Supporting Information for

Self-Assembly of a Novel Metal-organic Coordination Cage (MOCC) Based on a New Flexible Dicarboxylate Ligand: Synthesis, Crystal Structure and Magnetic Property

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General Information. Commercially available reagents were used as received without further purification. Elemental analyses (C, H, N, S) were obtained on a Perkin-Elmer 240 elemental analyzer. Thermal gravimetric analysis (TGA) was performed under N_2 on a Perkin Elmer TGA 7 instrument. NMR was collected on a Bruker 300 MHz spectrometer. Variable-temperature magnetic susceptibility data for polycrystalline samples of **MOCC-3** were obtained in an external field of 10.0 KG on a Quantum Design PPMS Model 6000 magnetometer from 275 to 4 K.

Synthesis of H_2**L**: Sodium methylate (1.78 g, 0.034 mol) was dissolved in absolute methanol (200 mL), to which o-mercaptobenzoic acid (4.7 g, 0.034 mol) was added. The mixture was stirred for 10 minutes, then, bis(bromomethyl)mesitylene (3.48 g, 0.0114 mol) was added. The reaction mixture was stirred under reflux for 6 hrs. The solid was filtered while still hot, and dissolved in water and filtered to remove any undissolved substance. The filtrate was acidified with dilute hydrochloric acid to give colorless solid, which was washed several times with water. Yield: 65 %. ^{1}H NMR (DMSO): 2.34, 6H; 2.43, 3H; 4.15, 4H; 6.97, 2H; 7.24, 2H; 7.58, 2H; 7.94, 2H.

Figure S1. The coordination environment of Mn1 and Mn2 in **MOCC-3**.

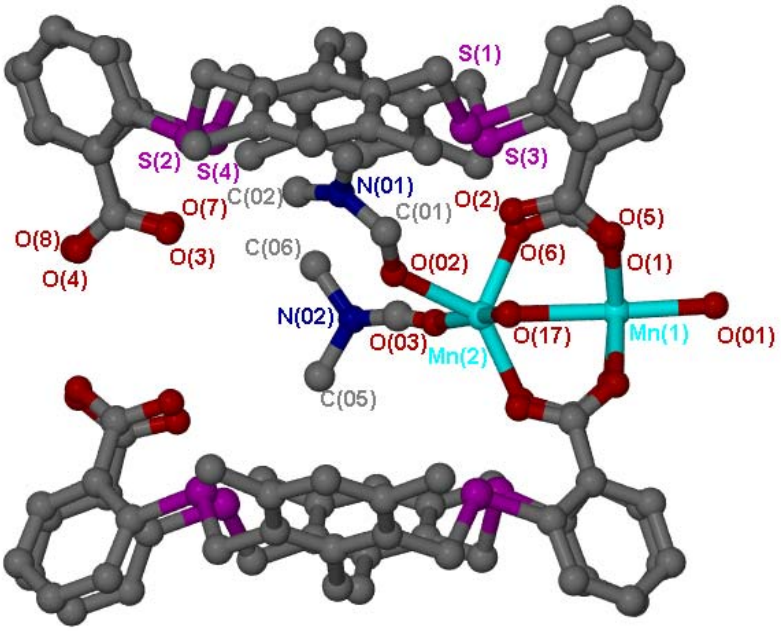

Figure S2. The coordination environment of Mn3 and Mn4 in **MOCC-3**.

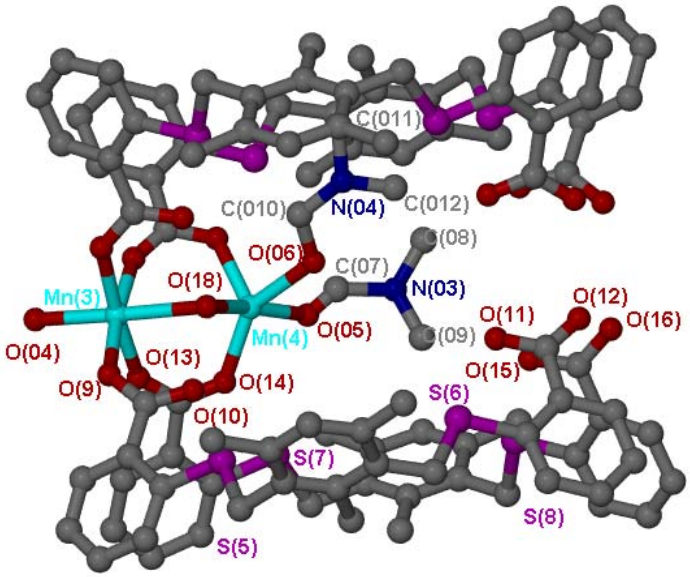

Figure S3. The packing of **MOCC-3** along *a* axis with space-filling representation of uncoordinated water and dmf molecules.

