Electronic Supplementary Material (ESI) for CrystEngComm

Supporting information

Mn^{II}, Cu^{II} and Co^{II} coordination polymers showing antiferromagnetism, coexience of spin frustration and long range magnetic ordering

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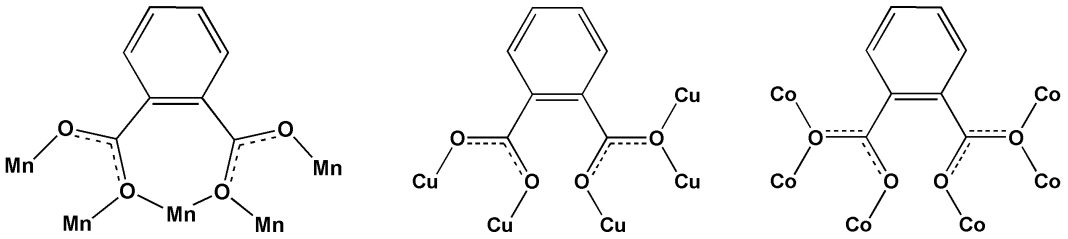


(a) (b) (c)

Scheme S1 Different coordination modes of the ligand 1,2-bdc^{2-} (a) in complex **1**, (b) in complex **2** and (c) in complex **3**.

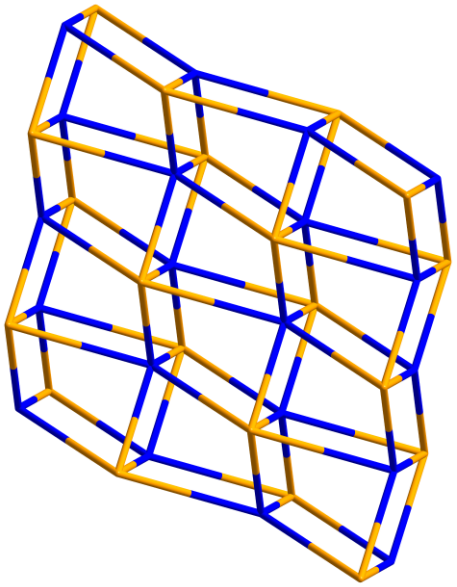


Fig. S1 A five-connected 2D network with point symbol of $\{4^8.6^2\}$ in **1** with Mn^{II} being represented as blue balls and the ligand bdc^{2-} as orange balls..

