Electronic Supplementary Material (ESI) for CrystEngComm

Supporting Information

Solvents influence on sizes of channels in three fry topological Mn(II)-MOFs based on metal-carboxylate chains: Syntheses, structures and magnetic properties†

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The Supporting Pictures For Article

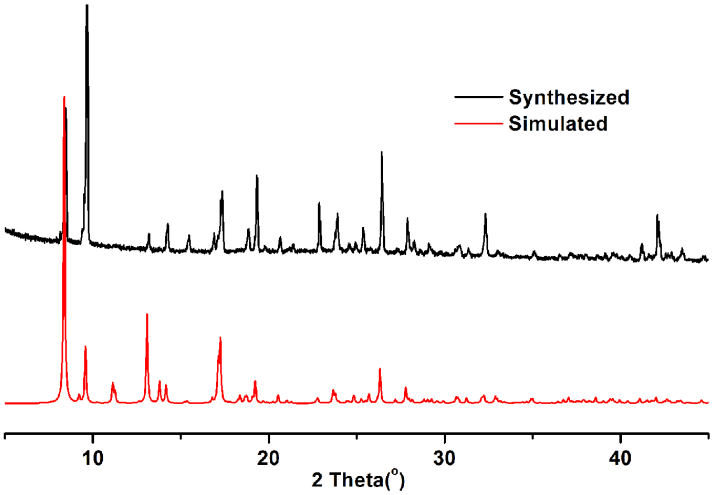


Fig. S1 Powder X-ray diffraction patterns of compound **1**.

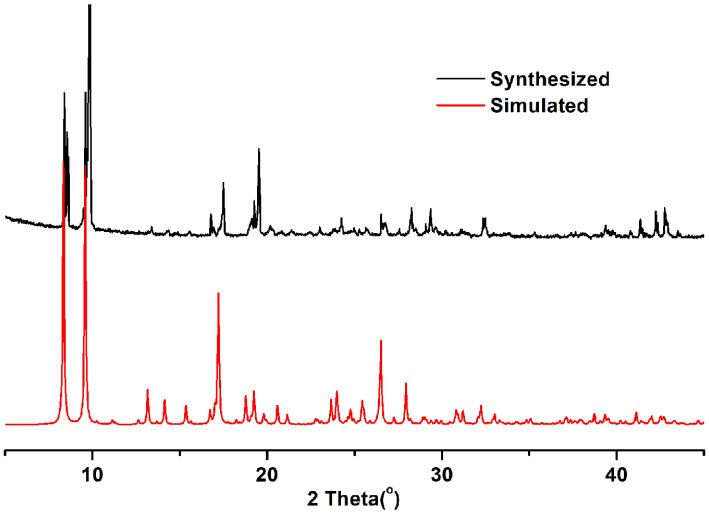


Fig. S2 Powder X-ray diffraction patterns of compound **2**.

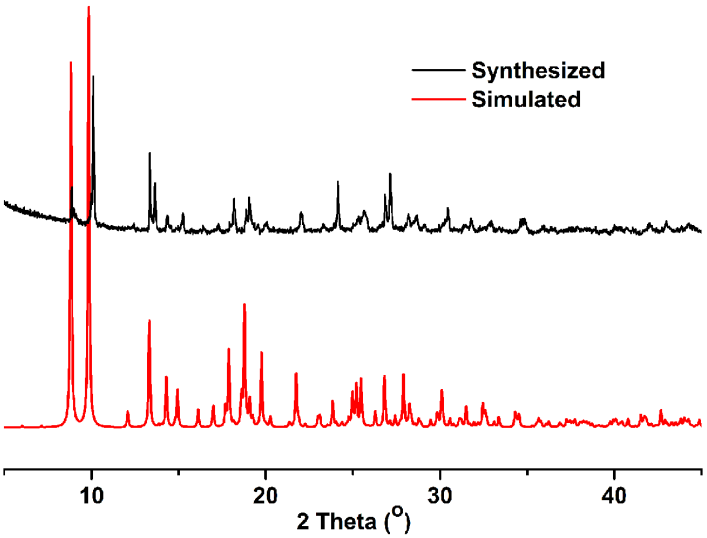


Fig. S3 Powder X-ray diffraction patterns of compound **3**.

