[Supporting information]

Five New Coordination Polymers Based on A Semi-rigid Dicarboxylic Acid and Versatile N-donor Ligands: Synthesis, Characterization and Properties

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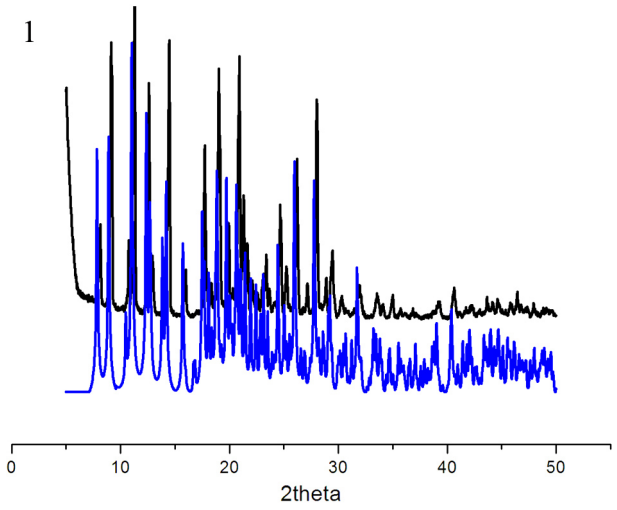

Figure S1. The simulated (blue) and experimental (black) XRPD patterns for **1**.

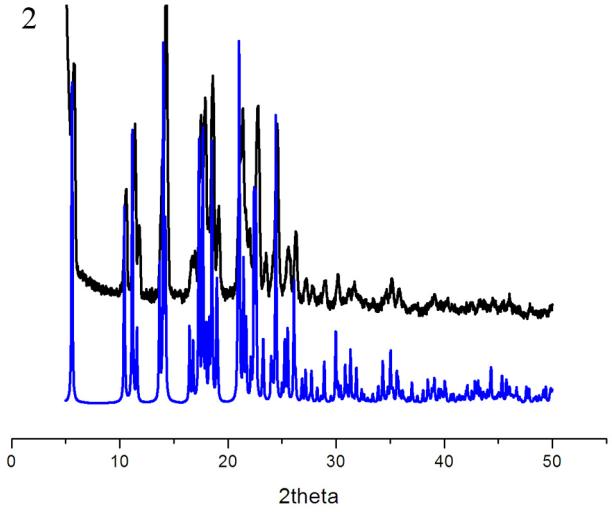

Figure S2. The simulated (blue) and experimental (black) XRPD patterns for **2**.

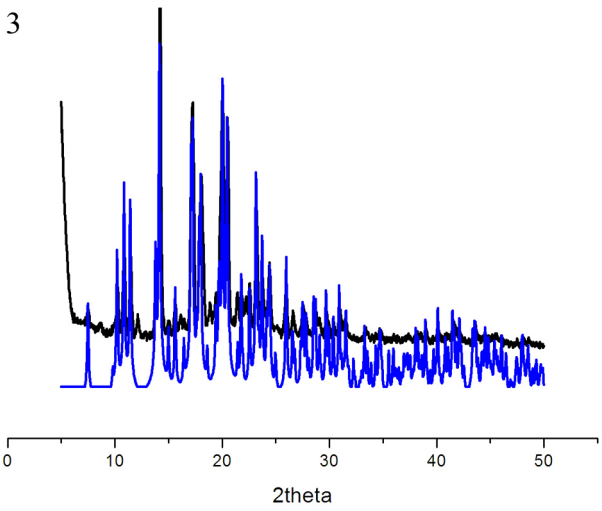

Figure S3. The simulated (blue) and experimental (black) XRPD patterns for **3**.

