Electronic Supplementary Material (ESI) for Dalton Transactions
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Electronic Supplementary Information

Structures and magnetic properties of copper(II) and manganese(II) polymers derived from pseudohalides and a flexible zwitterionic dicarboxylate ligand

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Table S1. Hydrogen bond lengths [Å] and angles [°] for compound **3.**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O3-H3C...O2#1	0.85(2)	2.21(6)	2.94(2)	143(8)
O4-H4C...O2#1	0.85(2)	1.95(3)	2.754(16)	158(7)
O4-H4B...N12#2	0.85(2)	2.07(4)	2.90(2)	165(9)
O3-H3D...N9#3	0.85(2)	2.08(6)	2.89(2)	157(15)
Symmetric code: #1 -x+2, -y, -z+1; #2 x, y, z-1; #3 x, y, z+1				

TOPOS outputs

Compound 2

V = $Mn_4(\mu_4\text{-}N_3)(\mu\text{-}OCO)_6$ cluster and Sc = C atoms of the carboxylate bridges between the clusters;

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Topology for Sc1
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Atom Sc1 links by bridge ligands and has
Common vertex with                                  R(A-A)
V 1      0.2513     -0.1095      0.7064     ( 0-1 0)      8.129A          1
V 1      0.2487      0.3905      0.2064     ( 0 0 0)     11.216A          1
V 1     -0.2487     -0.3905      0.7064     ( 0 0 0)     12.364A          1
Topology for Sc2
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Atom Sc2 links by bridge ligands and has

Common vertex with					R(A-A)	
V 1	0.2513	-0.1095	0.7064	(0-1 0)	8.050A	1
V 1	0.2487	0.3905	1.2064	(0 0 1)	11.186A	1
V 1	0.7513	-0.3905	0.7064	(1 0 0)	12.435A	1

Topology for V1

Atom V1 links by bridge ligands and has

Common vertex with					R(A-A)	
Sc 2	0.0968	0.5119	0.4545	(0 0-1)	8.050A	1
Sc 1	0.4076	0.5065	-0.0449	(0 0-1)	8.129A	1
Sc 2	0.4032	0.0119	-0.0455	(0 0-1)	11.186A	1
Sc 1	0.0924	0.0065	0.4551	(0 0 0)	11.216A	1
Sc 1	-0.0924	-0.0065	-0.0449	(0 0-1)	12.364A	1
Sc 2	0.5968	-0.0119	0.4545	(1 0-1)	12.435A	1
V 1	-0.2487	0.6095	-0.2936	(0 1-1)	17.134A	1
V 1	-0.2487	0.6095	0.7064	(0 1 0)	17.134A	1
V 1	0.7513	0.6095	-0.2936	(1 1-1)	17.170A	1
V 1	0.7513	0.6095	0.7064	(1 1 0)	17.170A	1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with VSc2

Coordination sequences

Sc1:	1	2	3	4	5	6	7	8	9	10
Num	3	26	88	154	331	479	591	940	1210	1276
Cum	4	30	118	272	603	1082	1673	2613	3823	5099

Sc2:	1	2	3	4	5	6	7	8	9	10
Num	3	26	88	154	331	479	591	940	1210	1276
Cum	4	30	118	272	603	1082	1673	2613	3823	5099

V1:	1	2	3	4	5	6	7	8	9	10
Num	10	42	108	230	342	506	772	938	1200	1634
Cum	11	53	161	391	733	1239	2011	2949	4149	5783

TD10=5327

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Vertex symbols for selected sublattice

Sc1 Point symbol:{4.5.6}

Extended point symbol:[4.5(4).6(12)]

Sc2 Point symbol:{4.5.6}

Extended point symbol:[4.5(4).6(12)]

V1 Point symbol:{4^6.5^18.6^19.7^2}

Extended point symbol:
[4.4.4.4.4.4.5.5.5.5.5.5.5.5.5.5.5.5.5.5.5.5.5(2).5(2).5(3).5(3).6.6.6.6.6.6.6(2).6(2).6(3).6(3).6(3).6(3).6(3).6(3).6(3).6(4).6(4).6(6).6(6).6(6).7(7).7(7)]

Point symbol for net: {4.5.6}2{4^6.5^18.6^19.7^2}

3,10-c net with stoichiometry (3-c)2(10-c); 2-nodal net

New topology, please, contact the authors (73705 types in 11 databases).