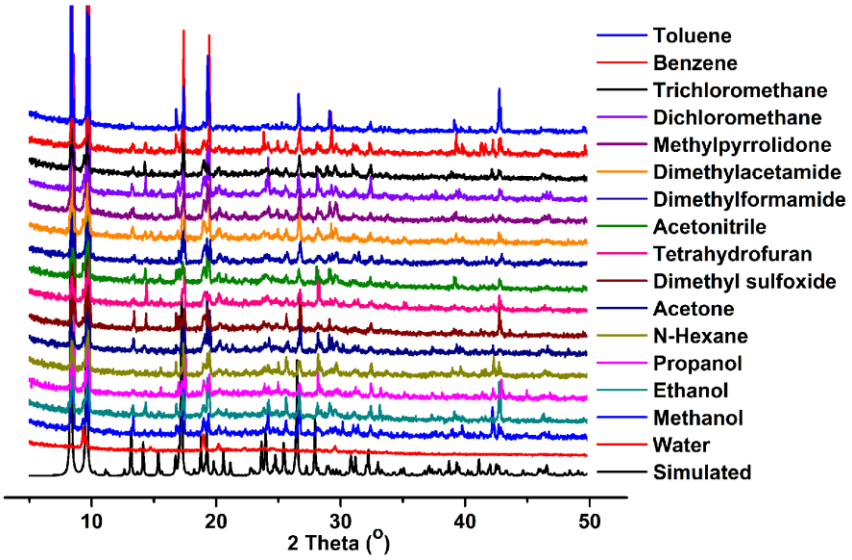


Fig. S4 The PXRD patterns of **2** after soaking in various solvents for 1 week.

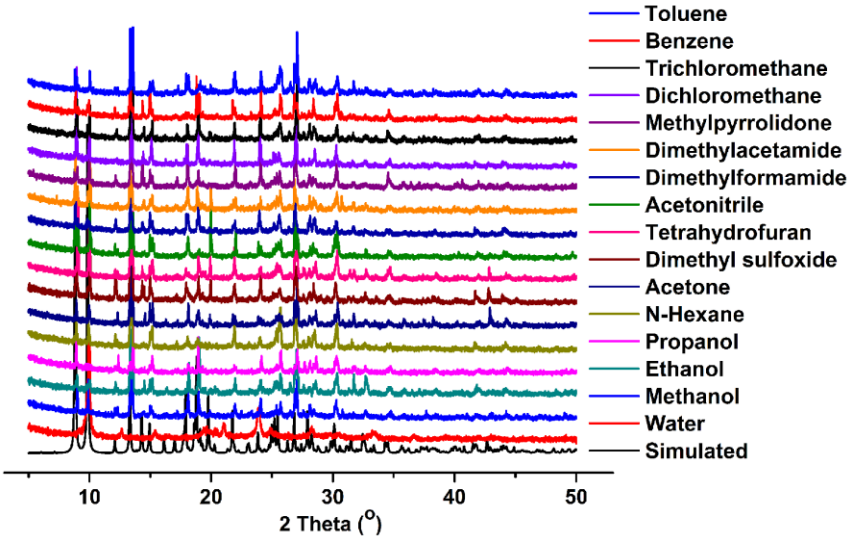


Fig. S5 The PXRD patterns of **3** after soaking in various solvents for 1 week.

