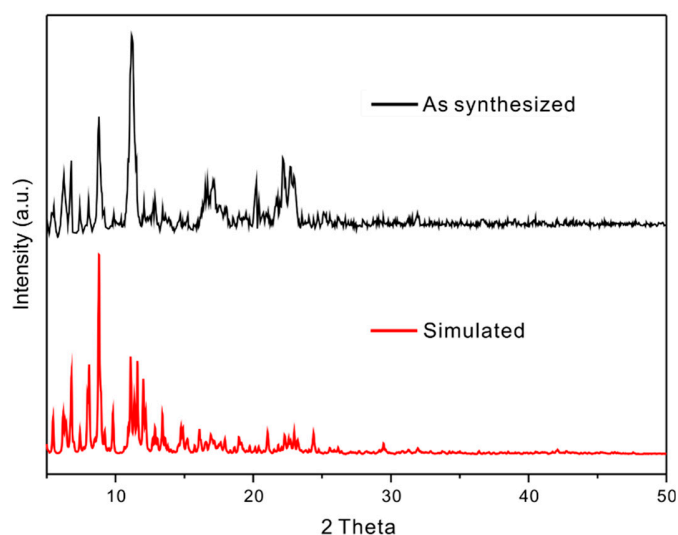


Figure S4. PXRD patterns for **3**: (top) as synthesized and (bottom) simulated from the single crystal X-ray data. The discrepancies in the intensities may be due to preferred orientations of the powder or partial removal of solvents during grinding.

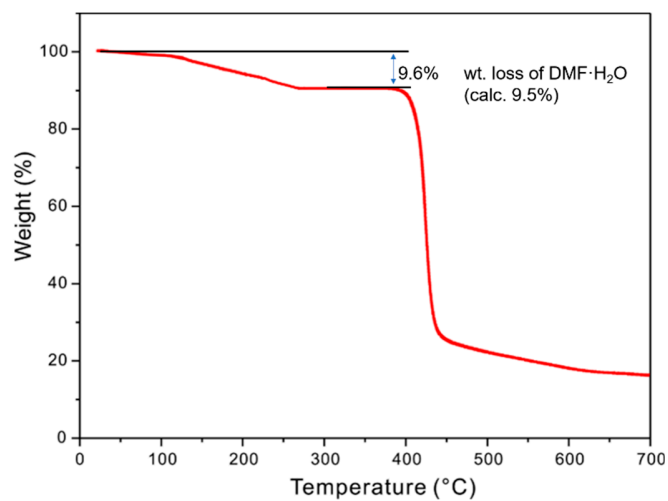


Figure S5. TGA curve of **1**.

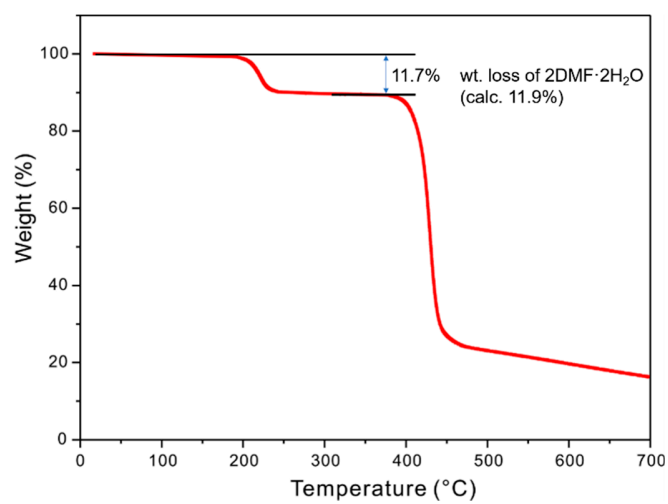


Figure S6. TGA curve of **2**.

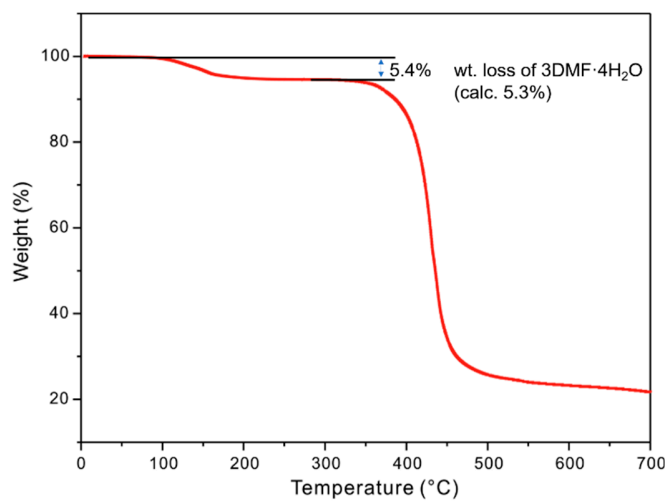


Figure S7. TGA curve of **3**.