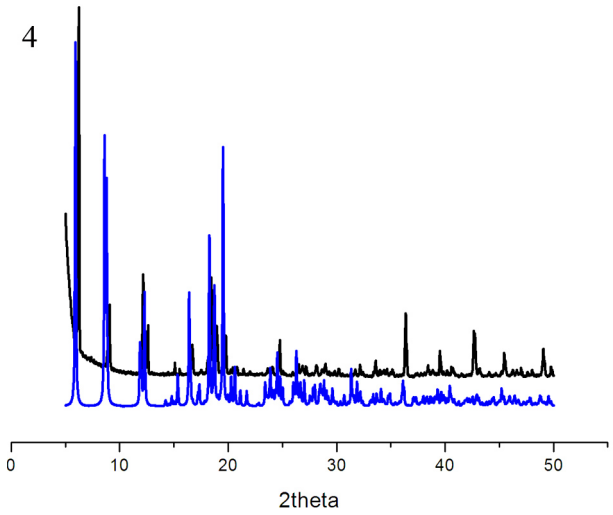

Figure S4. The simulated (blue) and experimental (black) XRPD patterns for **4**.

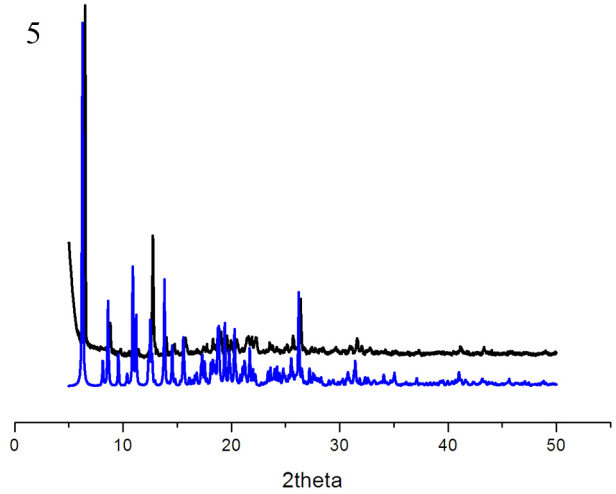

Figure S5. The simulated (blue) and experimental (black) XRPD patterns for **5**.

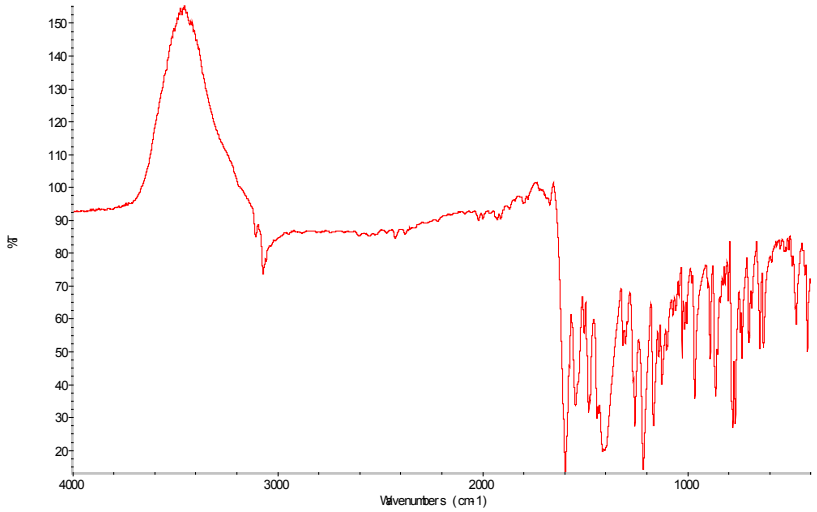

Figure S6. IR (4000-400 cm^{-1}) spectrum of the compound **1**.

