Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Synthesis, Structure, Topology and Catalytic Application of a Novel Cubane-based Copper(II) Metal–Organic Framework derived from a Flexible Amido Tripodal Acid

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Table S1: Crystal data and structure refinement detail for Compound 1

Formulae	$C_{20}H_{29}Cu_2N_3O_{13}$
Mol. wt.	646.54
Crystal system	Tetragonal
Space group	$P4_32_12$
Temperature /K	100
Wavelength /Å	0.71073
a /Å	18.9809(12)
b /Å	18.9809(12)
c /Å	17.5707(12)
α/°	90
β/°	90
γ/°	90
V/ Å^3	6330.3(9)
Z	8
Density/Mgm^{-3}	1.357
Abs. Coeff. /mm^{-1}	1.401
F(000)	2656
Refl. collected	40233
Refl. unique	9790
Max. 2θ/°	30.682
Ranges (h, k, l)	-27 <= h <= 23 -27 <= k <= 26 -25 <= l <= 25

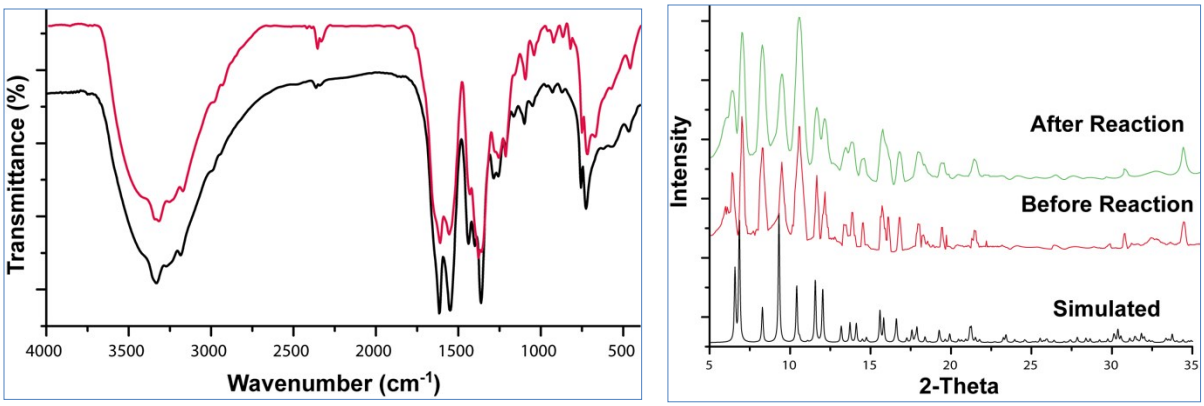
Complete to 2θ (%)	99.9
Refl. with I > 2σ(I)	7629
Data/ Restraints/Parameters	9790/ 184/ 412
Goof (F^2)	1.046
R1 [I > 2s(I)]	0.0566
wR2 [I > 2s(I)]	0.1588
R1 [all data]	0.0775
wR2 [all data]	0.1712

Table S2: Selected bond distances (Å) and angles (°) of 1

	Bond distances		Bond angles		Bond angles
Cu1–O1M2	1.945(4)	<OW1–Cu1–O1M1	92.81(17)	<OW2–Cu2 O1M2	101.80(19)
Cu1–O1M2’	1.961(4)	<O1M2–Cu1–OW1	95.71(19)	<O1M1 Cu2–OW2	167.64(19)
Cu1–OW1	2.004(5)	<O1M2–Cu1–OW1	174.44(19)	<O1M1–Cu2–OW2	91.74(19)
Cu1–O1M1	2.424(4)	<O1M2–Cu1–O1M1	84.22(15)	<O1M1–Cu2–O1M1	78.39(18)
Cu2–O1M1	1.951(4)	<O1M2–Cu1–O1M1	85.26(15)	<O1M1–Cu2–O1M2	84.95(16)
Cu2–O1M1’	1.967(4)	<O1M2–Cu1–O1M2	78.92(17)	<O1M1–Cu2–O1M2	85.31(15)
Cu1–O2	1.969(4)	<O1M2–Cu1–O2	93.36(17)	<O1M1–Cu2–O5	170.94(17)
Cu2–OW2	1.989(5)	<O1M2–Cu1–O2	170.85(17)	<O1M1–Cu2–O5	94.92(17)
Cu2–O1M2	2.405(4)	<O2–Cu1–OW1	91.86(19)	<O5–Cu2–OW2	95.6(2)
Cu1–Cu1	3.0155(13)	<O2–Cu1–O1M1	90.30(15)	<O5–Cu2–O1M2	88.05(16)
Cu2–Cu2	3.0362(13)				
Cu2–O5	1.977(4)				

