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Design of 1D and 2D molecule-based magnets with the ligand 4,5-dimethyl-1,2-phenylenebis(oxamato)

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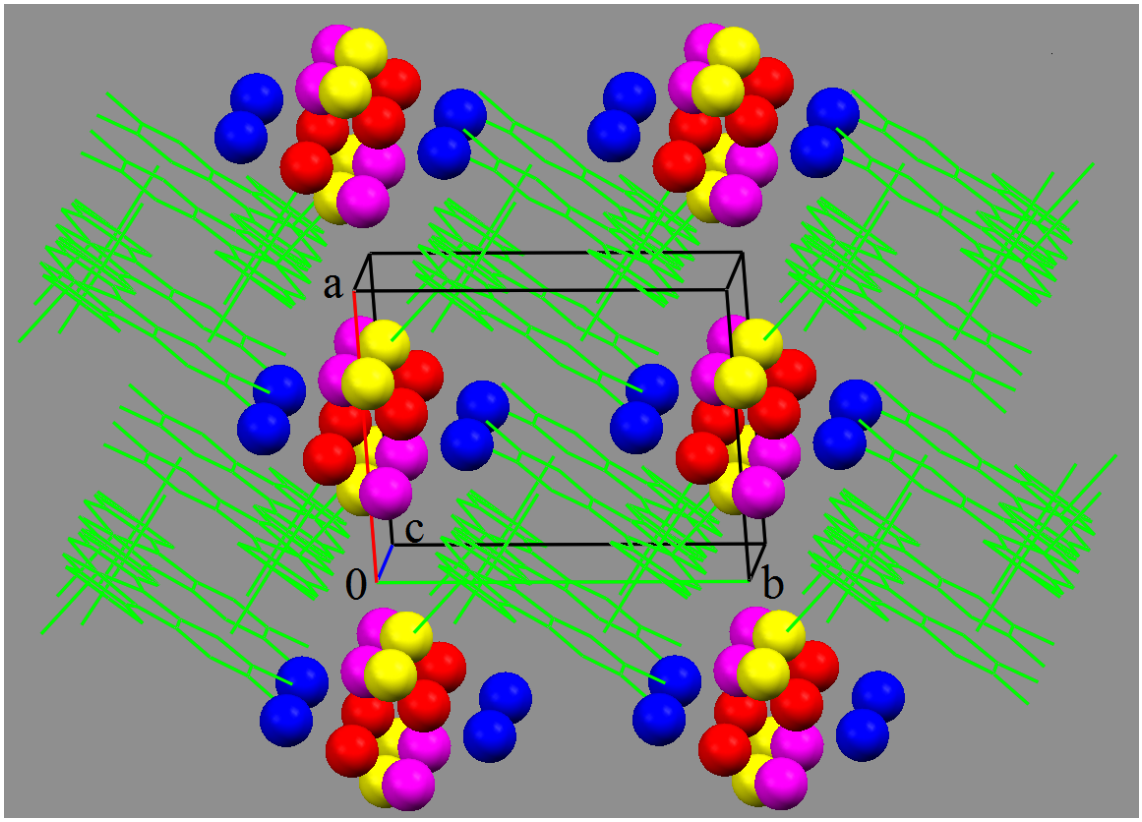
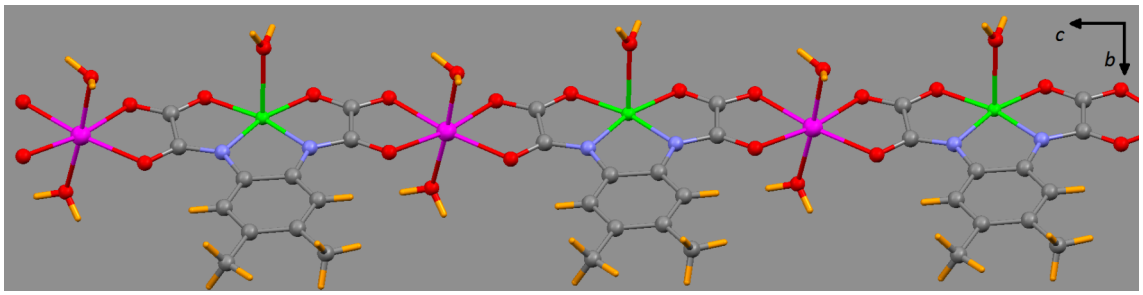
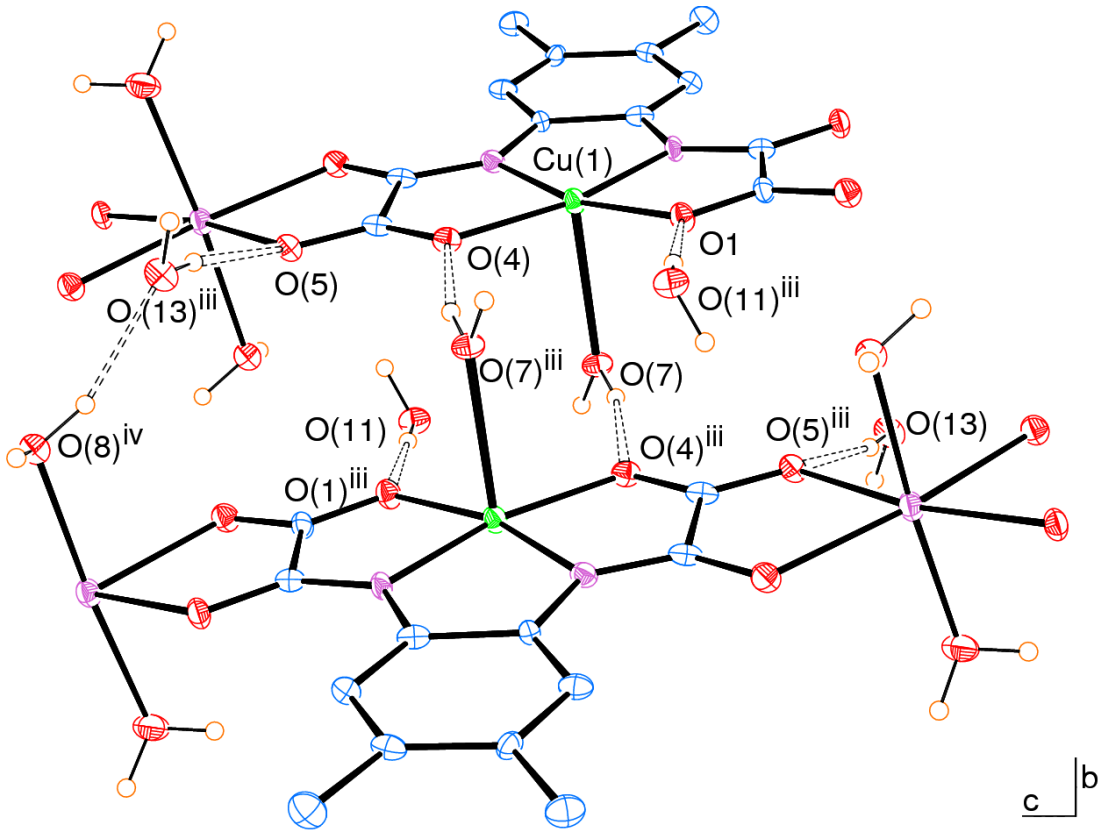
Crystallographic Supplementary Material for $[MnCu(dmopba)(H_2O)_3]_n \cdot 4nH_2O$ (**1**)