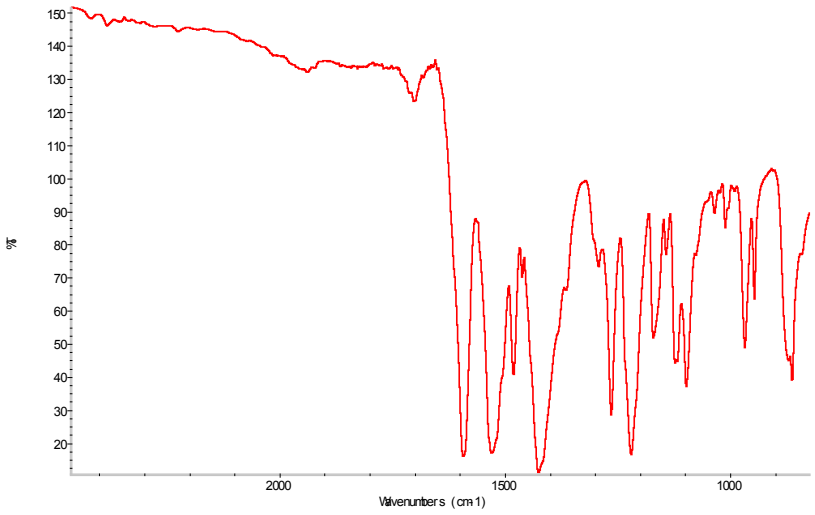

Figure S7. IR (4000-400 cm^{-1}) spectrum of the compound **2**.

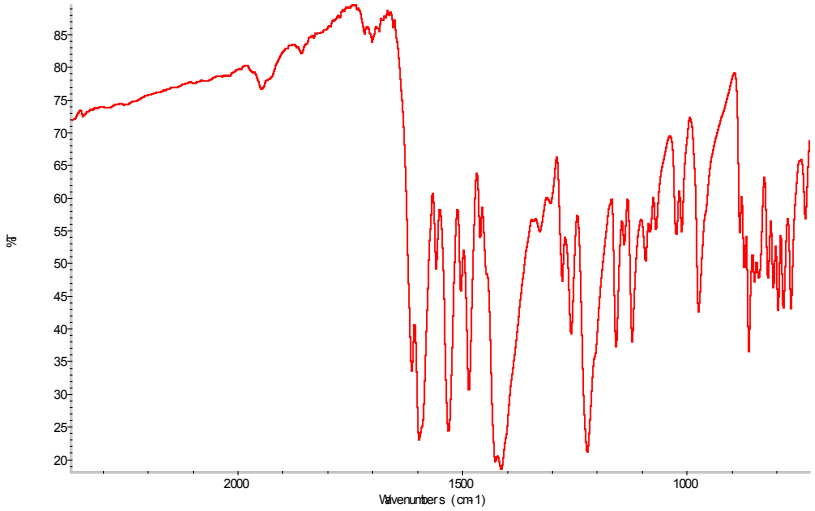

Figure S8. IR (4000-400 cm^{-1}) spectrum of the compound **3**.

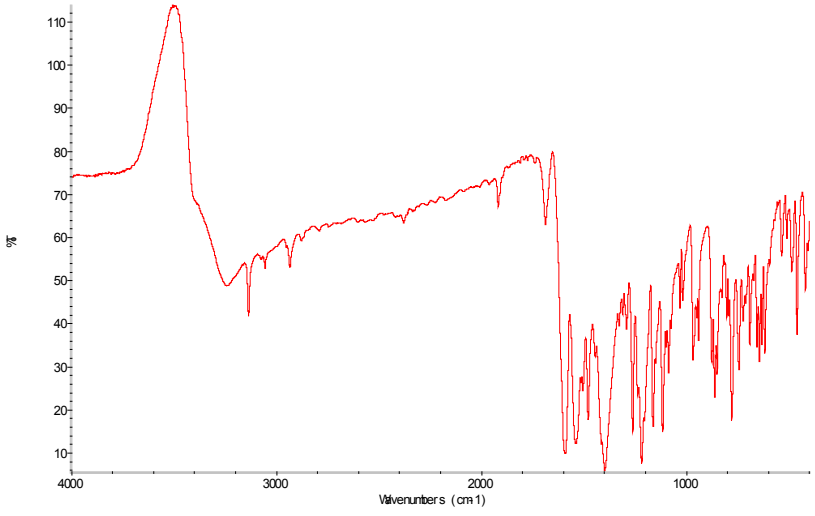

Figure S9. IR (4000-400 cm^{-1}) spectrum of the compound **4**.

