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Supporting Information

Synthesis and Structural Characterisation of the copper MOF: STAM-NMe_2.

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Experimental

Synthesis of 5-dimethylamino isophthalic acid:[1]

Formaldehyde solution (37 wt% in water, 6 mL, 10 eq.) was added to a solution of 5-amino isophthalic acid (1.38 g, 7.62 mmol) in DMF (10 mL) and the solution was stirred at ambient temperature for 20 minutes. The solution was cooled to 0 °C and sodium cyanoborohydride (1.42 g, 22.60 mmol) was slowly added. The solution was then stirred for 5 hours at ambient temperature. After evaporation of the solvent, the residue was dissolved in water and precipitated by addition of 2 M hydrochloric acid. The white precipitate was filtrated and washed with water until the pH value of the filtrate was neutral, to yield 5-dimethylamino isophthalic acid (5.28 g, 83 %) as a pale yellow solid. ^{1}H NMR (400 MHz, d_6-DMSO) δ_H 7.79 (1 H, t, J = 2.8 Hz, 1.6Hz), 7.44 (2 H, d, J = 1.2 Hz), 2.99 (6 H, s) ppm.

Crystallographic Data

Fig. S1 Comparison of bulk material with the single crystal phase by a whole-pattern (Le Bail type) refinement of the unit cell against the X-ray diffraction data to confirm sample purity.

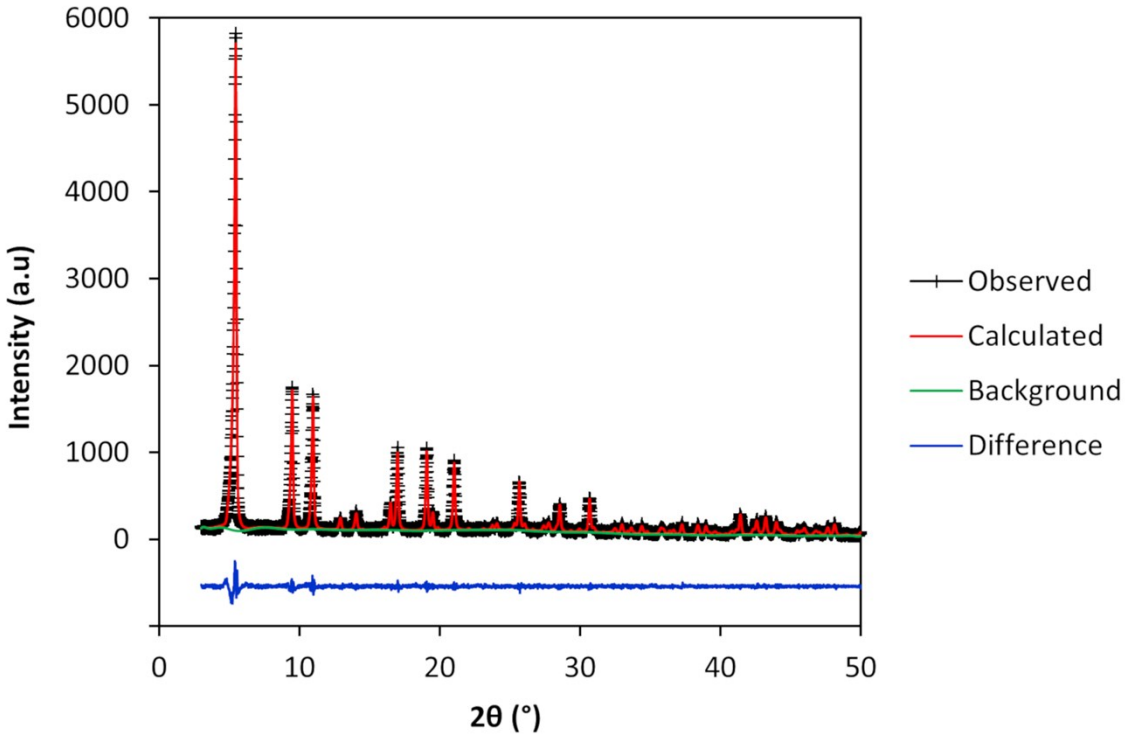

Table. S1 Crystallographic parameters from the Le Bail powder diffraction refinement of STAM-NMe_2 and comparison with single crystal data.