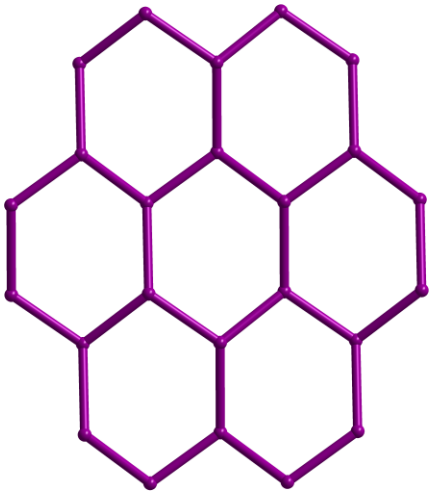
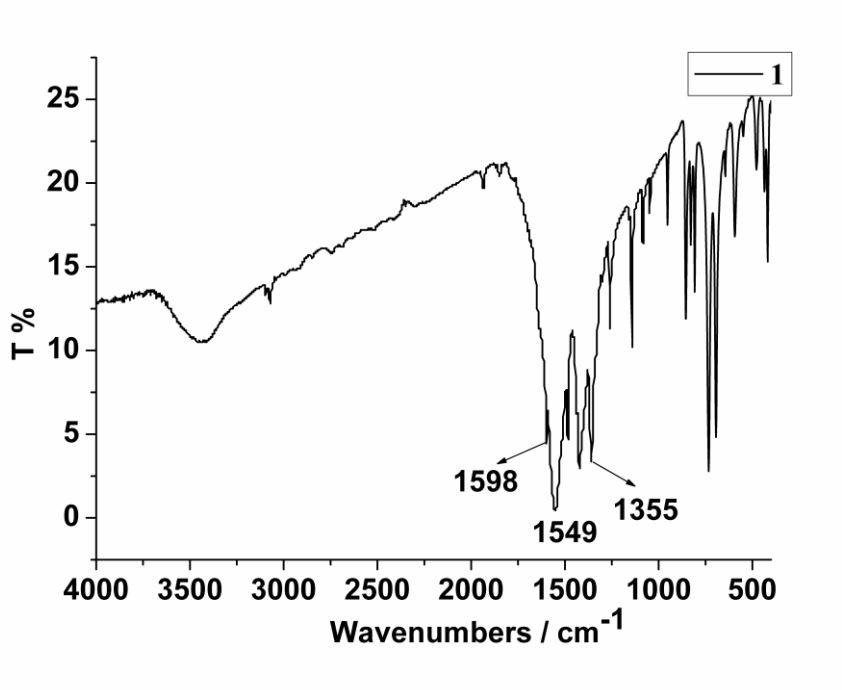
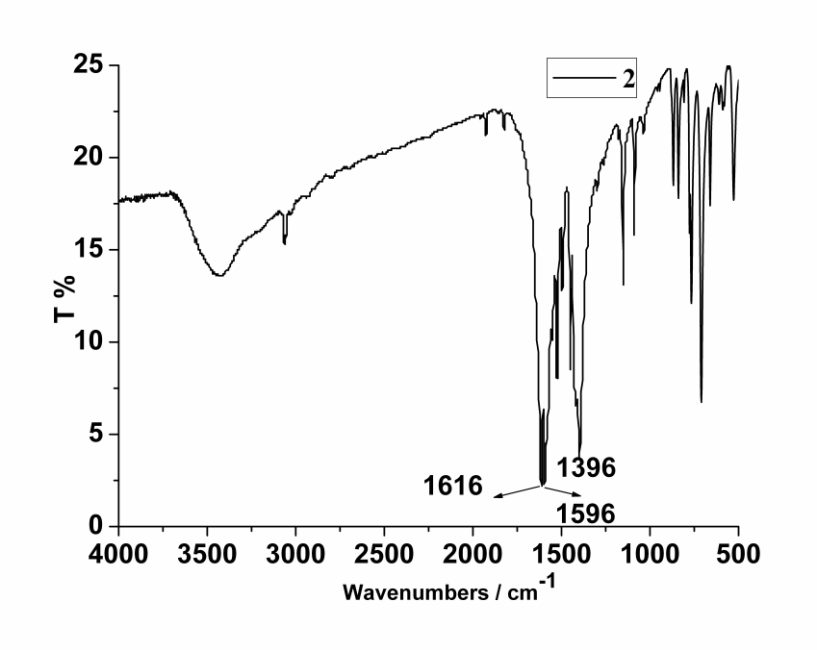


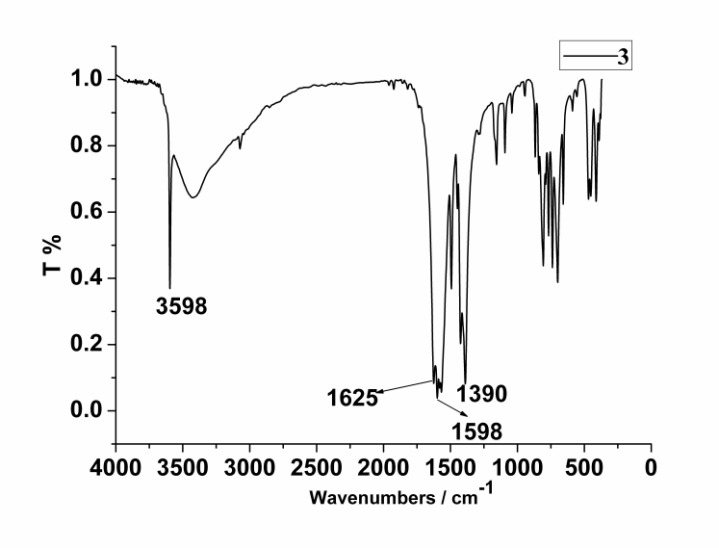
Fig. S2 A 3-connected **hcb** topological net in **3** with $Co_3(OH)$ being represented by purple balls.