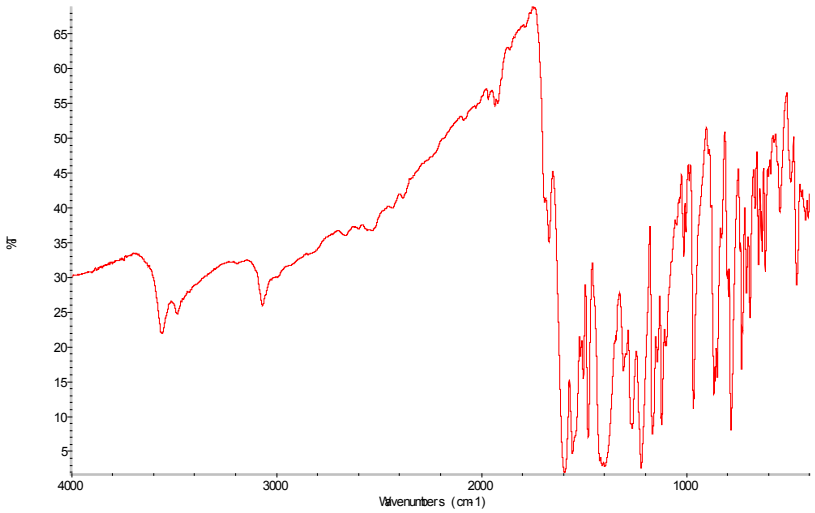

Figure S10. IR (4000-400 cm^{-1}) spectrum of the compound **5**.

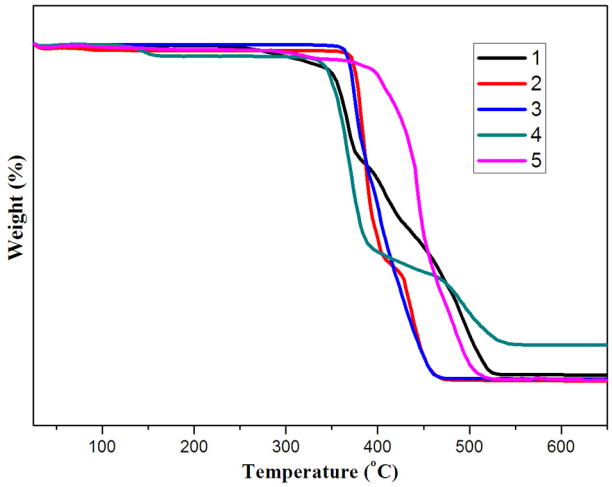

Figure S11. TGA curve of compound **1-5**.

Table S1. Selected bond distances (Å) and angles (°) for **1**.

Zn(1)-N(1)	2.1028(14)	Zn(1)-N(2)	2.0999(14)
Zn(1)-O(1)#1	2.2662(13)	Zn(1)-O(2)#1	2.1113(13)
Zn(1)-O(5)	2.1231(12)	Zn(1)-O(6)	2.1621(13)
N(2)-Zn(1)-N(1)	78.09(6)	N(2)-Zn(1)-O(2)#1	102.15(5)
N(1)-Zn(1)-O(2)#1	97.65(5)	N(2)-Zn(1)-O(5)	156.75(5)
N(1)-Zn(1)-O(5)	96.86(5)	O(2)#1-Zn(1)-O(5)	101.02(5)
N(2)-Zn(1)-O(6)	99.35(5)	N(1)-Zn(1)-O(6)	113.17(5)
O(2)#1-Zn(1)-O(6)	145.41(5)	O(5)-Zn(1)-O(6)	61.42(5)

N(2)-Zn(1)-O(1)#1	89.00(5)	N(1)-Zn(1)-O(1)#1	151.44(5)
O(2)#1-Zn(1)-O(1)#1	59.99(5)	O(5)-Zn(1)-O(1)#1	104.41(5)
O(6)-Zn(1)-O(1)#1	93.88(5)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1,y+1/2,-z+1/2.