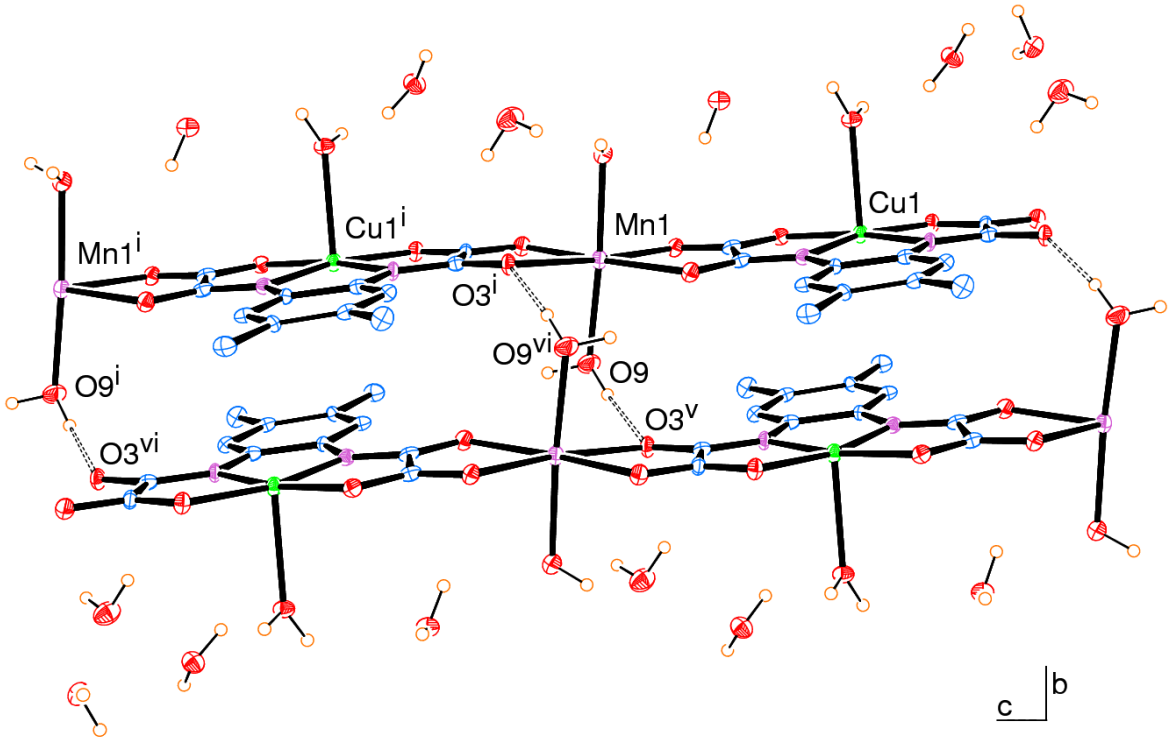
SM1. Mercury© view of compound **1** showing the crystal packing. It is possible to see the double chain (in green) formed along [001] direction and the channel filled by water molecules. Coloured balls represent the water molecules. Colour identification: O10 in blue, O11 in yellow, O12 in red, O13 in pink.



SM2. Mercury[*] view of compound **1** showing an individual chain along [001] direction. The aromatic rings lying in a same side of the chain. Non-coordinated water molecules were omitted for clarity.



SM3. Ortep-3[*] view of **1** showing the classical intermolecular hydrogen bonds stabilize the packing. Methyl and aromatic hydrogen were omitted for clarity. Symmetry codes: [iii] –x+2, –y, –z+1; [iv] –x+2, –y, –z+2.



SM4. Ortep-3* view of **1** showing the classical intermolecular hydrogen bonds that stabilize the double chain formed along [001]. Methyl and aromatic hydrogen were omitted for clarity. Symmetry codes: [i] x, y, z+1; [v] –x+2, –y+1, –z+1; [vi] –x+2, –y+1, –z+2.

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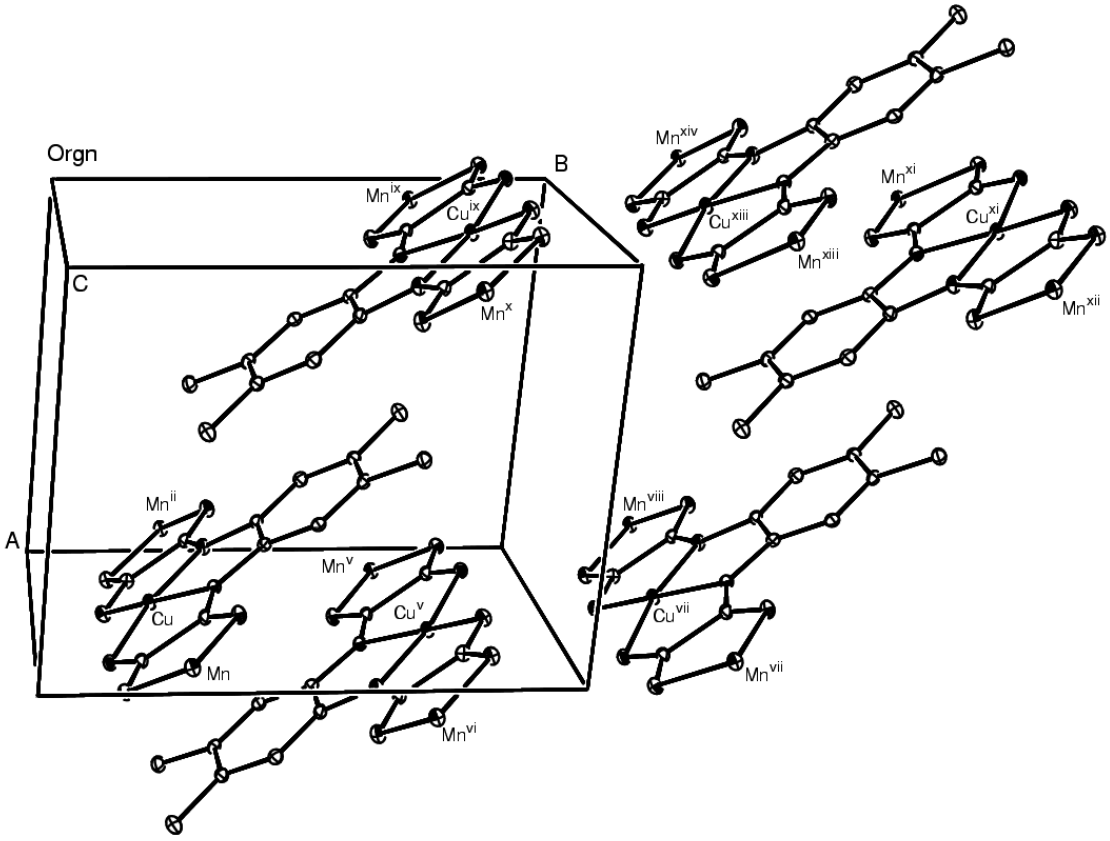