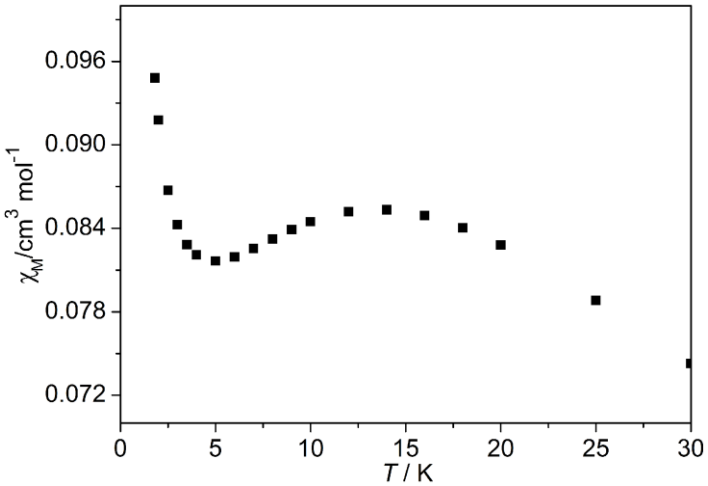


Fig. S6 The χ_M *VS.* T plot for compound **1**.

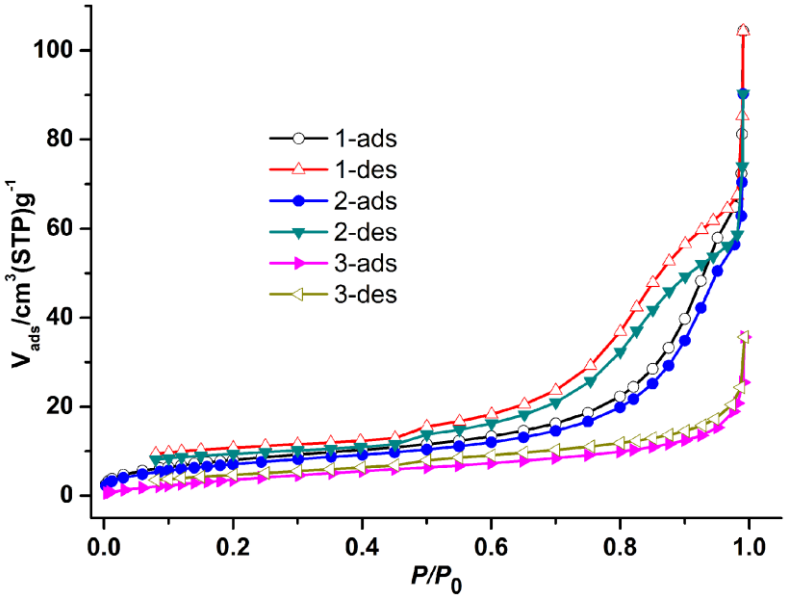


Fig. S7 Nitrogen adsorption–desorption isotherms of **1**–**3** at 77 K.