(a)

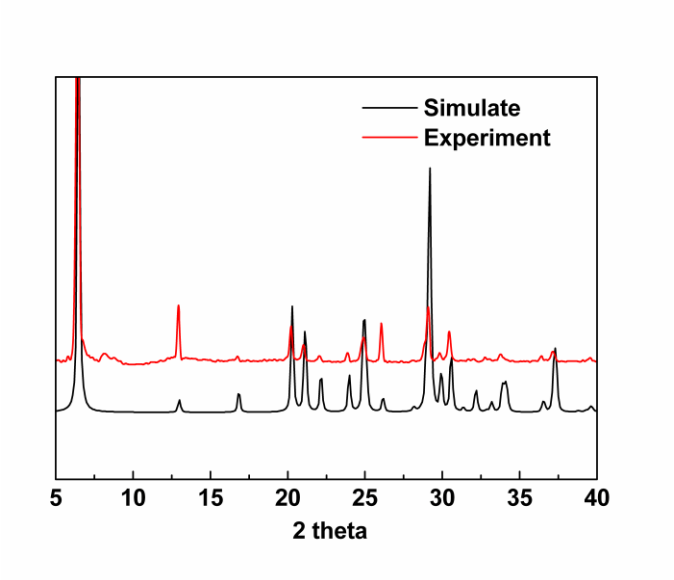


(b)

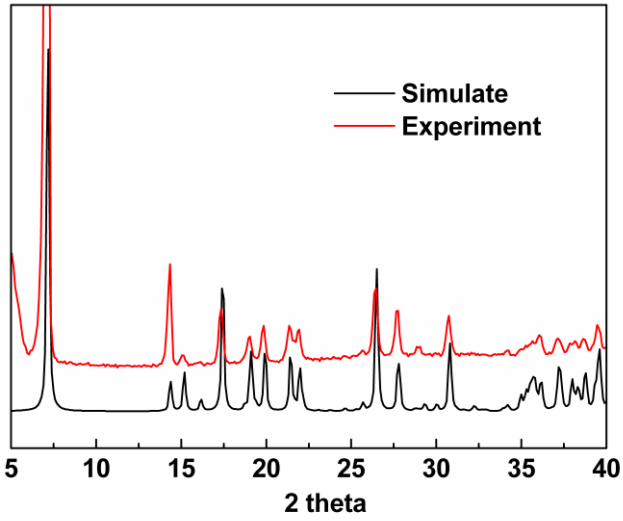


(c)

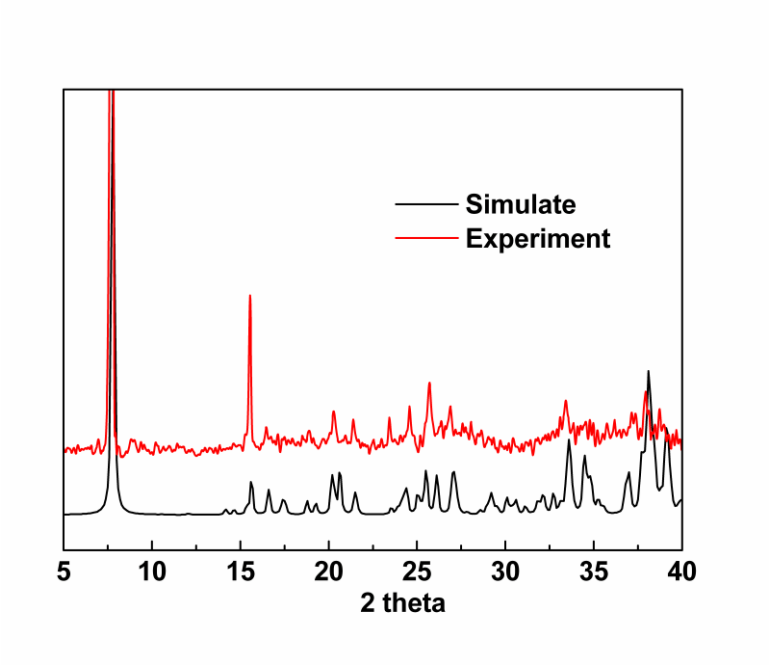
Fig. S3 IR spectra for three compounds.