SM5. Ortep-3 view of **1** highlighting the closest metal–metal separations: Mn–Cu = 5.430 Å, Cu–Mn^{ii} = 5.427 Å , Cu–Cu^{v} = 5.788 Å , Mn–Mn^{vi} = 4.788 Å, Cu^{v}–Cu^{vii} = 5.023 Å, Mn^{vi}–Mn^{vii} = 6.102 Å. All wáter molecules and hydrogen atoms were omitted for clarity. Symmetry codes: ^{ii} x, y, z–1; ^{v} –x+2, –y+1, –z+1; ^{vi} –x+2, –y+1, –z+2; ^{vii} x, y+1, z; ^{viii} x, y+1, z–1; ^{ix} –x+1, –y+1, –z+1; ^{x} –x+1, –y+1, –z+2; ^{xi} –x+1, –y+2, –z+1; ^{xii} –x+1, –y+2, –z+2; ^{xiii} x–1, y+1, z; ^{xiv} x–1, y+1, z–1

SM6. Crystal data and structure refinement for **1**.

Empirical formula	$C_{12}\ H_{22}\ Cu_1\ Mn_1\ N_2\ O_{13}$
Formula weight	520.80
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 8.4666(3) Å α = 89.873(4)°
	b = 10.5796(5) Å β = 95.912(4)°
	c = 10.7969(4) Å γ = 93.725(2)°
Volume	959.93(7) $Å^3$
Z	2
Density (calculated)	1.802 Mg/m^3
Absorption coefficient	1.836 mm^{-1}
F(000)	532
Crystal size	0.13 x 0.07 x 0.03 mm^3
Theta range for data collection	3.42 to 25.00°.
Index ranges	–10<=h<=9, –12<=k<=12, 0<=l<=12
Reflections collected	3242
Independent reflections	3242 [R(int) = 0.0000]
Completeness to theta = 25.00°	96.0 %
Max. and min. transmission	0.9470 and 0.7963
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3242 / 0 / 263
Goodness-of-fit on F^2	1.140
Final R indices [I>2sigma(I)]	R1 = 0.0617, wR2 = 0.1943
R indices (all data)	R1 = 0.0703, wR2 = 0.2062
Extinction coefficient	0.012(5)
Largest diff. peak and hole	0.894 and –0.951 $e.Å^{-3}$

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SM7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	10113(7)	1987(6)	2057(6)	20(1)
C(2)	9009(7)	3102(5)	2090(6)	20(1)
C(3)	7969(7)	4351(5)	3725(6)	21(1)
C(4)	7073(7)	5219(6)	3066(6)	21(1)
C(5)	6347(7)	6166(6)	3653(6)	22(1)
C(6)	6536(7)	6228(5)	4967(6)	19(1)
C(7)	7410(7)	5341(6)	5635(6)	22(1)
C(8)	8111(7)	4396(5)	5057(5)	17(1)
C(9)	9328(7)	3200(5)	6817(6)	21(1)
C(10)	10369(7)	2044(5)	6991(6)	22(1)
C(11)	5384(8)	7084(6)	2901(7)	29(2)
C(12)	5794(8)	7250(6)	5623(7)	27(1)
Cu(1)	9789(1)	2305(1)	4496(1)	20(1)
Mn(1)	9563(1)	2798(1)	9478(1)	22(1)
N(1)	8789(6)	3379(5)	3235(5)	19(1)
N(2)	8999(6)	3438(5)	5629(5)	20(1)
O(1)	10623(5)	1497(4)	3075(4)	23(1)
O(2)	10445(5)	1645(4)	1017(4)	24(1)
O(3)	8492(5)	3590(4)	1069(4)	23(1)
O(4)	10777(5)	1516(4)	6045(4)	21(1)
O(5)	10715(5)	1713(4)	8097(4)	22(1)
O(6)	8926(5)	3739(4)	7755(4)	24(1)
O(7)	7712(5)	679(4)	4386(4)	23(1)
O(8)	7404(5)	1540(4)	9133(4)	25(1)
O(9)	11741(6)	4011(4)	9952(5)	34(1)
O(10)	4649(6)	2682(5)	552(5)	41(1)
O(12)	5463(5)	892(4)	2380(4)	30(1)
O(11)	7222(5)	337(4)	6862(4)	26(1)
O(13)	6850(5)	–468(4)	700(4)	28(1)

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SM8. Bond lengths [Å] for **1**.

C(1)–O(2)	1.246(8)	C(9)–C(10)	1.553(9)
C(1)–O(1)	1.261(8)	C(10)–O(5)	1.255(8)
C(1)–C(2)	1.555(9)	C(10)–O(4)	1.255(8)
C(2)–O(3)	1.265(8)	Cu(1)–N(2)	1.913(5)
C(2)–N(1)	1.305(8)	Cu(1)–N(1)	1.934(5)
C(3)–C(4)	1.378(9)	Cu(1)–O(1)	1.973(4)
C(3)–N(1)	1.411(8)	Cu(1)–O(4)	1.998(4)
C(3)–C(8)	1.431(9)	Cu(1)–O(7)	2.372(4)
C(4)–C(5)	1.395(9)	Mn(1)–O(6)	2.144(5)
C(5)–C(6)	1.412(9)	Mn(1)–O(2) [i]	2.159(4)
C(5)–C(11)	1.494(9)	Mn(1)–O(8)	2.191(5)
C(6)–C(7)	1.388(9)	Mn(1)–O(9)	2.193(5)
C(6)–C(12)	1.500(8)	Mn(1)–O(3) [i]	2.215(4)
C(7)–C(8)	1.378(9)	Mn(1)–O(5)	2.223(4)
C(8)–N(2)	1.405(8)	O(2)–Mn(1) [ii]	2.159(4)
C(9)–O(6)	1.251(8)	O(3)–Mn(1) [ii]	2.215(4)
C(9)–N(2)	1.311(8)		

Symmetry transformations used to generate equivalent atoms:

[i] x,y,z+1 [ii] x,y,z–1

SM9. Bond angles [°] for **1**.