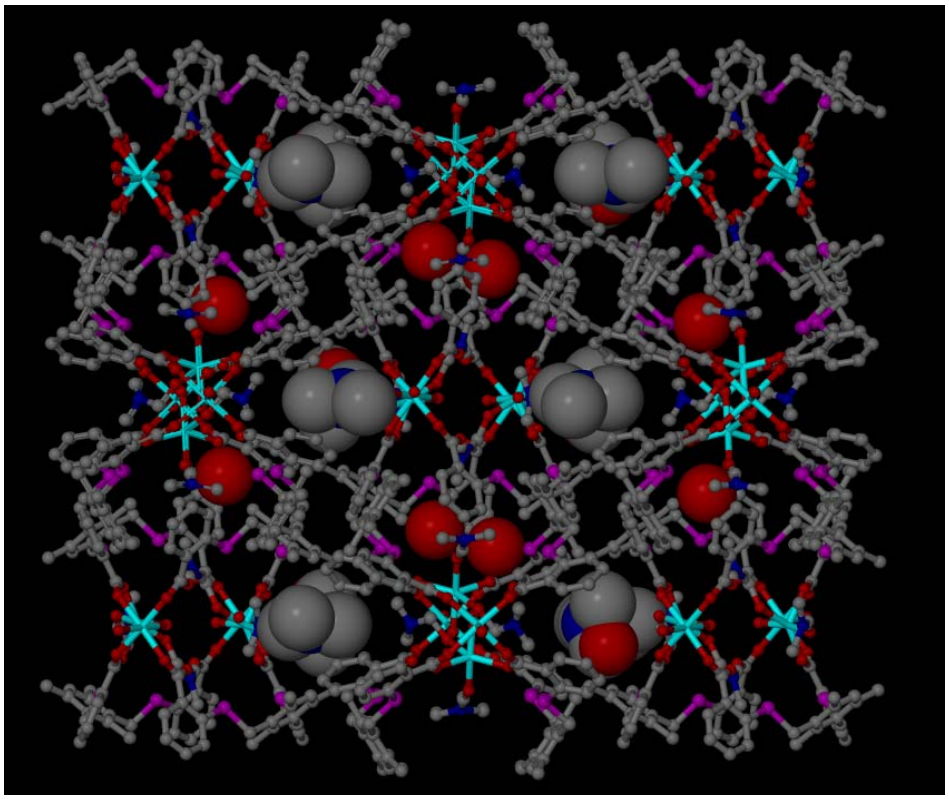

Figure S4. The packing of **MOCC-3** along *c* axis with space-filling representation of coordinated dmf molecules.

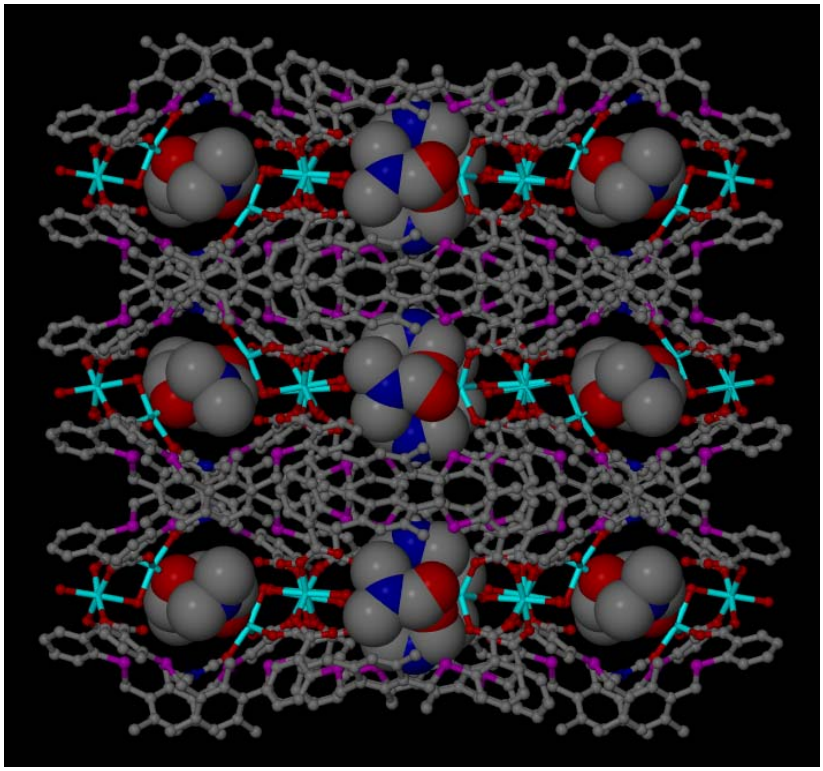

Figure S5. TGA of 1.