(a)



(b)



(c)

Fig. S4 PXRD curves for (a) **1**, (b) **2**, (c) **3**.

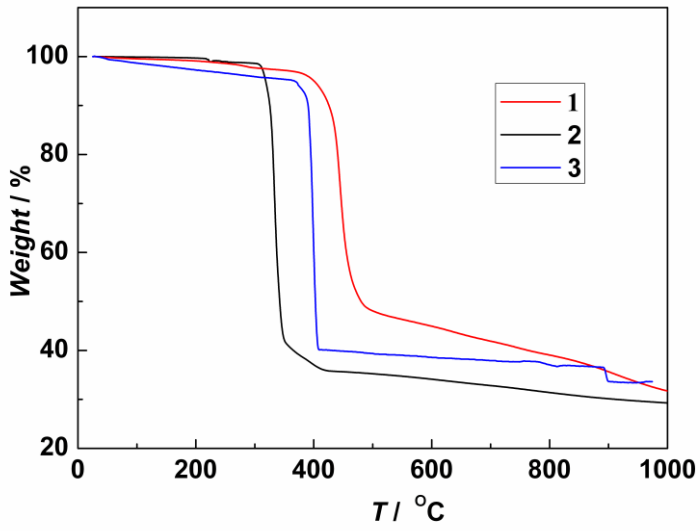


Fig. S5 TGA curves for three compounds.

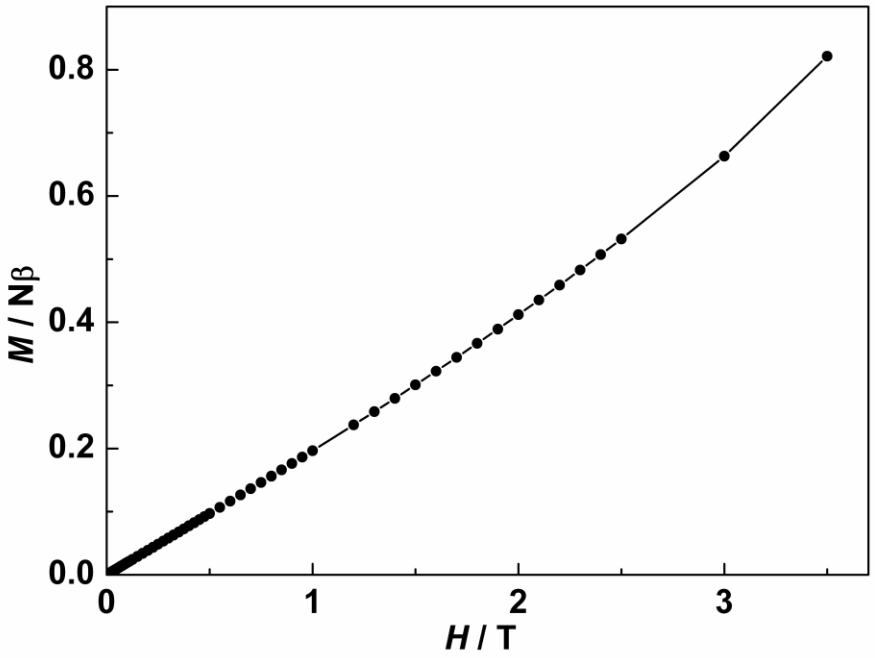


Fig. S6 The curve of magnetization *vs.* applied fields at 2 K in **1**.