O(2)–C(1)–O(1)	124.4(6)	N(2)–Cu(1)–O(7)	99.65(18)
O(2)–C(1)–C(2)	117.2(5)	N(1)–Cu(1)–O(7)	96.56(18)
O(1)–C(1)–C(2)	118.4(5)	O(1)–Cu(1)–O(7)	88.43(17)
O(3)–C(2)–N(1)	130.8(6)	O(4)–Cu(1)–O(7)	89.11(16)
O(3)–C(2)–C(1)	118.4(5)	O(6)–Mn(1)–O(2)^{i}	169.76(17)
N(1)–C(2)–C(1)	110.7(5)	O(6)–Mn(1)–O(8)	89.27(17)
C(4)–C(3)–N(1)	127.2(6)	O(2)^{i}–Mn(1)–O(8)	91.24(17)
C(4)–C(3)–C(8)	118.9(6)	O(6)–Mn(1)–O(9)	94.48(18)
N(1)–C(3)–C(8)	113.9(5)	O(2)^{i}–Mn(1)–O(9)	85.23(18)
C(3)–C(4)–C(5)	122.2(6)	O(8)–Mn(1)–O(9)	176.15(17)
C(4)–C(5)–C(6)	118.5(6)	O(6)–Mn(1)–O(3)^{i}	113.10(16)
C(4)–C(5)–C(11)	120.4(6)	O(2)^{i}–Mn(1)–O(3)^{i}	77.14(16)
C(6)–C(5)–C(11)	121.1(6)	O(8)–Mn(1)–O(3)^{i}	87.56(17)
C(7)–C(6)–C(5)	119.4(6)	O(9)–Mn(1)–O(3)^{i}	90.17(18)
C(7)–C(6)–C(12)	120.8(6)	O(6)–Mn(1)–O(5)	76.56(16)
C(5)–C(6)–C(12)	119.8(6)	O(2)^{i}–Mn(1)–O(5)	93.21(16)
C(8)–C(7)–C(6)	122.1(6)	O(8)–Mn(1)–O(5)	89.87(16)
C(7)–C(8)–N(2)	127.3(6)	O(9)–Mn(1)–O(5)	91.84(18)
C(7)–C(8)–C(3)	118.8(5)	O(3)^{i}–Mn(1)–O(5)	169.94(16)
N(2)–C(8)–C(3)	113.9(5)	C(2)–N(1)–C(3)	131.2(5)
O(6)–C(9)–N(2)	130.3(6)	C(2)–N(1)–Cu(1)	115.3(4)
O(6)–C(9)–C(10)	119.4(6)	C(3)–N(1)–Cu(1)	113.5(4)
N(2)–C(9)–C(10)	110.3(5)	C(9)–N(2)–C(8)	129.3(5)
O(5)–C(10)–O(4)	125.6(6)	C(9)–N(2)–Cu(1)	116.1(4)
O(5)–C(10)–C(9)	115.4(6)	C(8)–N(2)–Cu(1)	114.5(4)
O(4)–C(10)–C(9)	119.0(6)	C(1)–O(1)–Cu(1)	111.2(4)
N(2)–Cu(1)–N(1)	84.0(2)	C(1)–O(2)–Mn(1)^{ii}	115.0(4)
N(2)–Cu(1)–O(1)	166.4(2)	C(2)–O(3)–Mn(1)^{ii}	111.7(4)
N(1)–Cu(1)–O(1)	84.23(19)	C(10)–O(4)–Cu(1)	110.4(4)
N(2)–Cu(1)–O(4)	84.02(19)	C(10)–O(5)–Mn(1)	113.8(4)
N(1)–Cu(1)–O(4)	167.43(19)	C(9)–O(6)–Mn(1)	114.2(4)
O(1)–Cu(1)–O(4)	107.21(17)		

Symmetry transformations used to generate equivalent atoms:

^{i} x,y,z+1 ^{ii} x,y,z–1

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SM10. Hydrogen-Bonding Angles (in °) and Distances (in Å) for **1**. The characters D and A, resp., refer to hydrogen donor and acceptor

D	H	A	D–H	H...A	D...A	D–H...A	Symmetry*
O7	H71	O11	0.8500	2.3600	2.767(6)	110.00	x, y, z
O7	H72	O4	0.8600	1.9500	2.786(6)	167.00	–x+2, –y, –z+1
O8	H81	O10	0.8500	2.5300	3.218(7)	139.00	x, y, z
O8	H82	O13	0.8600	1.9300	2.759(6)	162.00	–x+1, –y, –z+1
O9	H92	O3	0.8500	1.9500	2.776(6)	162.00	–x+2, –y+1, –z
O10	H101	O9	0.8600	2.3800	2.928(7)	123.00	x–1, y, z
O11	H111	O8	0.8600	2.1900	2.751(6)	123.00	x, y, z+1
O11	H112	O1	0.8500	1.8900	2.745(6)	177.00	–x+2, –y, –z+1
O12	H121	O7	0.8600	2.4700	2.752(6)	100.00	x, y, z
O12	H122	O10	0.8500	2.4600	2.798(7)	104.00	x, y, z
O12	H122	O11	0.8500	2.3300	2.743(6)	110.00	–x+1, –y, –z+1
O13	H131	O10	0.8600	2.5300	2.863(7)	104.00	x, y, z+1
O13	H132	O5	0.8500	1.9000	2.733(6)	166.00	x–1, y, z
C4	H4	O3	0.9500	2.5600	3.143(8)	120.00	x, y, z
C7	H7	O6	0.9500	2.4800	3.069(7)	120.00	x, y, z

* Symmetry transformations used to generate equivalent A atoms (hydrogen acceptor).