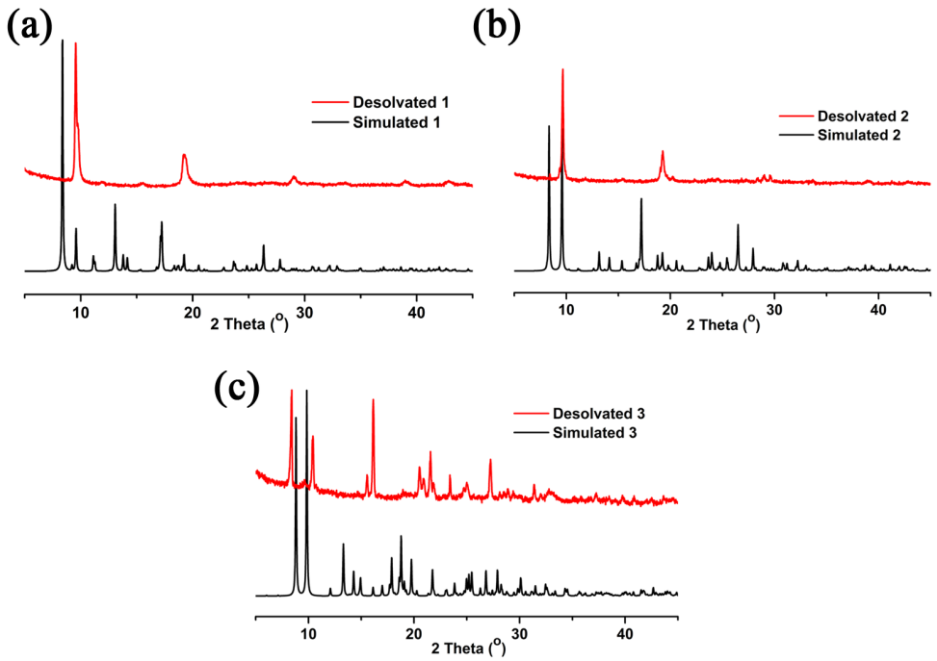
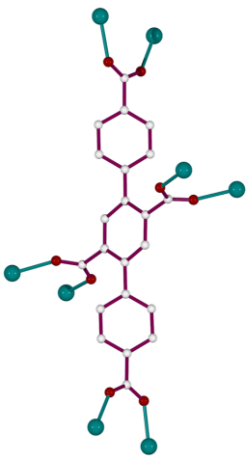


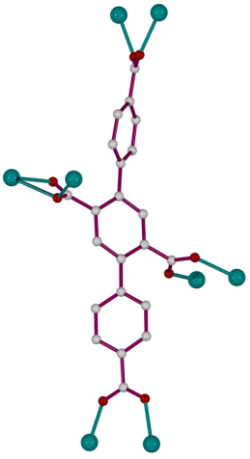
Fig. S8 PXRD patterns of **1** (a), **2** (b), **3** (c), desolvated **1**, **2** and **3**.

The Supporting Scheme For Article

Scheme S1. Coordination Modes of Ligands in Compounds **1** and **3**



1: $\eta^8\mu_8\chi^8$



3: $\eta^9\mu_8\chi^8$

Two coordination fashions of ligands H_4tptc in compounds **1** and **3**. The symbol of $\eta^x\mu_y\chi^z$ describes the coordination modes, where: η^x – number of coordination bonds donated from the ligand; μ_y – number of metal centers bonded to the ligand; χ^z – number of atoms donating coordination bonds.

The Supporting Table For Article

Table S1. Comparison of the diverse solvent-controlled Mn-tptc system

Compound	**1**	**2**	**3**
Crystallizing medium	H_2O/NMP	H_2O/DMA	H_2O/DMF
Coordinated solvents	H_2O/NMP	H_2O/DMA	DMF
Coordination modes of solvent	bridging	bridging	monodentate/bridging
Bridging fashions of carboxyl groups	μ_2-η^1:η^1	μ_2-η^1:η^1	μ_2-η^1:η^1/μ_2-η^1:η^2
Metal coordination	octahedron (MnO_6)	octahedron (MnO_6)	octahedron (MnO_6)
Intermetallic bridging modes	(μ-H_2O/NMP)(μ-COO)$_2$	(μ-H_2O/DMA)(μ-COO)$_2$	(μ-DMF)(μ-COO)$_2$ /(μ-COO)$_2$
Interchain Mn···Mn distances	9.494 Å, 12.628 Å	9.490 Å, 12.646 Å	8.880 Å, 12.463 Å
Size of channel	9.494 × 3.725 Å^2	9.490 ×3.706 Å^2	8.880 × 3.729 Å^2
Pore volume	1242.4 Å^3	1205.9 Å^3	1005.3 Å^3
Void ratio	41.4%	40.5%	37.0%

Table S2. Selected Bond Lengths (Å) and Angles (˚) for **1-3**.

