Electronic Supplementary Material (ESI) for Dalton Transactions.

Three Mn(II) Coordination Polymers with a Bispyridyl-based Quinolinate Ligand: the Anion-Controlled Tunable Structural and Magnetic Properties

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Table of Content

1. Table S1. Selected Bond lengths [Å] and angles [º] for L-MOM.

O(1)-C(2)	1.380(6)
O(1)-C(1)	1.413(7)
N(1)-C(11)	1.313(5)
N(1)-C(8)	1.367(4)
O(2)-C(3)	1.368(4)
O(2)-C(2)	1.436(5)
N(2)-C(16)	1.330(5)
N(2)-C(15)	1.338(5)
O(3)-C(24)	1.391(5)
O(3)-C(23)	1.430(5)
N(3)-C(20)	1.327(5)
N(3)-C(21)	1.343(5)
C(3)-C(4)	1.370(4)
C(3)-C(8)	1.448(5)
O(4)-C(25)	1.387(4)
O(4)-C(24)	1.420(4)
N(4)-C(33)	1.329(4)
N(4)-C(26)	1.363(4)
C(4)-C(5)	1.426(4)
C(4)-C(13)	1.498(4)
N(5)-C(37)	1.326(6)
N(5)-C(38)	1.328(6)
C(5)-C(6)	1.363(4)
N(6)-C(42)	1.336(5)
N(6)-C(43)	1.335(5)
C(6)-C(7)	1.423(5)
C(6)-C(18)	1.497(4)
C(7)-C(9)	1.410(5)
C(7)-C(8)	1.430(5)
C(9)-C(10)	1.357(5)
C(10)-C(11)	1.413(5)
C(11)-C(12)	1.519(5)
C(13)-C(17)	1.379(5)
C(13)-C(14)	1.399(4)
C(14)-C(15)	1.373(5)
C(16)-C(17)	1.386(5)
C(18)-C(19)	1.386(5)
C(18)-C(22)	1.402(4)
C(19)-C(20)	1.381(5)
C(21)-C(22)	1.386(5)
C(25)-C(30)	1.364(4)
C(25)-C(26)	1.442(4)
C(26)-C(27)	1.427(4)

C(27)-C(31)	1.415(4)
C(27)-C(28)	1.432(5)
C(28)-C(29)	1.372(4)
C(28)-C(40)	1.486(5)
C(29)-C(30)	1.417(4)
C(30)-C(35)	1.494(4)
C(31)-C(32)	1.368(5)
C(32)-C(33)	1.415(5)
C(33)-C(34)	1.496(5)
C(35)-C(39)	1.397(5)
C(35)-C(36)	1.414(5)
C(36)-C(37)	1.377(5)
C(38)-C(39)	1.387(5)
C(40)-C(44)	1.374(5)
C(40)-C(41)	1.400(5)
C(41)-C(42)	1.373(5)
C(43)-C(44)	1.384(5)

C(2)-O(1)-C(1)	114.8(4)
C(11)-N(1)-C(8)	118.4(3)
C(3)-O(2)-C(2)	118.7(3)
C(16)-N(2)-C(15)	115.3(3)
O(1)-C(2)-O(2)	112.1(4)
C(24)-O(3)-C(23)	113.6(3)
C(20)-N(3)-C(21)	115.0(3)
O(2)-C(3)-C(4)	120.1(3)
O(2)-C(3)-C(8)	119.3(3)
C(4)-C(3)-C(8)	120.5(3)
C(25)-O(4)-C(24)	113.7(3)
C(33)-N(4)-C(26)	118.4(3)
C(3)-C(4)-C(5)	118.7(3)
C(3)-C(4)-C(13)	123.3(3)
C(5)-C(4)-C(13)	117.9(3)
C(37)-N(5)-C(38)	116.8(3)
C(6)-C(5)-C(4)	123.3(3)
C(42)-N(6)-C(43)	115.5(3)
C(5)-C(6)-C(7)	118.8(3)
C(5)-C(6)-C(18)	117.3(3)
C(7)-C(6)-C(18)	123.9(3)
C(9)-C(7)-C(6)	124.1(3)
C(9)-C(7)-C(8)	116.1(3)
C(6)-C(7)-C(8)	119.7(3)
N(1)-C(8)-C(7)	123.1(3)
N(1)-C(8)-C(3)	118.0(3)

