Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Solvent-controlled Structural Diversity Observed in three Cu(II) MOFs with 2,2'-dinitro-biphenyl-4,4'-dicarboxylate Ligand: Synthesis, Structures and Magnetism

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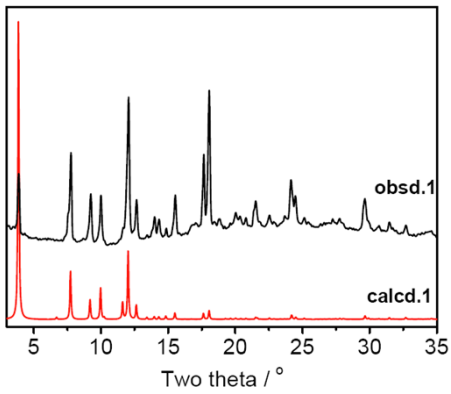

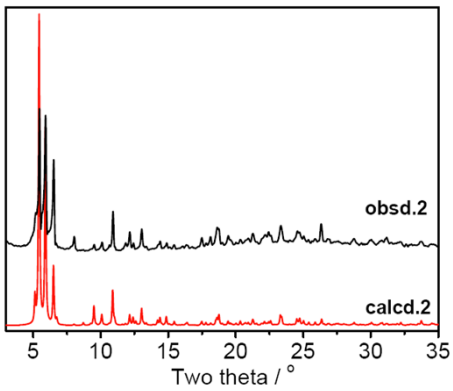

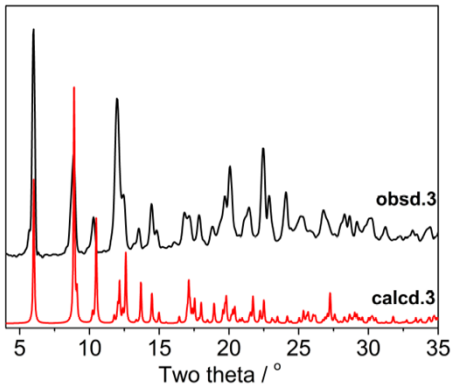

Figure S1. The experimental PXRD and calculated patterns from crystal data for compounds **1-3**.

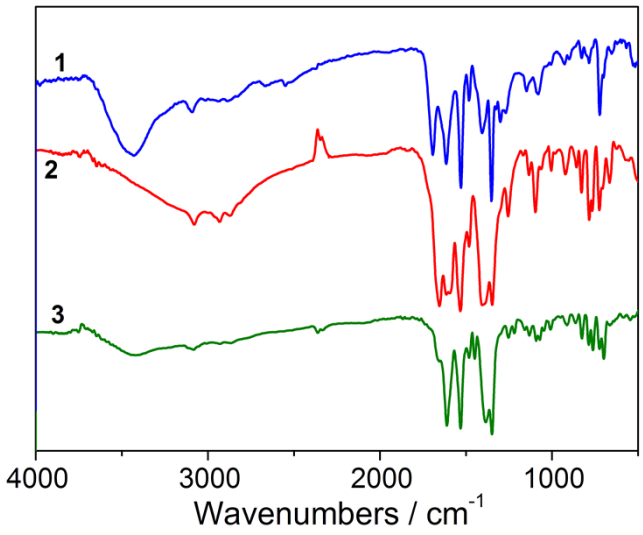

Figure S2. The FT-IR spectrum of compounds **1-3** .

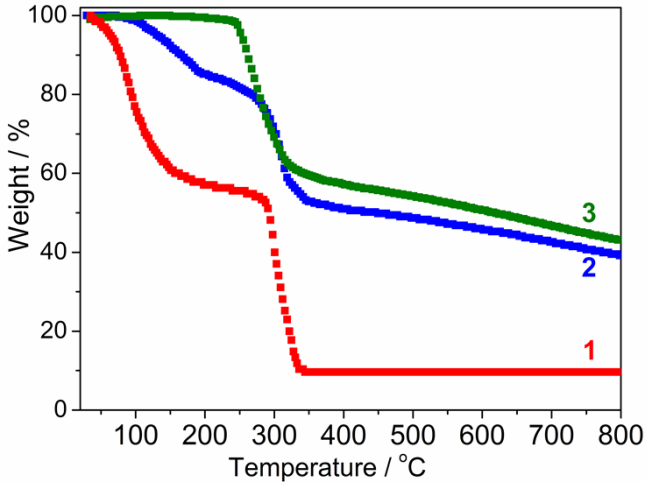

Figure S3. The TGA curves for compounds **1-3**. Compound **1** shows a rapid weight loss (46.3%) below 200°C, corresponding to the release of all four DMA and two water guest molecules per formula unit (calcd. 48.3%) and the framework finally collapsed from 255°C. Compound **3** shows no obvious weight loss until 190 °C, which is consistent with the absence of solvent molecules in the structure.