	Powder	**Single Crystal**
Temperature	298 K	173 K
Unit cell dimensions	a = 18.5669(5) Å	a = 18.5382(5) Å
	b = 18.5669(5) Å	b = 18.5382(5) Å
	c = 6.8288(3) Å	c = 6.7599(2)Å
Unit cell angles	α = 90	α = 90
	β = 90	β = 90
	γ = 120	γ = 120
Space Group	$P\bar{3}m1$	$P\bar{3}m1$

wRp	0.0643	-
Rp	0.0529	-

Table. S2 Full crystallographic data from the single crystal structure determination of STAM-NMe_2**.**

Identification code	**STAM-NMe_2**
Empirical formula	$C_{10}H_{11}CuNO_5$
Formula weight	288.74 g mol^{-1}
Temperature	173 K
Wavelength	0.71073 Å
Crystal system, space group	Trigonal, $P\bar{3}m1$
Unit cell dimensions	a = 18.5382(5) Å
	b = 18.5382(5) Å
	c = 6.7599(2)Å
Volume	2011.90(12) $Å^3$
Z	6
Calculated density	1.430 g cm^{-3}
Absorption coefficient	1.635 mm^{-1}
F(000)	882.0
GooF on F^2	1.124
Crystal size	0.04 x 0.04 x 0.02 mm^3
Theta range for data collection	4.394 to 57.87°
Reflections collected/unique	26670/1842 [R(int) = 0.0713]
Final R indices (I>2σ(I))	R_1 = 0.0367 wR_2 = 0.0941
Final R indices (all data)	R_1 = 0.0565 wR_2 = 0.0992

Table. S3 Bond lengths for STAM-NMe_2 from single crystal data.

Atom	Length (Å)	Atom	Length (Å)
Cu(1)-Cu(1)[1]	2.6032(7)	N(1)-C(5)	1.386(4)
Cu(1)-O(1W)	2.146(2)	N(1)-C(6)	1.443(3)
Cu(1)-O(2)[1]	1.9649(16)	N(1)-C(6)[4]	1.443(3)
Cu1()-O(2)[2]	1.9649(16)	C(1)-C(2)	1.491(3)
Cu(1)-O(1)	1.9524(18)	C(2)-C(4)	1.392(4)
Cu(1)-O(1)[3]	1.9523(18)	C(2)-C(3)	1.392(3)
O(2)-C(1)	1.253(3)	C(5)-C(4)	1.411(3)
O(1)-C(1)	1.251(3)	C(5)-C(4)[4]	1.411(3)

Symmetry transformations used to generate equivalent atoms:

[1] 1-X,1-Y,1-Z [2] +Y,+X,1-Z [3] 1-Y,1-X,+Z [4] +X,1+X-Y,+Z

Table. S4 Bond angles for STAM-NMe_2 from single crystal data.

Atom	Angle (°)	Atom	Angle (°)
O(1W) Cu(1) Cu(1)[1]	179.02(7)	C(1) O(1) Cu(1)	124.42(16)
O(2)[1] Cu(1) Cu(1)[1]	84.86(5)	C(5) N(1) C(6)[4]	119.29(16)
O(2)[2] Cu(1) Cu(1)[1]	84.86(5)	C(5) N(1) C(6)	119.29(16)
O(2)[1] Cu(1) O(1W)	95.83(7)	C(6)[4] N(1) C(6)	116.9(3)
O(2)[2] Cu(1) O(1W)	95.83(12)	O(2) C(1) O(1)	124.2(2)
O(2)[1] Cu(1) O(2)[2]	88.32(5)	O(2) C(1) C(2)	118.4(2)
O(1) Cu(1) Cu(1)[1]	83.82(5)	O(1) C(1) C(2)	117.4(2)
O(1)[3] Cu(1) Cu(1)[1]	83.82(5)	C(4) C(2) C(1)	119.9(2)
O(1) Cu(1) O(1W)	95.50(7)	C(3) C(2) C(1)	119.9(2)
O(1)[3] Cu(1) O(1W)	95.50(7)	C(3) C(2) C(4)	120.8(2)
O(1)[3] Cu(1) O(2)[2]	168.65(7)	N(1) C(5) C(4)	121.47(15)
O(1)[3] Cu(1) O(2)[1]	89.66(9)	N(1) C(5) C(4)[4]	121.47(15)

O(1) Cu(1) O(2)[1]	168.65(7)	C(4) C(5) C(4)[4]	117.0(3)
O(1) Cu(1) O(2)[2]	89.66(9)	C(2) C(4) C(5)	121.3(2)
O(1)[3] Cu(1) O(1)	89.86(13)	C(2)[4] C(3) C(2)	118.9(3)
C(1) O(2) Cu(1)[1]	122.66(15)		

Symmetry transformations used to generate equivalent atoms:

1 1-X,1-Y,1-Z **2** +Y,+X,1-Z **3** 1-Y,1-X,+Z **4** +X,1+X-Y,+Z

Reference

[1] D. Lagnoux, E. Delort, C Douat-Casassus, A. Esposito and J-L. Reymond, *Chem. Eur. J.*, 2004, **10**, 1215-1226.