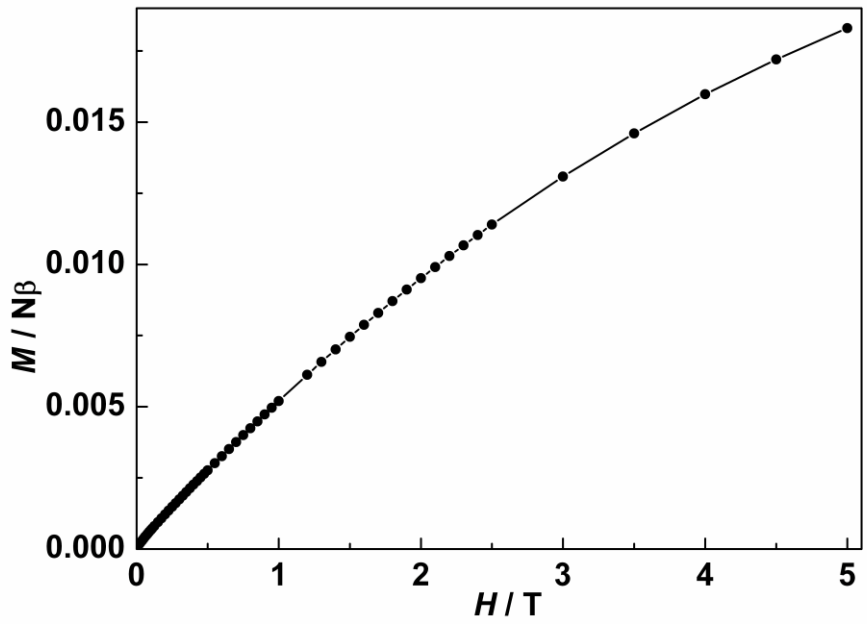


Fig. S7 The curve of magnetization *vs.* applied fields at 2 K in **2**.