Compound 3

Topology for Mn1

Atom Mn1 links by bridge ligands and has

Common vertex with					R(A-A)	
Mn 1	0.7499	0.3811	0.9890	(0 0 0)	6.131A	1
Mn 1	0.7499	0.3811	-0.0110	(0 0-1)	6.131A	1
Mn 1	1.2501	-0.1189	0.5110	(2 0 1)	6.314A	1
Mn 1	0.2501	-0.1189	0.5110	(1 0 1)	6.360A	1
Mn 1	2.2501	0.8811	0.5110	(3 1 1)	19.590A	1

Structural group analysis

Structural group No 1

Structure consists of 3D framework with Mn

Coordination sequences

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Mn1: 1 2 3 4 5 6 7 8 9 10
Num 5 20 52 102 170 254 354 470 602 750
Cum 6 26 78 180 350 604 958 1428 2030 2780

TD10=2780

Vertex symbols for selected sublattice

Mn1 Point symbol:{6^10}
Extended point symbol:[6.6(3).6(3).6(3).6(3).6(3).6(3).6(3).6(5).6(5).6(7)]

Point symbol for net: {6^10}
5-c net; uninodal net

ATTENTION! If the name below is written in a long notation s/... or s-d-G-n, this net is a subnet of the net s (see Manual for details)
Topological type: hxg-d /P n -3 m->P b c n (-a+b,2c,a+b; 1/2,0,0);Bond sets: 3,5,6,7:hxg-d (uninodal.ttd) {6^10} - VS [6.6(3).6(3).6(3).6(3).6(3).6(3).6(3).6(5).6(5).6(7)] (73705 types in 11 databases).

Compound 4

Topology for F1

Atom F1 links by bridge ligands and has
Common vertex with R(A-A)
F 2 0.9432 0.9636 0.3739 (0 0 0) 3.093A 1
F 1 1.0568 1.0364 -0.1239 (2 2 0) 3.303A 1
F 1 -0.9432 0.0364 -0.1239 (0 1 0) 17.393A 1
Topology for F2

Atom F2 links by bridge ligands and has
Common vertex with R(A-A)
F 1 0.9432 0.9636 0.1239 (0 0 0) 3.093A 1
F 2 1.0568 1.0364 0.6261 (2 2 1) 3.246A 1
F 2 0.0568 -0.9636 0.6261 (1 0 1) 19.508A 1

Structural group analysis

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Structural group No 1

Structure consists of 3D framework with F
There are 3 interpenetrating nets
FIV: Full interpenetration vectors

[1,0,0] (10.11A)

PIC: [3,0,0][0,0,1][1,-1,0] (PICVR=3)

Zt=3; Zn=1

Class Ia Z=3

Coordination sequences

F1: 1 2 3 4 5 6 7 8 9 10
Num 3 6 12 24 38 56 77 102 129 160
Cum 4 10 22 46 84 140 217 319 448 608

F2: 1 2 3 4 5 6 7 8 9 10
Num 3 6 12 24 38 56 77 102 129 160
Cum 4 10 22 46 84 140 217 319 448 608

TD10=608

Vertex symbols for selected sublattice

F1 Point symbol:{10^3}
Extended point symbol:[10(2).10(4).10(4)]

F2 Point symbol:{10^3}
Extended point symbol:[10(2).10(4).10(4)]

Point symbol for net: {10^3}
3-c net; uninodal net

Topological type: ths ThSi2; 3/10/t4 (topos&RCSR.ttd) {10^3} - VS [10(2).10(4).10(4)] (73705 types in 11 databases).