Table S1. Selected bond lengths [Å] and angles [°] for compound **1**.

Cu1-O1	1.9533(18)	Cu1-O2C	1.9448(18)
Cu1-O3B	1.9436(18)	Cu1-O4A	1.9515(18)
Cu1-OW1	2.115(3)	Cu1E-O3	1.9439(18)
O4A-Cu1-O3B	167.87(9)	O4A-Cu1-O1	90.19(11)
O3B-Cu1-O1	88.99(11)	O4A-Cu1-O2C	88.93(11)
O3B-Cu1-O2C	89.33(11)	O1-Cu1-O2C	167.77(9)
O4A-Cu1-OW1	94.17(12)	O3B-Cu1-OW1	97.95(12)
O1-Cu1-OW1	94.13(12)	O2C-Cu1-OW1	98.09(12)

Symmetry codes: A y, -x+y, -z; B -y+1/3, x-y+2/3, z+2/3; C -x+1/3, -y+2/3, -z+2/3; D x-y, x, -z; E -x+y-1/3, -x+1/3, z-2/3.

Table S2. Selected bond distances [Å] and angles [°] for compound **3**.

Cu1-N1	1.978(4)	Cu2-N2	1.997(4)
Cu2-O1	1.950(3)	Cu2-O5	2.198(4)
Cu1-O6	1.913(3)	Cu1-O7	1.956(5)
Cu2-O7	1.986(4)	Cu1-O7A	1.951(4)
Cu2-O4B	2.000(3)		
O6-Cu1-O7A	168.71(18)	O7A-Cu1-O7	81.53(16)

O6-Cu1-O7	93.26(15)	O6-Cu1-N1	93.98(17)
O7A-Cu1-N1	93.93(18)	O7-Cu1-N1	162.08(18)
O1-Cu2-O7	93.48(16)	O1-Cu2-O4B	171.12(17)
O7-Cu2-O4B	88.22(15)	O1-Cu2-N2	88.66(17)
O7-Cu2-N2	173.31(18)	O4B-Cu2-N2	88.71(17)
O1-Cu2-O5	90.75(17)	O7-Cu2-O5	91.65(17)
O4B-Cu2-O5	97.92(16)	N2-Cu2-O5	94.65(17)

Symmetry codes: A –x+3/2, -y+3/2, -z+1; B x, -y+2, z-1/2.

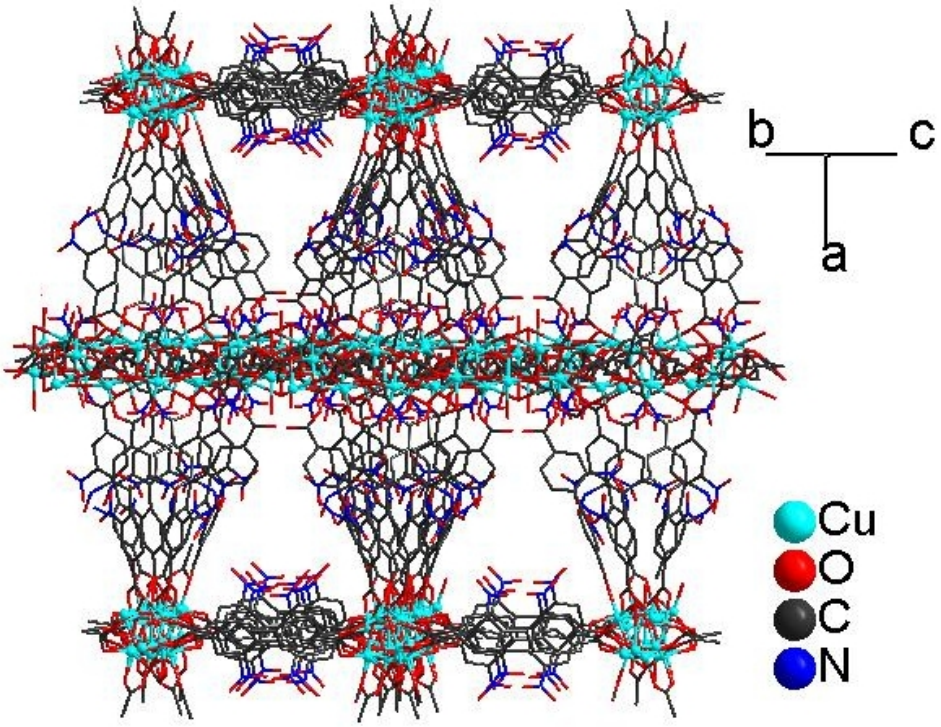

Figure S4. View of the 3D frameworks in compound **2**.