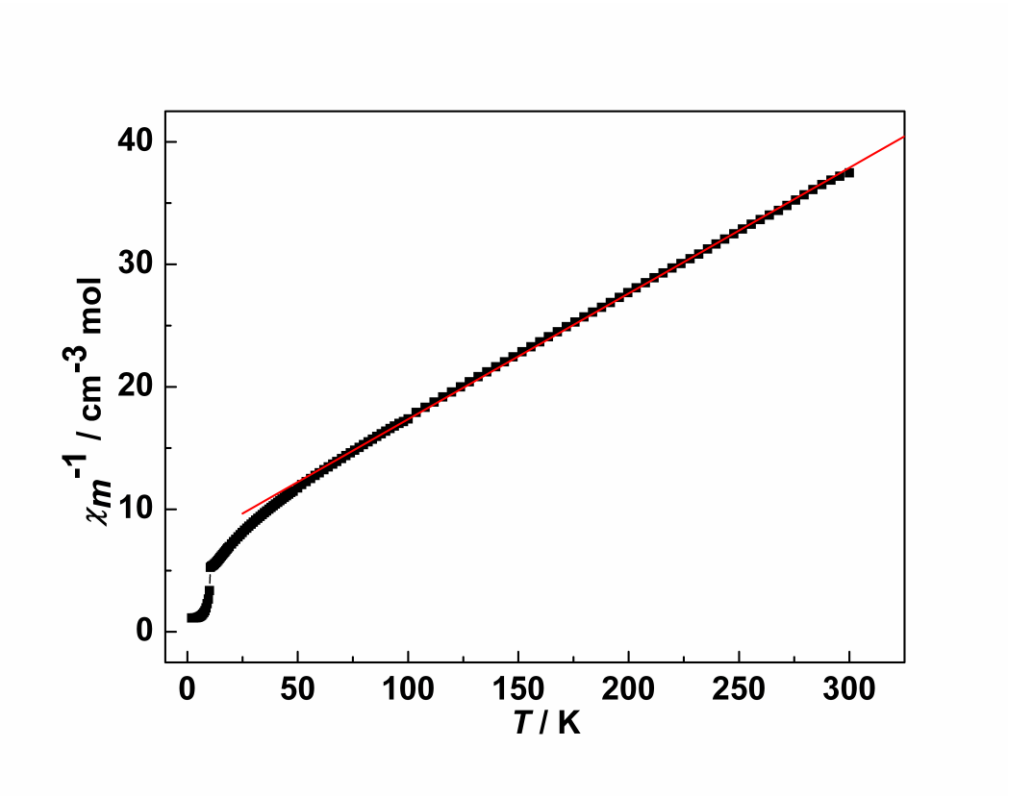


Fig. S8 The χ_m^{-1} *vs.* *T* plot of **3** in the range 2-300 K at 1 kOe. The solid line is the best-fit above 50 K according to the Curie-Weiss law.

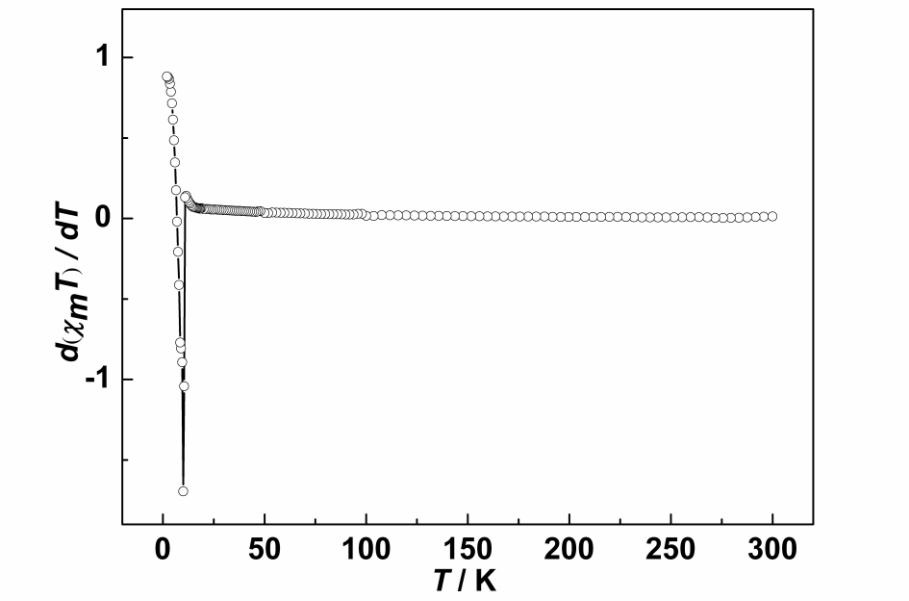


Fig. S9 The d($\chi_m T$)/dT derivative curve of **3**.

Table S1 Crystallographic data for compound **1~3**.

	1	**2**	**3**
Empirical formula	$C_8H_4MnO_4$	$C_8H_4CuO_4$	$C_{16}H_{10}Co_3O_{10}$
Formula weight	219.05	227.65	539.03
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	*P*2/c	$P2_1/c$	$P2_1/c$
Unit cell dimensions			
a (Å)	4.664(2)	13.171(5)	11.648(2)
b (Å)	13.625(6)	5.1292(18)	12.091(3)
c (Å)	6.339(2)	11.719(4)	11.846(3)
B (º)	115.82(3)	110.745(6)	103.245(4)
V (Å^3)	362.6(3)	740.3(5)	1624.0(6)
Z	2	4	4
ρ calcd.(Mg/m^3)	2.006	2.042	2.205
μ (mm^{-1})	1.790	2.920	3.090
F(000)	218	452	1068
θ limits (º)	2.99 to 24.99 deg	1.65 to 25.00	1.80 to 25.00
h, *k*, *l* limits	-5 to 5, -15 to 16, -7 to 7	-13 to 15, -3 to 6, -13 to 13	-13 to 12, -14 to 13, -14 to 13
Reflections collected	2341	3523	7928
GOOF	1.218	1.064	0.966
R index [$I>2\sigma(I)$]	R_1 = 0.0435, wR_2 = 0.1193	R_1 = 0.0444, wR_2 = 0.1070	R_1 = 0.0409, wR_2 = 0.1045
R (all data)	R_1 = 0.0459, wR_2 = 0.1199	R_1 = 0.0535, wR_2 = 0.1106	R_1 = 0.0601, wR_2 = 0.1136
Largest diff. peak and hole (e·Å^{-3})	1.162 and -0.487	1.357 and -0.781	1.394 and -0.757

