Supplementary Information

Title: A novel polythreaded metal-organic framework with inherent features of different side arms and five fold interpenetration

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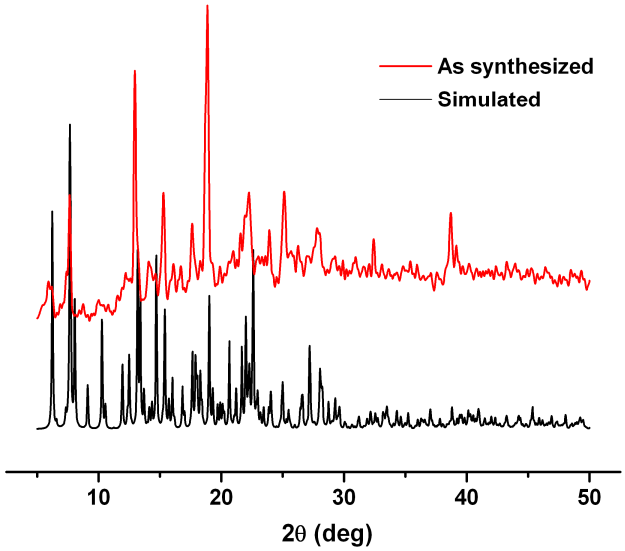

Fig. S1. Comparison of XRPD patterns of the simulated pattern and as-synthesized product.

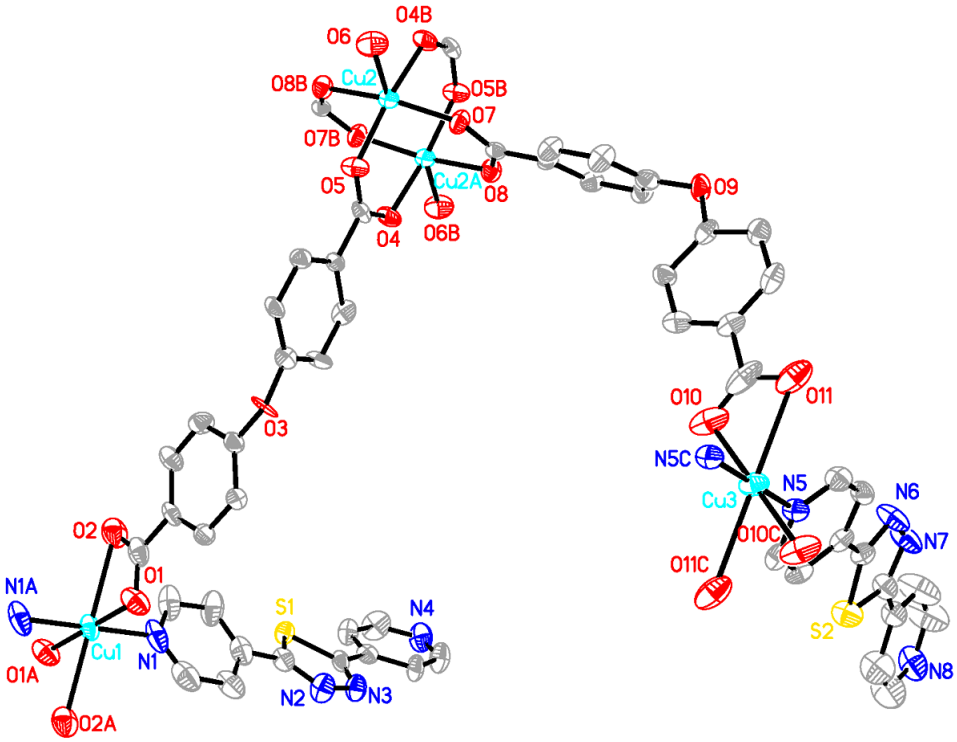

Fig. S2. ORTEP plot (30% thermal probability ellipsoids) of the crystal structure. Cu1 and Cu3 are situated on inversion centres while Cu2 is in a general position. The metal site Cu1 is half-occupied. Solvent molecules and hydrogen atoms are omitted for clarity. Symmetry codes: A: -x+1, -y+1, -z-1; B: -x, -y+2, -z; C: -x-1, -y, -z.