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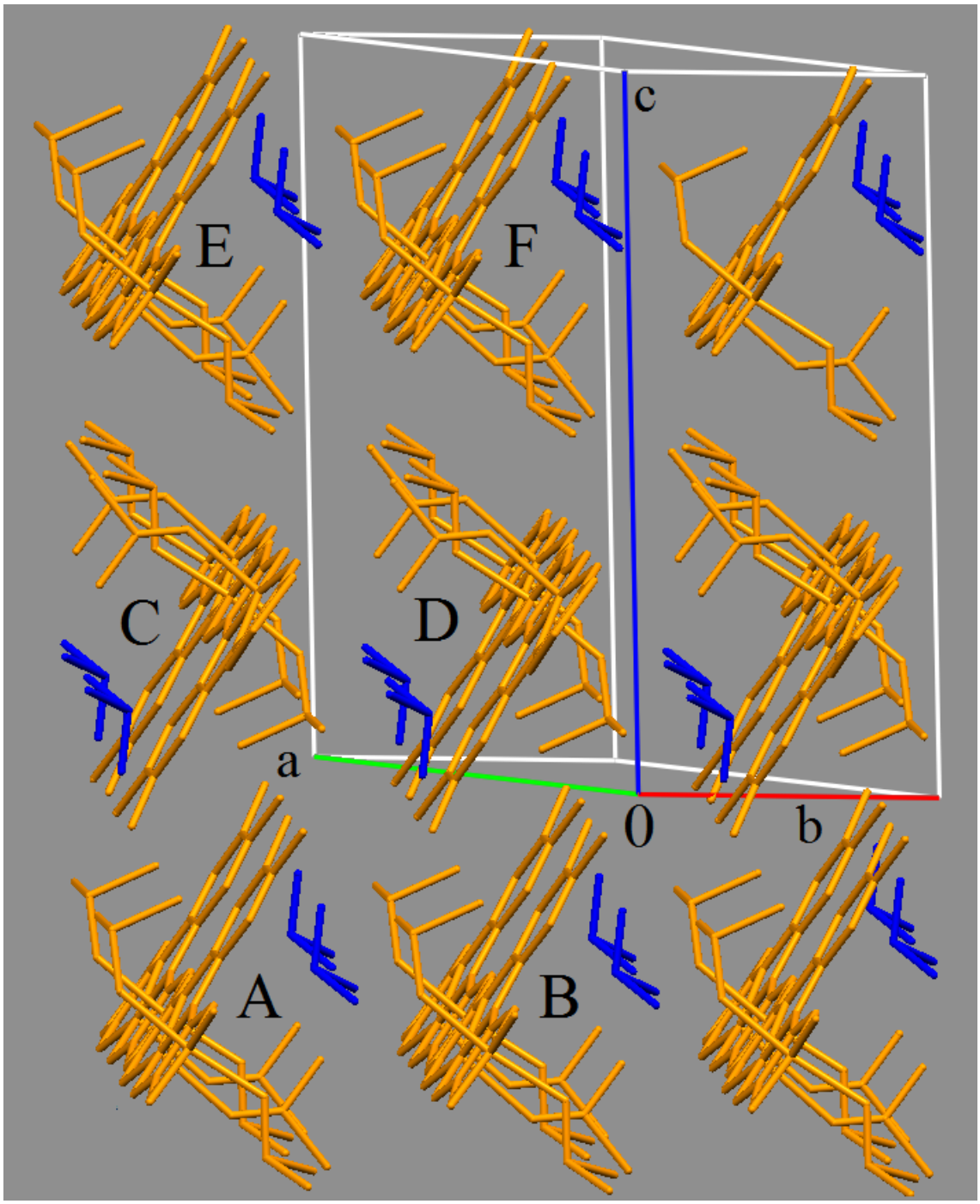
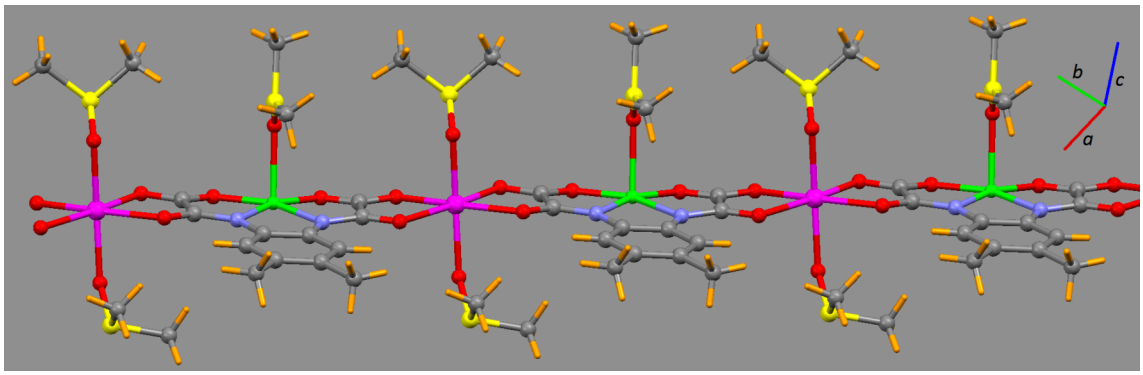
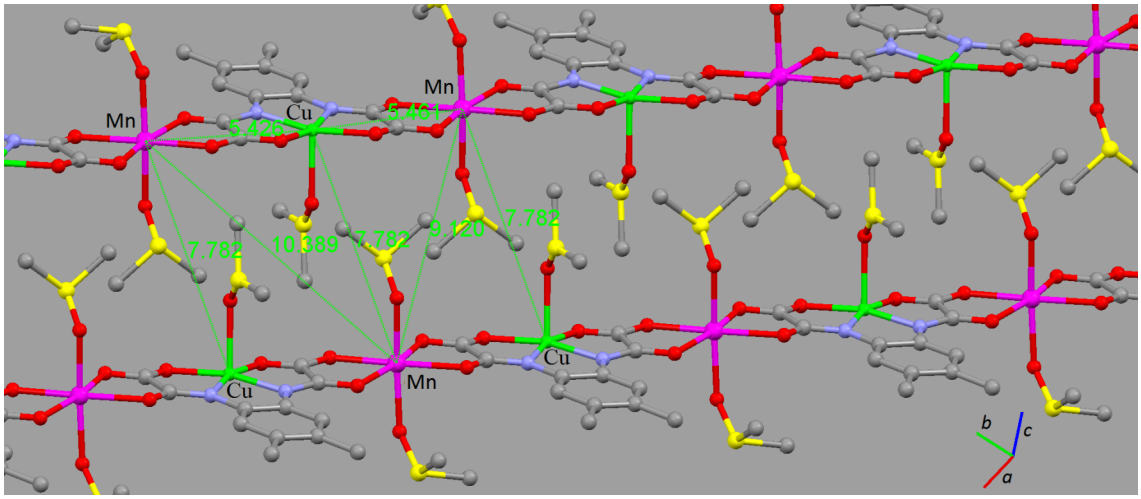
Crystallographic Supplementary Material for $[MnCu(dmopba)(DMSO)_3]_n \cdot nDMSO$ (**2**)



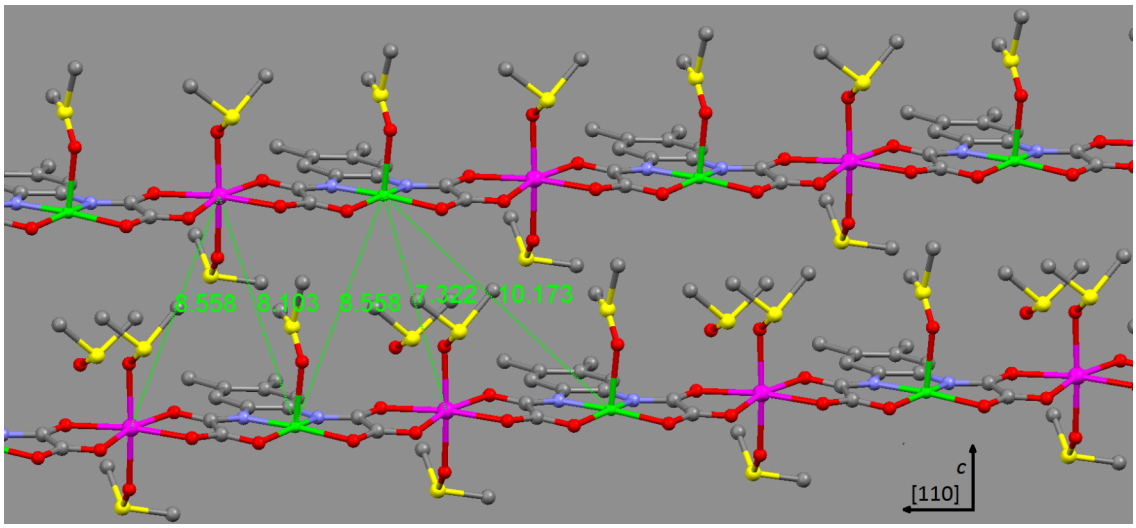
SM11. Mercury© view of **2** displaying the crystal packing onto plane (110). It is possible to see the double chain (in orange) formed along [110] and the channel filled by non-coordinated DMSO molecules (in blue). Capital letter identify parallel chains along [110].