Table S2. Selected bond distances (Å) and angles (°) for **2**.

Ni(1)-N(3)	2.011(4)	Ni(1)-N(1)	2.060(5)
Ni(1)-O(5)#1	2.083(3)	Ni(1)-O(1)	2.125(4)
Ni(1)-O(2)	2.134(4)	Ni(1)-O(6)#1	2.148(3)
N(3)-Ni(1)-N(1)	96.72(18)	N(3)-Ni(1)-O(5)#1	96.60(16)
N(1)-Ni(1)-O(5)#1	94.20(17)	N(3)-Ni(1)-O(1)	99.11(19)
N(1)-Ni(1)-O(1)	99.96(18)	O(5)#1-Ni(1)-O(1)	157.40(15)
N(3)-Ni(1)-O(2)	92.04(17)	N(1)-Ni(1)-O(2)	160.93(16)
O(5)#1-Ni(1)-O(2)	101.61(15)	O(1)-Ni(1)-O(2)	61.80(15)
N(3)-Ni(1)-O(6)#1	158.45(15)	N(1)-Ni(1)-O(6)#1	88.32(16)
O(5)#1-Ni(1)-O(6)#1	62.05(13)	O(1)-Ni(1)-O(6)#1	100.63(16)
O(2)-Ni(1)-O(6)#1	89.71(15)		

Symmetry transformations used to generate equivalent atoms: #1 x+1/2,y+1/2,z

Table S3. Selected bond distances (Å) and angles (°) for **3**.

Ni(1)-N(1)	2.062(3)	Ni(1)-N(2)	2.069(4)
Ni(1)-O(5)#1	2.083(3)	Ni(1)-O(2)	2.097(3)
Ni(1)-O(1)	2.100(3)	Ni(1)-O(6)#1	2.144(3)
N(1)-Ni(1)-N(2)	94.42(13)	N(1)-Ni(1)-O(5)#1	94.03(13)
N(2)-Ni(1)-O(5)#1	101.70(13)	N(1)-Ni(1)-O(2)	107.20(14)
N(2)-Ni(1)-O(2)	92.78(13)	O(5)#1-Ni(1)-O(2)	153.31(12)
N(1)-Ni(1)-O(1)	169.70(14)	N(2)-Ni(1)-O(1)	89.57(14)

O(5)#1-Ni(1)-O(1)	94.45(11)	O(2)-Ni(1)-O(1)	63.06(12)
N(1)-Ni(1)-O(6)#1	89.07(13)	N(2)-Ni(1)-O(6)#1	164.14(13)
O(5)#1-Ni(1)-O(6)#1	62.58(11)	O(2)-Ni(1)-O(6)#1	100.96(12)
O(1)-Ni(1)-O(6)#1	89.66(12)		

Symmetry transformations used to generate equivalent atoms: #1 x,y,z-1

Table S4. Selected bond distances (Å) and angles (°) for **4**.