Complex **1**					
Mn(1)-O(2)	2.114(3)	Mn(1)-O(8)#1	2.132(4)	Mn(1)-O(6)#2	2.136(3)
Mn(1)-O(4) #3	2.155(3)	Mn(1)-O(9)	2.240(3)	Mn(1)-O(10)	2.383(3)
Mn(2)-O(7) #3	2.155(3)	Mn(2)-O(5)#6	2.159(3)	Mn(2)-O(9)#6	2.261(3)
Mn(3)-O(3) #3	2.133(3)	Mn(3)-O(1)	2.149(3)	Mn(3)-O(10)	2.253(3)
O(2)-Mn(1)-O(8)#1	162.87(14)		O(4)#3-Mn(1)-O(10)	99.89(12)	
O(2)-Mn(1)-O(6)#2	91.49(14)		O(9)-Mn(1)-O(10)	169.79(11)	
O(8)#1-Mn(1)-O(6)#2	96.44(14)		O(7)#3-Mn(2)-O(7)#4	180.00(15)	
O(2)-Mn(1)-O(4)#3	87.59(14)		O(7)#3-Mn(2)-O(5)#5	91.85(13)	
O(8)#1-Mn(1)-O(4)#3	85.75(14)		O(7)#4-Mn(2)-O(5)#5	88.15(13)	
O(6)#2-Mn(1)-O(4)#3	175.04(13)		O(7)#3-Mn(2)-O(5)	88.15(13)	
O(2)-Mn(1)-O(9)	94.10(12)		O(7)#4-Mn(2)-O(5)	91.85(13)	
O(8)#1-Mn(1)-O(9)	101.67(13)		O(5)#5-Mn(2)-O(5)	180.0	
O(6)#2-Mn(1)-O(9)	85.14(13)		O(7)#3-Mn(2)-O(9)#6	87.63(12)	
O(4)#3-Mn(1)-O(9)	90.07(13)		O(7)#4-Mn(2)-O(9)#6	92.37(12)	
O(2)-Mn(1)-O(10)	88.60(12)		O(5)#5-Mn(2)-O(9)#6	90.07(12)	
O(8)#1-Mn(1)-O(10)	77.05(13)		O(5)-Mn(2)-O(9)#6	89.93(12)	
O(6)#2-Mn(1)-O(10)	84.95(12)		O(7)#3-Mn(2)-O(9)#7	92.37(12)	
O(7)#4-Mn(2)-O(9)#7	87.63(12)		O(1)#9-Mn(3)-O(1)	180.000(1)	
O(5)#5-Mn(2)-O(9)#7	89.93(12)		O(3)#3-Mn(3)-O(10)	86.98(13)	
O(5)-Mn(2)-O(9)#7	90.07(12)		O(3)#8-Mn(3)-O(10)	93.02(13)	
O(9)#6-Mn(2)-O(9)#7	180.000(1)		O(1)#9-Mn(3)-O(10)	86.58(12)	
O(3)#3-Mn(3)-O(3)#8	180.000(1)		O(1)-Mn(3)-O(10)	93.42(12)	
O(3)#3-Mn(3)-O(1)#9	84.39(14)		O(3)#3-Mn(3)-O(10)#9	93.02(13)	
O(3)#8-Mn(3)-O(1)#9	95.61(13)		O(3)#8-Mn(3)-O(10)#9	86.98(13)	
O(3)#3-Mn(3)-O(1)	95.61(13)		O(1)#9-Mn(3)-O(10)#9	93.42(12)	
O(3)#8-Mn(3)-O(1)	84.39(14)		O(1)-Mn(3)-O(10)#9	86.58(12)	
O(10)-Mn(3)-O(10)#9	180.000(1)		Mn(1)-O(9)-Mn(2)#12	111.70(13)	
Mn(3)-O(10)-Mn(1)	109.22(12)				