C(7)-C(8)-C(3)	118.8(3)
C(10)-C(9)-C(7)	119.8(3)
C(9)-C(10)-C(11)	120.3(3)
N(1)-C(11)-C(10)	122.3(3)
N(1)-C(11)-C(12)	116.6(4)
C(10)-C(11)-C(12)	121.1(3)
C(17)-C(13)-C(14)	116.5(3)
C(17)-C(13)-C(4)	119.8(3)
C(14)-C(13)-C(4)	123.6(3)
C(15)-C(14)-C(13)	119.4(3)
N(2)-C(15)-C(14)	124.6(4)
N(2)-C(16)-C(17)	124.5(4)
C(13)-C(17)-C(16)	119.6(3)
C(19)-C(18)-C(22)	116.9(3)
C(19)-C(18)-C(6)	120.0(3)
C(22)-C(18)-C(6)	123.0(3)
C(20)-C(19)-C(18)	119.1(3)
N(3)-C(20)-C(19)	125.5(4)
N(3)-C(21)-C(22)	124.6(3)
C(21)-C(22)-C(18)	118.8(3)
O(3)-C(24)-O(4)	112.1(3)
C(30)-C(25)-O(4)	121.4(3)
C(30)-C(25)-C(26)	121.3(3)
O(4)-C(25)-C(26)	117.3(3)
N(4)-C(26)-C(27)	123.3(3)
N(4)-C(26)-C(25)	118.5(3)
C(27)-C(26)-C(25)	118.2(3)
C(31)-C(27)-C(26)	116.2(3)
C(31)-C(27)-C(28)	123.3(3)
C(26)-C(27)-C(28)	120.4(3)
C(29)-C(28)-C(27)	117.6(3)
C(29)-C(28)-C(40)	119.2(3)
C(27)-C(28)-C(40)	123.1(3)
C(28)-C(29)-C(30)	123.7(3)
C(25)-C(30)-C(29)	118.6(3)
C(25)-C(30)-C(35)	122.3(3)
C(29)-C(30)-C(35)	119.0(3)
C(32)-C(31)-C(27)	119.9(3)
C(31)-C(32)-C(33)	119.9(3)
N(4)-C(33)-C(32)	122.2(3)
N(4)-C(33)-C(34)	117.5(3)
C(32)-C(33)-C(34)	120.3(3)
C(39)-C(35)-C(36)	116.9(3)

C(39)-C(35)-C(30)	120.0(3)
C(36)-C(35)-C(30)	123.1(3)
C(37)-C(36)-C(35)	118.6(4)
N(5)-C(37)-C(36)	124.6(4)
N(5)-C(38)-C(39)	124.1(4)
C(38)-C(39)-C(35)	119.0(4)
C(44)-C(40)-C(41)	116.1(3)
C(44)-C(40)-C(28)	121.7(3)
C(41)-C(40)-C(28)	122.1(3)
C(42)-C(41)-C(40)	119.3(4)
N(6)-C(42)-C(41)	124.8(4)
N(6)-C(43)-C(44)	123.6(4)
C(40)-C(44)-C(43)	120.6(3)