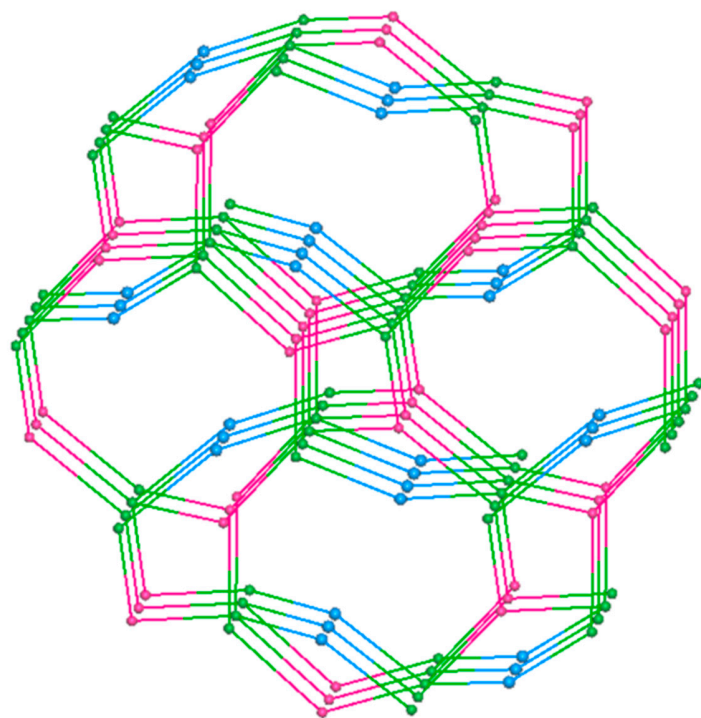


Figure S8. Topological representation of **1**. Color codes: bpeb node (blue), Zn node (green), and btb node (pink).

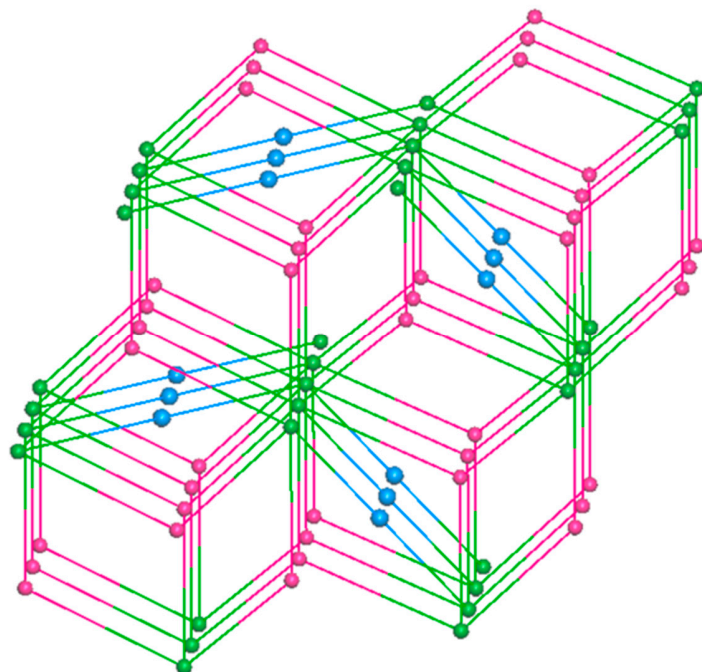


Figure S9. Topological representation of **2**. Color codes: bpeb node (blue), Zn node (green), and btb node (pink).

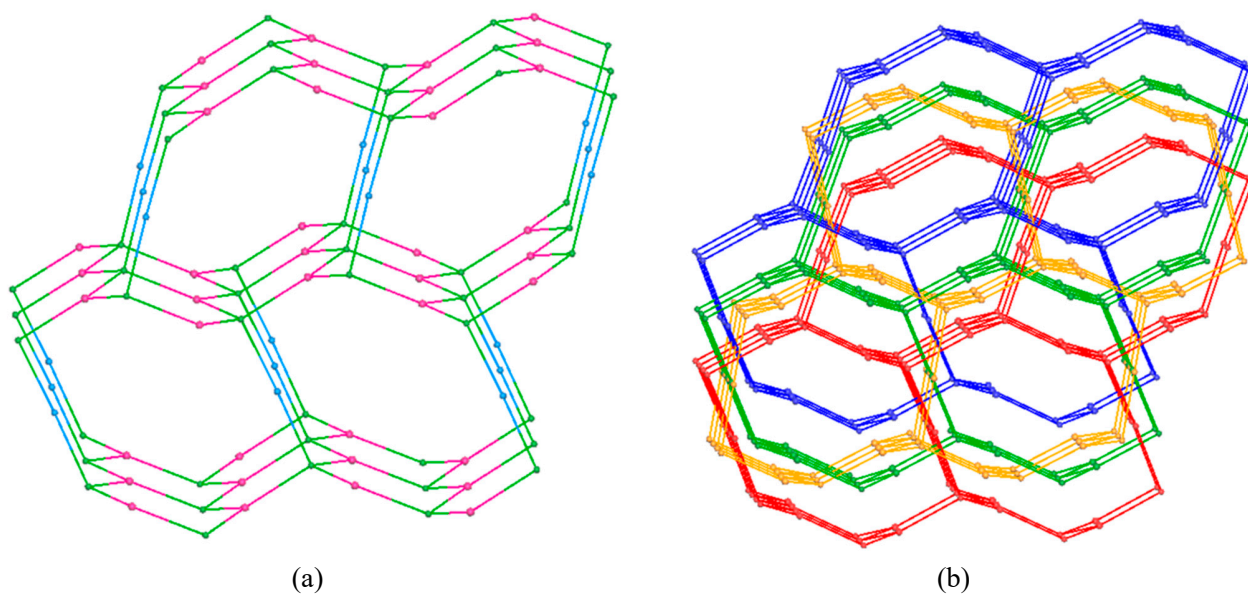


Figure S10. Topological representation of **3** showing (a) a single network and (b) four-fold interpenetration. Color codes: bpeb node (blue), Zn node (green), and btb node (pink).

References:

- S1. J. Duan, M. Higuchi, M. L. Foo, S. Horike, K. P. Rao and S. Kitagawa, *Inorg. Chem.*, 2013, **52**, 8244.
 S2. S. Henke, R. Schmid, J.-D. Grunwaldt and R. A. Fischer, *Chem. Eur. J.*, 2010, **16**, 14296.
 S3. W. Kaneko, M. Ohba and S. Kitagawa, *J. Am. Chem. Soc.*, 2007, **129**, 13706.