Symmetry transformations used to generate equivalent atoms: #1 x-1, -y+3/2, z+1/2; #2 x, -y+3/2, z+1/2; #3 x-1, y, z; #4 -x+1, -y+1, -z+1; #5 -x, -y+1, -z+1; #6 -x, y-1/2, -z+3/2; #7 x, -y+3/2, z-1/2; #8 -x+1, -y+1, -z+2; #9 -x, -y+1, -z+2; #12 -x, y+1/2, -z+3/2

Complex **2**					
Mn(1)-O(8)#1	2.114(4)	Mn(1)-O(5)	2.135(3)	Mn(1)-O(3)#2	2.141(4)
Mn(1)-O(1)#3	2.149(4)	Mn(1)-O(9)	2.246(3)	Mn(1)-O(10)	2.373(3)
Mn(2)-O(6)	2.155(3)	Mn(2)-O(2)#3	2.165(4)	Mn(2)-O(9)	2.276(3)
Mn(3)-O(4)#2	2.118(4)	Mn(3)-O(7)#1	2.175(4)	Mn(3)-O(10)	2.236(3)
O(8)#1-Mn(1)-O(5)	91.58(16)		O(2)#5-Mn(2)-O(9)#4	93.96(14)	
O(8)#1-Mn(1)-O(3)#2	87.90(17)		O(2)#3-Mn(2)-O(9)#4	86.04(14)	
O(5)-Mn(1)-O(3)#2	175.00(15)		O(6)#4-Mn(2)-O(9)	91.10(14)	
O(8)#1-Mn(1)-O(1)#3	162.04(16)		O(6)-Mn(2)-O(9)	88.90(14)	

O(5)-Mn(1)-O(1)#3	96.26(16)	O(2)#5-Mn(2)-O(9)	86.04(14)
O(3)#2-Mn(1)-O(1)#3	85.65(17)	O(2)#3-Mn(2)-O(9)	93.96(14)
O(8)#1-Mn(1)-O(9)	93.14(15)	O(9)#4-Mn(2)-O(9)	180.000(1)
O(5)-Mn(1)-O(9)	84.77(14)	O(4)#2-Mn(3)-O(4)#6	180.000(1)
O(3)#2-Mn(1)-O(9)	90.29(15)	O(4)#2-Mn(3)-O(7)#1	95.99(16)
O(1)#3-Mn(1)-O(9)	103.62(15)	O(4)#6-Mn(3)-O(7)#1	84.01(17)
O(8)#1-Mn(1)-O(10)	89.44(15)	O(4)#2-Mn(3)-O(7)#7	84.01(17)
O(5)-Mn(1)-O(10)	84.45(14)	O(4)#6-Mn(3)-O(7)#7	95.99(16)
O(3)#2-Mn(1)-O(10)	100.51(14)	O(7)#1-Mn(3)-O(7)#7	180.000(2)
O(1)#3-Mn(1)-O(10)	75.33(15)	O(4)#2-Mn(3)-O(10)#8	92.28(15)
O(9)-Mn(1)-O(10)	168.98(13)	O(4)#6-Mn(3)-O(10)#8	87.72(15)
O(6)#4-Mn(2)-O(6)	180.000(1)	O(7)#1-Mn(3)-O(10)#8	86.07(14)
O(6)#4-Mn(2)-O(2)#5	88.58(16)	O(7)#7-Mn(3)-O(10)#8	93.93(14)
O(6)-Mn(2)-O(2)#5	91.42(16)	O(4)#2-Mn(3)-O(10)	87.72(15)
O(6)#4-Mn(2)-O(2)#3	91.42(16)	O(4)#6-Mn(3)-O(10)	92.28(15)
O(6)-Mn(2)-O(2)#3	88.58(16)	O(7)#1-Mn(3)-O(10)	93.93(14)
O(2)#5-Mn(2)-O(2)#3	180.000(2)	O(7)#7-Mn(3)-O(10)	86.07(14)
O(6)#4-Mn(2)-O(9)#4	88.90(14)	O(10)#8-Mn(3)-O(10)	180.000(1)
O(6)-Mn(2)-O(9)#4	91.10(14)	Mn(1)-O(9)-Mn(2)	110.05(15)
Mn(3)-O(10)-Mn(1)	108.61(15)		