[a] $R = \Sigma(||F_o|-|F_c||)/\Sigma|F_o|$, [b] $wR = \{\Sigma w[(F_o^2-F_c^2)^2]/\Sigma w[(F_o^2)^2]\}^{1/2}$, $w = 1/[\sigma^2(F_o^2)+(aP)^2+bP]$, P = $(F_o^2+2F_c^2)/3$]. **1**, a = 0.0694, b = 0.5648; **2**, a = 0.0653, b = 0.5533; **3**, a = 0.0722, b = 0.0000.

Table S2 Selected bond lengths and bond angles for compound **1~3**.

		1	
Mn(1)-O(2)#1	2.114(3)	Mn(1)-O(1)#3	2.170(3)
Mn(1)-O(1)	2.243(3)	Mn(1)-Mn(1)#4	3.4812(11)
O(2)#1-Mn(1)-O(2)#2	101.03(15)	O(2)#1-Mn(1)-O(1)#3	154.82(10)
O(2)#2-Mn(1)-O(1)#3	94.47(10)	O(1)#3-Mn(1)-O(1)#4	78.78(13)
O(2)#1-Mn(1)-O(1)	87.13(10)	O(2)#2-Mn(1)-O(1)	85.16(10)
O(1)#3-Mn(1)-O(1)	114.08(10)	O(1)#4-Mn(1)-O(1)	75.85(10)
O(1)-Mn(1)-O(1)#5	167.86(13)		
		2	
Cu(1)-O(2)	1.935(3)	Cu(1)-O(1)	1.953(3)
Cu(1)-O(3)	1.957(3)	Cu(1)-O(4)	2.033(3)
Cu(1)-O(4)#1	2.204(3)	Cu(1)-Cu(1)#2	2.6229(12)
O(2)-Cu(1)-O(1)	168.68(14)	O(2)-Cu(1)-O(3)	86.24(14)
O(1)-Cu(1)-O(3)	91.67(14)	O(2)-Cu(1)-O(4)	88.61(14)
O(1)-Cu(1)-O(4)	91.25(13)	O(3)-Cu(1)-O(4)	167.96(13)
O(2)-Cu(1)-O(4)#1	90.46(13)	O(1)-Cu(1)-O(4)#1	100.65(13)
O(3)-Cu(1)-O(4)#1	111.33(12)		
		3	
Co(1)-O(10)	2.005(3)	Co(2)-O(9)#4	2.082(3)
Co(1)-O(9)	2.007(3)	Co(2)-O(10)	2.088(3)
Co(1)-O(6)	2.060(3)	Co(2)-O(4)#1	2.104(3)
Co(1)-O(1)#1	2.064(3)	Co(2)-O(5)	2.106(3)
Co(1)-O(3)#2	2.345(3)	Co(2)-O(7)#4	2.109(3)
Co(1)-O(8)#3	2.367(3)	Co(2)-O(2)	2.109(3)
Co(3)-O(9)	2.088(3)	Co(4)-O(10)	2.082(3)
Co(3)-O(5)#1	2.098(3)	Co(4)-O(2)	2.091(3)
Co(3)-O(3)#2	2.099(3)	Co(4)-O(8)#3	2.118(3)
O(10)-Co(1)-O(9)	173.73(12)	O(9)#4-Co(2)-O(10)	179.07(12)
O(10)-Co(1)-O(6)	95.72(12)	O(9)#4-Co(2)-O(4)#1	86.27(12)
O(9)-Co(1)-O(6)	88.19(12)	O(10)-Co(2)-O(4)#1	92.91(12)
O(10)-Co(1)-O(1)#1	88.58(13)	O(9)#4-Co(2)-O(5)	78.87(11)
O(9)-Co(1)-O(1)#1	95.66(13)	O(10)-Co(2)-O(5)	101.61(11)
O(6)-Co(1)-O(1)#1	99.01(14)	O(4)#1-Co(2)-O(5)	93.22(12)
O(10)-Co(1)-O(3)#2	101.28(11)	O(9)#4-Co(2)-O(7)#4	92.99(12)
O(9)-Co(1)-O(3)#2	74.79(11)	O(10)-Co(2)-O(7)#4	86.66(12)
O(6)-Co(1)-O(3)#2	162.97(12)	O(4)#1-Co(2)-O(7)#4	95.13(12)
O(1)#1-Co(1)-O(3)#2	82.59(13)	O(5)-Co(2)-O(7)#4	167.93(12)
O(10)-Co(1)-O(8)#3	74.81(12)	O(9)#4-Co(2)-O(2)	102.09(12)
O(9)-Co(1)-O(8)#3	100.88(12)	O(10)-Co(2)-O(2)	78.79(12)
O(6)-Co(1)-O(8)#3	83.18(13)	O(4)#1-Co(2)-O(2)	167.42(12)