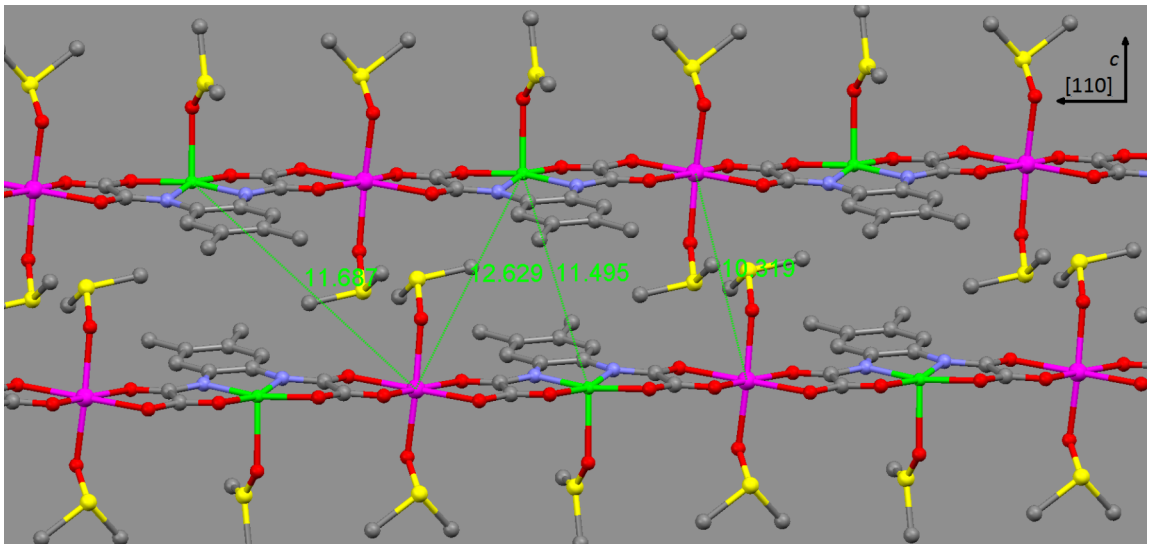
SM12. Mercury® view of **2** displaying an individual chain along [110] direction. The aromatic rings lying in a same side of the chain. Non-coordinated DMSO molecules were omitted for clarity.



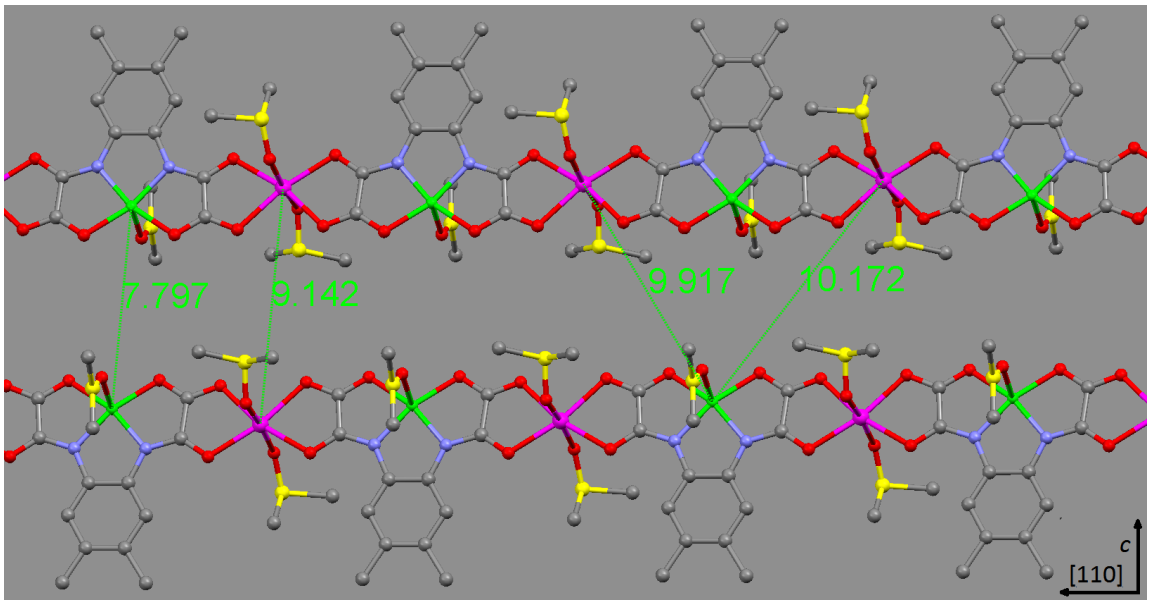
SM13. Mercury® view of **2** highlighting the closest metal–metal separations between chains C and E (see SM11). Non-coordinated DMSO and hydrogen atoms were omitted for clarity.



SM14. Mercury® view of **2** highlighting the closest metal–metal separations between chains C and D (see SM11). Hydrogen atoms were omitted for clarity.



SM15. Mercury® view of **2** highlighting the closest metal–metal separations between chains A and C (see SM11). Non-coordinated DMSO and hydrogen atoms were omitted for clarity.



SM16. Mercury® view of **2** highlighting the closest metal–metal separations between chains C and F (see SM11). Non-coordinated DMSO and hydrogen atoms were omitted for clarity.

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SM17. Crystal data and structure refinement for **2**.

Empirical formula	$C_{20}\ H_{32}\ Cu_1\ Mn_1\ N_2\ O_{10}\ S_4$
Formula weight	707.2
Temperature	250(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 8.558(1) Å α = 93.146(17)□
	b = 10.173(2) Å β = 98.93(2)□
	c = 18.201(6) Å γ = 110.158(14)□
Volume	1459.4(6) $Å^3$
Z	2
Density (calculated)	1.609 Mg/m^3
Absorption coefficient	1.499 mm^{-1}
F(000)	728
Crystal size	0.21 x 0.18 x 0.03 mm^3
Theta range for data collection	3.03 to 30°.
Index ranges	–12<=h<=10, –14<=k<=14, –24<=l<=25
Reflections collected	23081
Independent reflections	8152 [R(int) = 0.0581]
Completeness to theta = 30°	98.9 %
Absorption correction	multi–scan
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8152 / 0 / 373
Goodness-of-fit on F^2	1.056
Final R indices [I>2sigma(I)]	R1 = 0.053, wR2 = 0.1281
R indices (all data)	R1 = 0.1013, wR2 = 0.1543
Largest diff. peak and hole	2.017 and –2.176 $e.Å^{-3}$