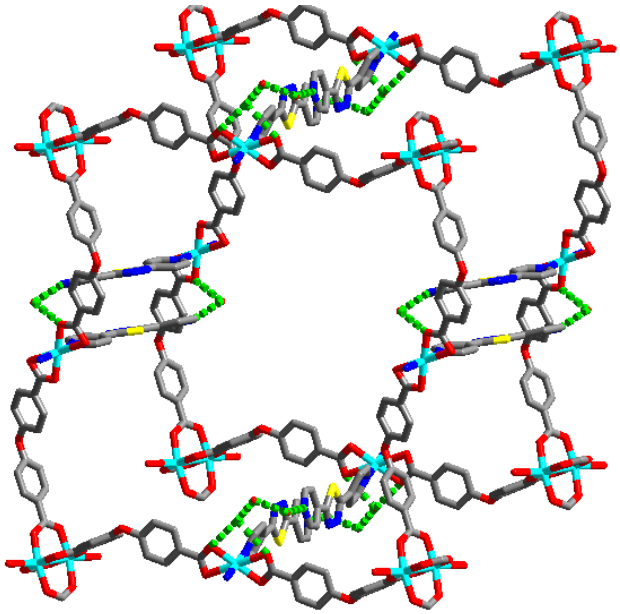

Fig. S3. View of a single distorted cube-like unit.

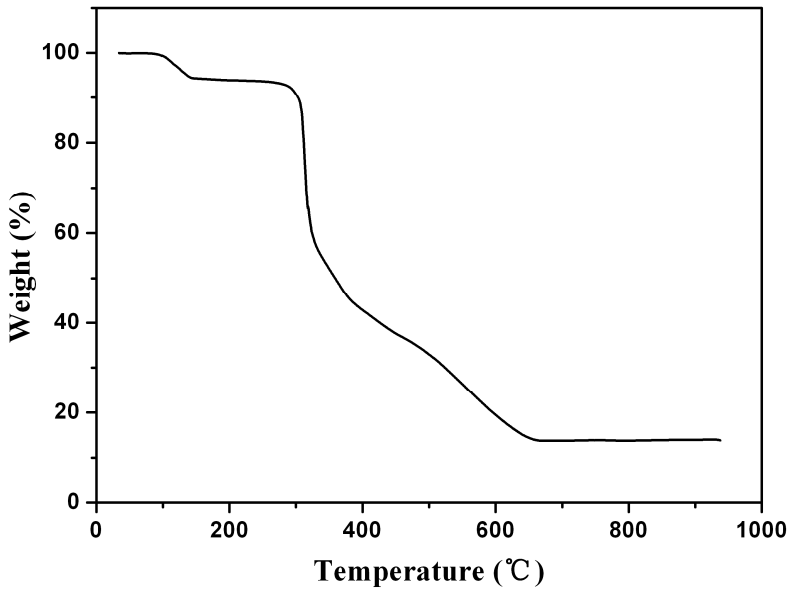

Fig. S4. TG graph of complex **1**.

Table S1. Selected bond lengths (Å) and angles (°) of complex **1**[a]

Cu1–N1	2.013(7)	Cu1–O1	2.032(4)	Cu1–O2	2.445(5)
Cu2–O5	1.941(4)	Cu2–O4#2	1.952(4)	Cu2–O7	1.971(4)
Cu2–O8#2	1.972(4)	Cu2–O6	2.160(4)	Cu3–O10	1.991(5)
Cu3–N5	1.991(5)	Cu3–O11	2.506(5)		
N1–Cu1–O1	89.0(2)	N1–Cu1–O2	88.1(2)	O1–Cu1–O2	58.15(18)
O5–Cu2–O4#2	168.19(17)	O5–Cu2–O7	89.52(17)	O4#2–Cu2–O7	89.74(17)
O5–Cu2–O8#2	87.65(17)	O7–Cu2–O8#2	168.30(16)	O4–Cu2–O8	90.71(17)
O5–Cu2–O6	99.83(17)	O4#2–Cu2–O6	91.96(17)	O10–Cu3–N5	89.0(2)
O10–Cu3–O11	56.6(2)	O7–Cu2–O6	90.37(16)	O8#2–Cu2–O6	101.30(16)
O11–Cu3–N5	88.7(2)				

[a] Symmetry codes: #2 -x, -y+2, -z.

Table S2. Possible hydrogen bond geometries for complex **1**[a]

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	<DHA (°)
O15–H15A···O1	0.829(11)	2.52(3)	2.940(10)	112(2)
O14–H14B···.O6#4	0.84	2.12	2.964(8)	173.0
O14–H14A···O15#5	0.78	1.92	2.700(16)	173.8
O13–H13B···N4#6	0.79	2.02	2.812(10)	176.4
O13–H13A···O14	0.79	2.01	2.795(12)	175.2
O12–H12B···O10#7	0.77	2.21	2.972(9)	175.2
O12–H12A···N8#8	0.78	2.11	2.891(8)	174.6
O6–H6WB···O12#2	0.80	1.95	2.752(6)	178.6
O6–H6WA···O11#9	0.83	2.38	3.059(7)	138.9

[a] Symmetry codes: #2 -x, -y+2, -z; #4 x+1, y, z+1; #5 -x+1, -y+1, -z; #6 x-1, y, z; #7 -x, -y+1, -z; #8 –x+1, -y+1, -z+1; #9 –x-1, -y+1, -z.