Symmetry transformations used to generate equivalent atoms: #1 x, -y+3/2, z+1/2; #2 x+1, -y+3/2, +1/2; #3 x+1, y, z; #4 -x+2, -y+2, -z+2; #5 -x+1, -y+2, -z+2; #6 -x+1, y-1/2, -z+3/2; #7 -x+2, y-1/2, -z+3/2; #8 -x+2, -y+1, -z+2

Complex **3**

Mn(1)-O(1)#1	2.071(2)	Mn(1)-O(3)	2.195(2)	Mn(1)-O(9)	2.327(3)
Mn(2)-O(4)	2.105(2)	Mn(2)-O(2)#2	2.146(2)	Mn(2)-O(9)#3	2.396(3)
Mn(3)-O(8)#7	2.099(3)	Mn(3)-O(5)#8	2.166(2)	Mn(3)-O(7)#9	2.178(2)
Mn(3)-O(10)	2.180(3)	Mn(3)-O(6)	2.214(3)	Mn(3)-O(5)	2.408(2)

O(1)#1-Mn(1)-O(1)#2	180.000(1)	O(1)#1-Mn(1)-O(3)	84.33(10)
O(1)#2-Mn(1)-O(3)	95.67(10)	O(3)#3-Mn(1)-O(3)	180.0
O(1)#1-Mn(1)-O(9)	92.69(10)	O(1)#2-Mn(1)-O(9)	87.31(10)
O(3)#3-Mn(1)-O(9)	89.82(10)	O(3)-Mn(1)-O(9)	90.18(9)
O(9)#3-Mn(1)-O(9)	180.0	O(4)-Mn(2)-O(4)#4	180.000(1)
O(4)-Mn(2)-O(2)#5	87.28(10)	O(4)#4-Mn(2)-O(2)#5	92.72(10)
O(2)#5-Mn(2)-O(2)#2	180.0	O(4)-Mn(2)-O(9)#3	87.26(10)
O(4)#4-Mn(2)-O(9)#3	92.74(10)	O(2)#5-Mn(2)-O(9)#3	82.78(9)
O(2)#2-Mn(2)-O(9)#3	97.22(9)	O(9)#3-Mn(2)-O(9)#6	180.00(11)
O(8)#7-Mn(3)-O(5)#8	98.36(10)	O(8)#7-Mn(3)-O(7)#9	170.07(10)
O(5)#8-Mn(3)-O(7)#9	91.54(10)	O(8)#7-Mn(3)-O(10)	86.47(12)
O(5)#8-Mn(3)-O(10)	96.58(11)	O(7)#9-Mn(3)-O(10)	93.17(11)
O(8)#7-Mn(3)-O(6)	91.70(11)	O(5)#8-Mn(3)-O(6)	94.67(9)
O(7)#9-Mn(3)-O(6)	86.71(10)	O(10)-Mn(3)-O(6)	168.75(11)
O(8)#7-Mn(3)-O(5)	87.30(9)	O(5)#8-Mn(3)-O(5)	151.07(6)
O(7)#9-Mn(3)-O(5)	83.64(9)	O(10)-Mn(3)-O(5)	112.12(10)

O(6)-Mn(3)-O(5)	56.67(9)	Mn(3)#10-O(5)-Mn(3)	116.74(10)
Mn(1)-O(9)-Mn(2)#12	104.28(10)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1, -y+1, -z+1; #2 x-1, y, z; #3 -x, -y+1, -z+1; #4 -x, -y+2, -z+1; #5 -x+1, -y+2, -z+1; #6 x, y+1, z; #7 x+1, y, z; #8 -x+1, y-1/2, -z+1/2; #9 -x, y-1/2, -z+1/2; #10 -x+1, y+1/2, -z+1/2; #12 x, y-1, z