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SM18. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	7577(1)	728(1)	3164(1)	31(1)
Mn(1)	12136(2)	5871(1)	2859(1)	32(1)
S(1)	11149(5)	7266(4)	4294(2)	61(1)
S(2)	12870(3)	4247(3)	1302(1)	42(1)
S(3)	5428(16)	2482(15)	3863(4)	224(6)
O(1)	6939(8)	–1029(6)	3659(3)	37(1)
O(2)	4679(8)	–3012(6)	3551(3)	38(1)
O(3)	3229(7)	–2338(6)	2262(3)	37(1)
O(4)	9872(7)	2023(6)	3679(3)	39(1)
O(5)	11639(8)	4206(7)	3619(3)	38(1)
O(6)	9652(7)	4342(6)	2331(3)	35(1)
O(7)	6373(15)	1787(13)	3966(5)	88(4)
O(8)	10949(10)	7064(8)	3456(4)	51(2)
O(9)	13180(9)	4730(8)	2128(4)	50(2)
N(1)	5619(8)	–322(7)	2412(4)	30(1)
N(2)	7912(8)	2104(7)	2447(4)	30(1)
C(1)	5483(11)	–1866(8)	3330(5)	33(2)
C(2)	4647(9)	–1520(8)	2595(5)	29(2)
C(3)	5356(9)	379(8)	1793(4)	27(2)
C(4)	4002(10)	–125(8)	1182(4)	30(2)
C(5)	3904(10)	684(8)	592(4)	29(2)
C(6)	5131(11)	2016(9)	610(4)	32(2)
C(7)	6459(10)	2522(9)	1224(4)	30(2)
C(8)	6602(10)	1717(8)	1805(4)	28(2)
C(9)	9248(10)	3252(8)	2658(4)	27(2)
C(10)	10312(9)	3157(8)	3374(4)	26(2)
C(11)	2453(12)	45(11)	–67(5)	40(2)
C(12)	5036(13)	2907(11)	–17(5)	42(2)
C(13A)	11810(170)	9170(50)	4600(50)	270(70)
C(14A)	9080(80)	6790(100)	4490(20)	140(30)
C(13B)	11330(90)	8950(50)	4525(16)	120(20)
C(14B)	9090(70)	6240(90)	4430(30)	150(40)
C(15)	11422(15)	4967(14)	841(6)	57(3)
C(16)	11442(17)	2473(12)	1197(8)	63(3)
C(17)	4680(30)	3120(30)	4596(8)	122(9)
C(18)	4320(60)	2640(60)	3145(11)	300(30)
S(4)	–681(3)	–2834(3)	1673(1)	44(1)
O(10)	–1025(13)	–2908(12)	827(4)	75(3)
C(19)	–75(18)	–1032(13)	2033(8)	68(3)
C(20)	–2662(16)	–3453(15)	1965(8)	67(3)

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SM19. Bond lengths [Å] for **2**.

Cu(1)–N(1)	1.927(6)	O(3)–C(2)#1	1.246(9)
Cu(1)–N(2)	1.945(6)	O(4)–C(10)	1.271(9)
Cu(1)–O(1)	1.991(6)	O(5)–C(10)	1.258(9)
Cu(1)–O(4)	1.995(6)	O(6)–C(9)	1.255(9)
Cu(1)–O(7)	2.327(9)	N(1)–C(2)	1.311(10)
Mn(1)–O(3)	2.175(6)	N(1)–C(3)	1.397(10)
Mn(1)–O(8)	2.176(8)	N(2)–C(9)	1.309(10)
Mn(1)–O(6)	2.188(6)	N(2)–C(8)	1.420(9)
Mn(1)–O(9)	2.198(7)	C(1)–O(2)#2	1.256(10)
Mn(1)–O(2)	2.214(6)	C(1)–C(2)	1.534(11)
Mn(1)–O(5)	2.216(6)	C(2)–O(3)#2	1.246(9)
S(1)–O(8)	1.503(7)	C(3)–C(4)	1.403(10)
S(1)–C(13B)	1.69(4)	C(3)–C(8)	1.407(10)
S(1)–C(14B)	1.77(5)	C(4)–C(5)	1.398(11)
S(1)–C(14A)	1.77(6)	C(5)–C(6)	1.394(11)
S(1)–C(13A)	1.84(4)	C(5)–C(11)	1.517(10)
S(2)–O(9)	1.510(7)	C(6)–C(7)	1.395(11)
S(2)–C(15)	1.774(12)	C(6)–C(12)	1.505(11)
S(2)–C(16)	1.777(12)	C(7)–C(8)	1.389(11)
S(3)–O(7)	1.246(10)	C(9)–C(10)	1.497(10)
S(3)–C(18)	1.54(2)	S(4)–O(10)	1.515(8)
S(3)–C(17)	1.749(16)	S(4)–C(20)	1.771(12)
O(1)–C(1)	1.272(10)	S(4)–C(19)	1.780(13)
O(2)–C(1)#1	1.256(10)		

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y+1,z #2 x–1,y–1,z

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SM20. Bond angles [°] for **2**.

N(1)–Cu(1)–N(2)	82.8(3)	C(10)–O(4)–Cu(1)	110.3(5)
N(1)–Cu(1)–O(1)	84.1(2)	C(10)–O(5)–Mn(1)	113.4(5)
N(2)–Cu(1)–O(1)	165.1(3)	C(9)–O(6)–Mn(1)	112.0(5)
N(1)–Cu(1)–O(4)	163.3(3)	S(3)–O(7)–Cu(1)	133.0(7)
N(2)–Cu(1)–O(4)	82.8(3)	S(1)–O(8)–Mn(1)	124.1(4)
O(1)–Cu(1)–O(4)	109.0(2)	S(2)–O(9)–Mn(1)	136.3(4)
N(1)–Cu(1)–O(7)	101.0(4)	C(2)–N(1)–C(3)	129.7(6)
N(2)–Cu(1)–O(7)	97.8(4)	C(2)–N(1)–Cu(1)	115.0(5)
O(1)–Cu(1)–O(7)	91.5(4)	C(3)–N(1)–Cu(1)	114.9(5)
O(4)–Cu(1)–O(7)	89.4(4)	C(9)–N(2)–C(8)	131.3(7)
O(3)–Mn(1)–O(8)	90.5(3)	C(9)–N(2)–Cu(1)	114.7(5)
O(3)–Mn(1)–O(6)	117.0(2)	C(8)–N(2)–Cu(1)	113.9(5)
O(8)–Mn(1)–O(6)	90.8(3)	O(2)#2–C(1)–O(1)	124.3(8)
O(3)–Mn(1)–O(9)	85.4(3)	O(2)#2–C(1)–C(2)	116.2(7)
O(8)–Mn(1)–O(9)	172.9(3)	O(1)–C(1)–C(2)	119.4(7)
O(6)–Mn(1)–O(9)	86.1(3)	O(3)#2–C(2)–N(1)	129.2(7)
O(3)–Mn(1)–O(2)	76.4(2)	O(3)#2–C(2)–C(1)	120.1(7)
O(8)–Mn(1)–O(2)	93.5(3)	N(1)–C(2)–C(1)	110.7(6)
O(6)–Mn(1)–O(2)	165.9(2)	N(1)–C(3)–C(4)	126.4(7)
O(9)–Mn(1)–O(2)	91.1(3)	N(1)–C(3)–C(8)	114.7(6)
O(3)–Mn(1)–O(5)	166.5(2)	C(4)–C(3)–C(8)	118.9(7)
O(8)–Mn(1)–O(5)	92.8(3)	C(5)–C(4)–C(3)	120.5(7)
O(6)–Mn(1)–O(5)	76.1(2)	C(6)–C(5)–C(4)	120.5(7)
O(9)–Mn(1)–O(5)	92.6(3)	C(6)–C(5)–C(11)	121.9(7)
O(2)–Mn(1)–O(5)	90.3(2)	C(4)–C(5)–C(11)	117.7(7)
O(8)–S(1)–C(13B)	106.3(12)	C(7)–C(6)–C(5)	118.8(7)
O(8)–S(1)–C(14B)	102(2)	C(7)–C(6)–C(12)	120.0(8)
C(13B)–S(1)–C(14B)	105(4)	C(5)–C(6)–C(12)	121.2(7)
O(8)–S(1)–C(14A)	106.4(15)	C(8)–C(7)–C(6)	121.5(7)
C(13B)–S(1)–C(14A)	86(4)	C(7)–C(8)–C(3)	119.8(7)
O(8)–S(1)–C(13A)	108(3)	C(7)–C(8)–N(2)	126.6(7)
C(14B)–S(1)–C(13A)	115(5)	C(3)–C(8)–N(2)	113.7(6)
C(14A)–S(1)–C(13A)	96(5)	O(6)–C(9)–N(2)	126.8(7)
O(9)–S(2)–C(15)	107.4(5)	O(6)–C(9)–C(10)	121.2(7)
O(9)–S(2)–C(16)	104.6(6)	N(2)–C(9)–C(10)	112.0(6)
C(15)–S(2)–C(16)	96.9(6)	O(5)–C(10)–O(4)	124.1(7)
O(7)–S(3)–C(18)	131.3(12)	O(5)–C(10)–C(9)	116.8(6)
O(7)–S(3)–C(17)	122.2(9)	O(4)–C(10)–C(9)	119.1(6)
C(18)–S(3)–C(17)	104.7(10)	O(10)–S(4)–C(20)	107.6(6)
C(1)–O(1)–Cu(1)	109.4(5)	O(10)–S(4)–C(19)	107.0(7)
C(1)#1–O(2)–Mn(1)	113.7(5)	C(20)–S(4)–C(19)	97.3(7)
C(2)#1–O(3)–Mn(1)	113.2(5)		