Cd(1)-N(4)	2.266(5)	Cd(1)-O(2)	2.518(5)
Cd(1)-O(1W)	2.295(4)	Cd(1)-O(1)	2.340(5)
Cd(1)-O(5)	2.353(5)	Cd(1)-O(5)#3	2.387(4)
Cd(1)-O(6)#3	2.502(5)	Cd(2)-N(1)	2.257(5)
Cd(2)-O(12)#2	2.516(5)	Cd(2)-O(2W)	2.292(4)
Cd(2)-O(11)	2.330(5)	Cd(2)-O(10)#1	2.357(5)
Cd(2)-O(11)#2	2.407(4)	Cd(2)-O(9)#1	2.506(5)
N(1)-Cd(2)-O(2W)	174.87(17)	N(1)-Cd(2)-O(11)	100.63(19)
O(2W)-Cd(2)-O(11)	83.46(16)	N(1)-Cd(2)-O(10)#1	89.76(19)
O(2W)-Cd(2)-O(10)#1	86.68(17)	O(11)-Cd(2)-O(10)#1	96.46(17)
N(1)-Cd(2)-O(11)#2	86.94(18)	O(2W)-Cd(2)-O(11)#2	97.35(16)
O(11)-Cd(2)-O(11)#2	71.61(18)	O(10)#1-Cd(2)-O(11)#2	166.76(19)
N(1)-Cd(2)-O(9)#1	88.26(18)	O(2W)-Cd(2)-O(9)#1	86.65(15)
O(11)-Cd(2)-O(9)#1	149.07(15)	O(10)#1-Cd(2)-O(9)#1	53.66(18)
O(11)#2-Cd(2)-O(9)#1	138.92(17)	N(1)-Cd(2)-O(12)#2	94.81(19)
O(2W)-Cd(2)-O(12)#2	85.60(17)	O(11)-Cd(2)-O(12)#2	121.29(15)
O(10)#1-Cd(2)-O(12)#2	140.17(18)	O(11)#2-Cd(2)-O(12)#2	52.99(15)
O(9)#1-Cd(2)-O(12)#2	86.89(16)	N(4)-Cd(1)-O(1W)	175.14(18)
N(4)-Cd(1)-O(1)	91.49(19)	O(1W)-Cd(1)-O(1)	85.51(17)
N(4)-Cd(1)-O(5)	101.0(2)	O(1W)-Cd(1)-O(5)	83.09(17)
O(1)-Cd(1)-O(5)	96.14(18)	N(4)-Cd(1)-O(5)#3	85.36(18)

O(1W)-Cd(1)-O(5)#3	98.44(17)	O(1)-Cd(1)-O(5)#3	166.40(19)
O(5)-Cd(1)-O(5)#3	71.58(19)	N(4)-Cd(1)-O(6)#3	94.3(2)
O(1W)-Cd(1)-O(6)#3	85.70(16)	O(1)-Cd(1)-O(6)#3	140.90(17)
O(5)-Cd(1)-O(6)#3	120.43(15)	O(5)#3-Cd(1)-O(6)#3	52.66(15)
N(4)-Cd(1)-O(2)	88.84(18)	O(1W)-Cd(1)-O(2)	86.30(16)
O(1)-Cd(1)-O(2)	54.18(18)	O(5)-Cd(1)-O(2)	149.25(16)
O(5)#3-Cd(1)-O(2)	138.76(17)	O(6)#3-Cd(1)-O(2)	87.27(15)

Symmetry transformations used to generate equivalent atoms: #1 x-1,y-1,z+1; #2 -x+1,-y+1,-z; #3 -x+3,-y+2,-z

Table S5. Selected bond distances (Å) and angles (°) for **5**.