O(1)#1-Co(1)-O(8)#3	163.38(12)	O(5)-Co(2)-O(2)	79.39(12)
O(3)#2-Co(1)-O(8)#3	100.17(11)	O(7)#4-Co(2)-O(2)	93.81(12)
O(9)#5-Co(3)-O(9)	180.00(12)	O(10)-Co(4)-O(10)#2	180.00(13)
O(9)-Co(3)-O(5)#1	78.92(11)	O(10)-Co(4)-O(2)#2	100.67(11)
O(9)-Co(3)-O(5)#3	101.08(11)	O(10)-Co(4)-O(2)	79.33(11)
O(5)#1-Co(3)-O(5)#3	180.0	O(10)#2-Co(4)-O(2)	100.67(11)
O(9)-Co(3)-O(3)#6	101.24(12)	O(2)#2-Co(4)-O(2)	180.00(8)
O(5)#1-Co(3)-O(3)#6	81.72(12)	O(10)-Co(4)-O(8)#3	78.96(12)
O(9)-Co(3)-O(3)#2	78.76(12)	O(2)-Co(4)-O(8)#3	98.27(12)
O(5)#1-Co(3)-O(3)#2	98.28(12)	O(10)-Co(4)-O(8)#4	101.04(12)
O(5)#3-Co(3)-O(3)#2	81.72(12)	O(2)-Co(4)-O(8)#4	81.73(12)
O(3)#6-Co(3)-O(3)#2	180.0	O(8)#3-Co(4)-O(8)#4	180.00(9)

Symmetry transformations used to generate equivalent atoms: 1: #1 *x*-1, *y*, *z*; #2 -*x*+1, *y*, -*z*+3/2; #3 *x*, -*y*+1, *z*+1/2; #4 -*x*, -*y*+1, -*z*+1; #5 -*x*, *y*, -*z*+3/2; 2, #1 -*x*+1, -*y*+3, -*z*+1; #2 -*x*+1, -*y*+2, -*z*+1; 3, #1 -*x*, *y*+1/2, -*z*+1/2; #2 -*x*, -*y*, -*z*+1; #3 *x*, -*y*+1/2, *z*+1/2; #4 -*x*, *y*-1/2, -*z*+1/2; #5 -*x*, -*y*+1, -*z*+1; #6 *x*, *y*+1, *z*.