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y+1,z #2 x–1,y–1,z

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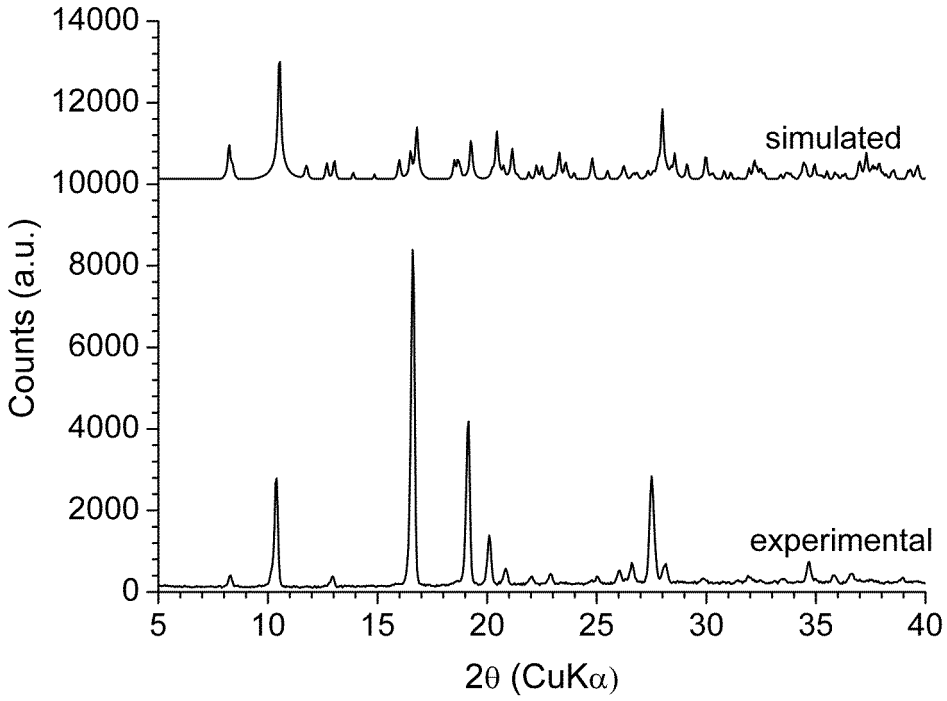

SM21. X-ray powder pattern for the compound **1** with 2 θ in the 5–40 range. Simulated X-ray powder diffraction pattern was calculated using Mercury®.

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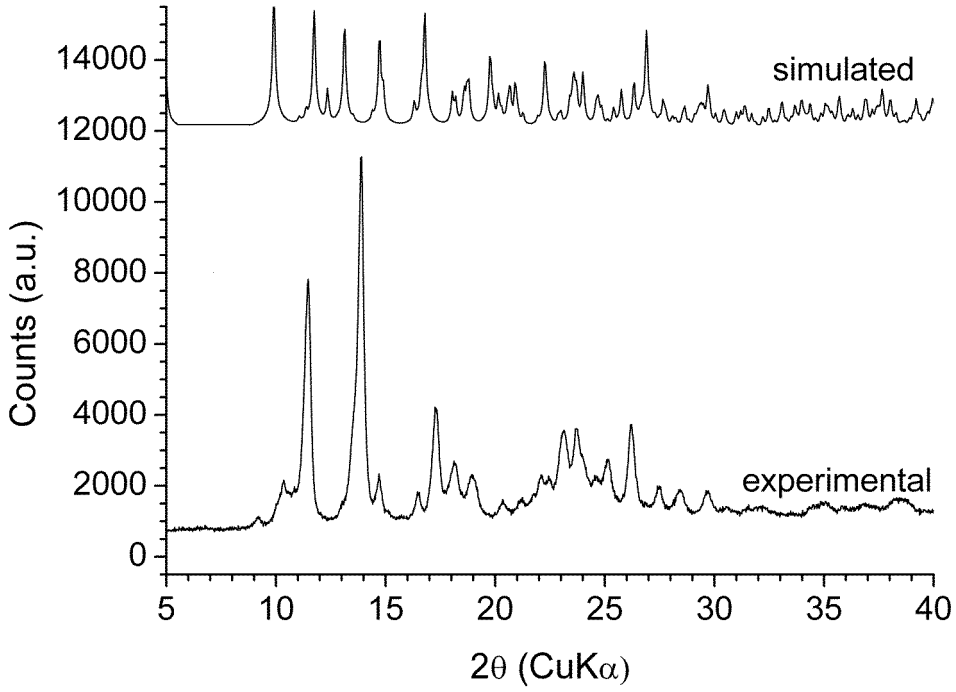

SM22. X-ray powder pattern for the compound **2** with 2 θ in the 5–40 range. Simulated X-ray powder diffraction pattern was calculated using Mercury®.