Mn(1)-N(1)	2.296(2)	Mn(1)-N(2)	2.2566(19)
Mn(1)-O(8)	2.1623(16)	Mn(1)-O(12)	2.0863(17)
Mn(1)-O(13)	2.4416(18)	Mn(1)-O(14)	2.2260(16)
Mn(2)-O(7)	2.2591(16)	Mn(2)-O(11)	2.1131(16)
Mn(2)-O(13)	2.1305(15)	Mn(3)-N(3)	2.253(2)
Mn(3)-N(4)	2.319(2)	Mn(3)-O(1)	2.2486(18)
Mn(3)-O(2)	2.418(2)	Mn(3)-O(6)	2.1225(17)
Mn(3)-O(18)	2.1067(17)	Mn(4)-O(1)	2.2028(16)
Mn(4)-O(5)	2.1436(17)	Mn(4)-O(17)	2.1305(17)
O(12)-Mn(1)-O(8)	145.72(7)	O(12)-Mn(1)-O(14)	102.53(7)
O(8)-Mn(1)-O(14)	95.50(6)	O(12)-Mn(1)-N(2)	97.44(7)
O(8)-Mn(1)-N(2)	113.34(7)	O(14)-Mn(1)-N(2)	84.19(6)
O(12)-Mn(1)-N(1)	87.06(7)	O(8)-Mn(1)-N(1)	87.77(7)
O(14)-Mn(1)-N(1)	156.47(7)	N(2)-Mn(1)-N(1)	73.19(7)
O(12)-Mn(1)-O(13)	83.46(6)	O(8)-Mn(1)-O(13)	83.13(6)
O(14)-Mn(1)-O(13)	55.54(6)	N(2)-Mn(1)-O(13)	138.47(6)
N(1)-Mn(1)-O(13)	147.85(6)	O(11)#3-Mn(2)-O(11)	180.00(7)
O(11)#3-Mn(2)-O(13)	90.77(7)	O(11)-Mn(2)-O(13)	89.23(7)

O(11)#3-Mn(2)-O(13)#3	89.23(7)	O(11)-Mn(2)-O(13)#3	90.77(7)
O(13)-Mn(2)-O(13)#3	180.00(7)	O(11)#3-Mn(2)-O(7)#3	91.95(7)
O(11)-Mn(2)-O(7)#3	88.05(7)	O(13)-Mn(2)-O(7)#3	90.16(6)
O(13)#3-Mn(2)-O(7)#3	89.84(6)	O(11)#3-Mn(2)-O(7)	88.05(7)
O(11)-Mn(2)-O(7)	91.95(7)	O(13)-Mn(2)-O(7)	89.84(6)
O(13)#3-Mn(2)-O(7)	90.16(6)	O(7)#3-Mn(2)-O(7)	180.0
O(18)-Mn(3)-O(6)	93.75(7)	O(18)-Mn(3)-O(1)	112.58(7)
O(6)-Mn(3)-O(1)	101.78(7)	O(18)-Mn(3)-N(3)	89.45(7)
O(6)-Mn(3)-N(3)	111.56(7)	O(1)-Mn(3)-N(3)	138.66(7)
O(18)-Mn(3)-N(4)	161.77(8)	O(6)-Mn(3)-N(4)	90.96(7)
O(1)-Mn(3)-N(4)	83.55(7)	N(3)-Mn(3)-N(4)	72.46(8)
O(18)-Mn(3)-O(2)	99.80(7)	O(6)-Mn(3)-O(2)	157.14(7)
O(1)-Mn(3)-O(2)	55.98(6)	N(3)-Mn(3)-O(2)	87.05(7)
N(4)-Mn(3)-O(2)	81.89(7)	O(17)#4-Mn(4)-O(17)	180.000(1)
O(17)#4-Mn(4)-O(5)	91.65(7)	O(17)-Mn(4)-O(5)	88.35(8)
O(17)#4-Mn(4)-O(5)#4	88.35(8)	O(17)-Mn(4)-O(5)#4	91.65(7)
O(5)-Mn(4)-O(5)#4	180.000(1)	O(17)#4-Mn(4)-O(1)	92.17(7)
O(17)-Mn(4)-O(1)	87.83(7)	O(5)-Mn(4)-O(1)	90.26(7)
O(5)#4-Mn(4)-O(1)	89.74(7)	O(17)#4-Mn(4)-O(1)#4	87.83(7)
O(17)-Mn(4)-O(1)#4	92.17(7)	O(5)-Mn(4)-O(1)#4	89.74(7)
O(5)#4-Mn(4)-O(1)#4	90.26(7)	O(1)-Mn(4)-O(1)#4	180.0

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