Table S3: C-H····O interactions (Å, °) in complex 1

Complex	D-H---A	D···H (Å)	H···A (Å)	D···A (Å)	<D–H···A(°)	Symmetry
1	C2–H2A····O1	0.95	2.44	3.3464(2)	160	1/2-y,1/2+x,-1/4+z
	C1M2–H1MF····O2	0.98	2.59	3.1125(2)	113	-
	C16A–H16A····O7	1.00	2.38	2.7986(2)	104	-
	C17A–H17E····O9A	0.98	2.54	2.9553(2)	105	-



A B

Figure S1: (A) FT-IR spectra of **1** before (black line) and after (red line) the Henry reaction. (B) PXRD diffractograms of **1** before (red line) and after (green line) the Henry reaction.

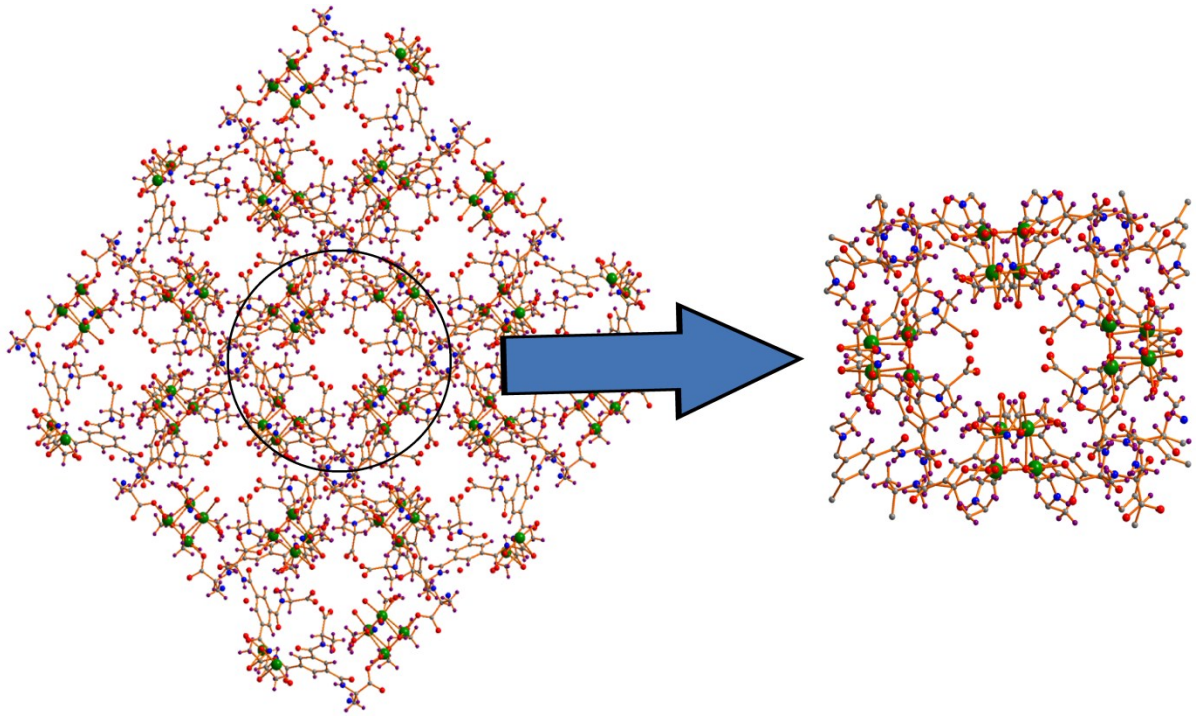


Figure S2

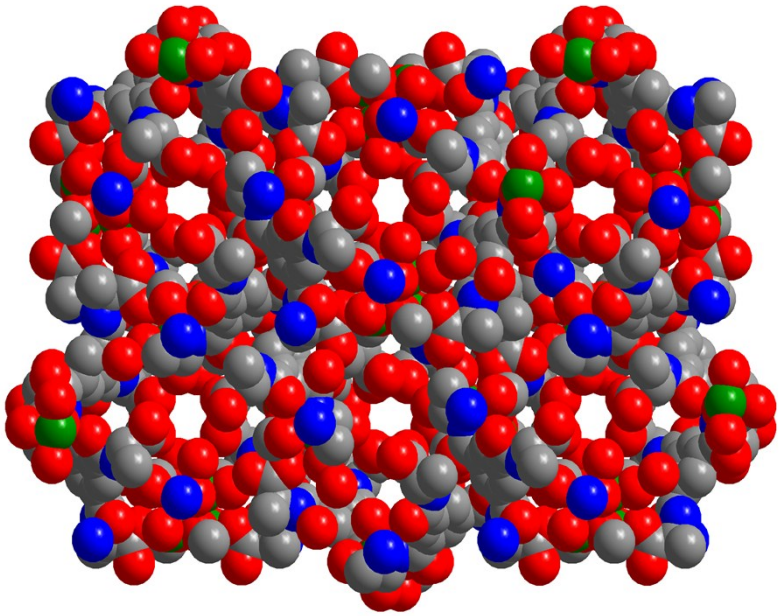


Figure S3 Space-filling model of MOF **1**

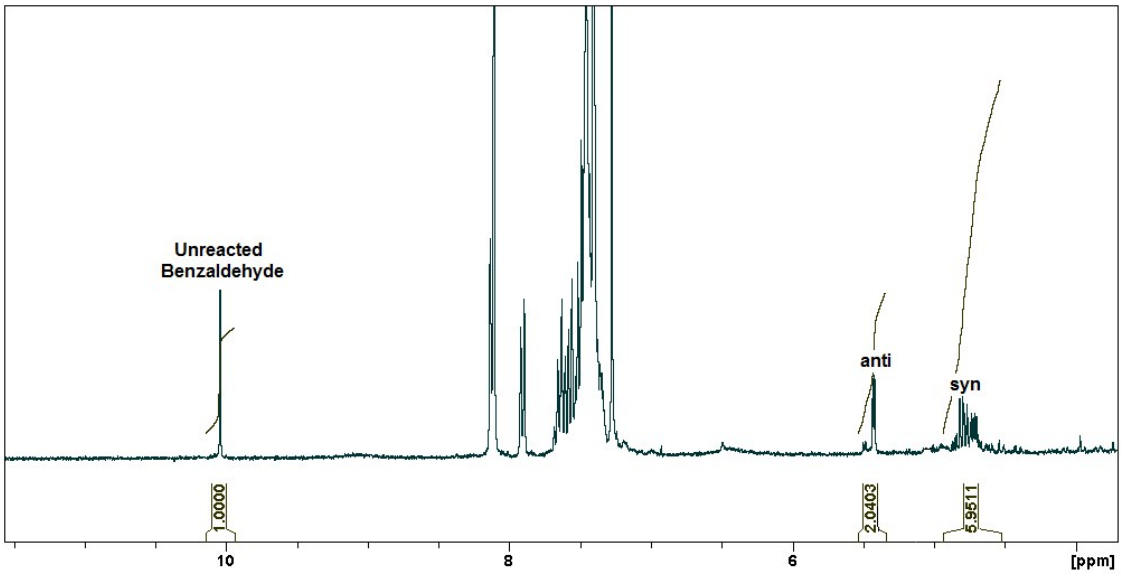


Figure S4 Example of integration in the ^{1}H-NMR spectrum for the determination of Henry reaction products (Table 1, Entry 6).

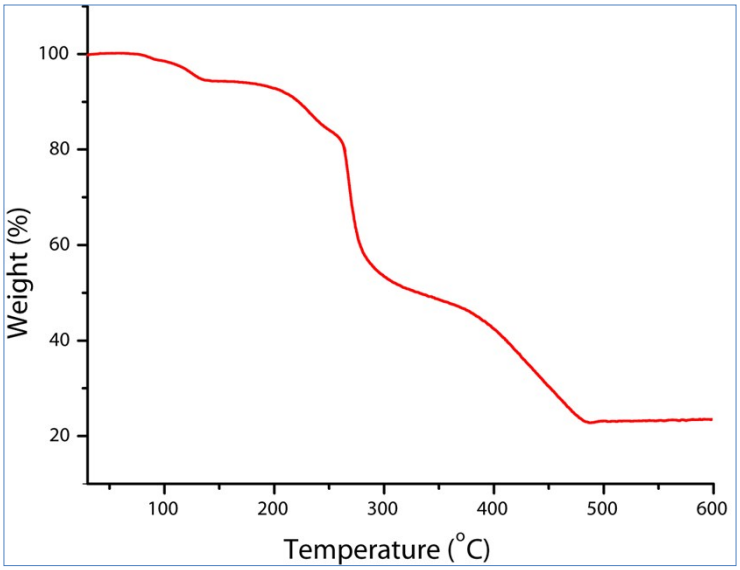


Figure S5 Thermogravimetric curve for framework **1**.