2. Table S2. Selected Bond lengths [Å] and angles [º] for **1**.

Mn(1)-O(3)	2.041(5)
Mn(1)-O(3)#1	2.041(5)
Mn(1)-N(1)#1	2.234(7)
Mn(1)-N(1)	2.234(7)
Mn(1)-N(5)#1	2.261(6)
Mn(1)-N(5)	2.261(6)
O(1)-Mn(2)	1.977(5)
Mn(2)-O(2)	1.934(5)
Mn(2)-N(2)#2	2.088(8)
Mn(2)-N(4)	2.181(7)
Mn(2)-N(7)	2.271(8)
N(2)-Mn(2)#3	2.088(8)
O(3)-Mn(1)-O(3)#1	180.0
O(3)-Mn(1)-N(1)#1	102.3(2)
O(3)#1-Mn(1)-N(1)#1	77.7(2)
O(3)-Mn(1)-N(1)	77.7(2)
O(3)#1-Mn(1)-N(1)	102.3(2)
N(1)#1-Mn(1)-N(1)	180.0
O(3)-Mn(1)-N(5)#1	91.5(2)
O(3)#1-Mn(1)-N(5)#1	88.5(2)
N(1)#1-Mn(1)-N(5)#1	86.3(2)
N(1)-Mn(1)-N(5)#1	93.7(2)
O(3)-Mn(1)-N(5)	88.5(2)
O(3)#1-Mn(1)-N(5)	91.5(2)
N(1)#1-Mn(1)-N(5)	93.7(2)
N(1)-Mn(1)-N(5)	86.3(2)

N(5)#1-Mn(1)-N(5)	180.00(5)
C(27)-O(1)-Mn(2)	116.0(4)
C(2)-N(1)-C(6)	117.5(8)
C(2)-N(1)-Mn(1)	131.7(6)
C(6)-N(1)-Mn(1)	110.1(5)
O(2)-Mn(2)-O(1)	136.6(3)
O(2)-Mn(2)-N(2)#2	116.2(3)
O(1)-Mn(2)-N(2)#2	107.1(3)
O(2)-Mn(2)-N(4)	97.4(2)
O(1)-Mn(2)-N(4)	80.1(2)
N(2)#2-Mn(2)-N(4)	93.9(3)
O(2)-Mn(2)-N(7)	79.5(3)
O(1)-Mn(2)-N(7)	98.5(2)
N(2)#2-Mn(2)-N(7)	92.1(3)
N(4)-Mn(2)-N(7)	174.0(3)
C(47)-O(2)-Mn(2)	118.9(5)
C(14)-N(2)-Mn(2)#3	129.1(6)
C(13)-N(2)-Mn(2)#3	116.4(6)
C(7)-O(3)-Mn(1)	115.2(5)
C(22)-N(4)-Mn(2)	131.6(6)
C(26)-N(4)-Mn(2)	108.5(4)
C(39)-N(5)-Mn(1)	124.6(5)
C(38)-N(5)-Mn(1)	121.7(5)

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

3. Table S3. Selected Bond lengths [Å] and angles [º] for **2**.

Mn(1)-O(1)	2.073(3)
Mn(1)-O(1)#1	2.073(3)
Mn(1)-N(2)#2	2.254(4)
Mn(1)-N(2)#3	2.254(4)
Mn(1)-N(1)#1	2.295(4)
Mn(1)-N(1)	2.295(4)
N(2)-Mn(1)#4	2.254(4)
O(1)-Mn(1)-O(1)#1	180.000(1)
O(1)-Mn(1)-N(2)#2	89.56(14)
O(1)#1-Mn(1)-N(2)#2	90.44(14)
O(1)-Mn(1)-N(2)#3	90.44(14)
O(1)#1-Mn(1)-N(2)#3	89.56(14)
N(2)#2-Mn(1)-N(2)#3	180.00(17)

O(1)-Mn(1)-N(1)#1	103.74(14)
O(1)#1-Mn(1)-N(1)#1	76.26(14)
N(2)#2-Mn(1)-N(1)#1	93.27(16)
N(2)#3-Mn(1)-N(1)#1	86.73(16)
O(1)-Mn(1)-N(1)	76.26(14)
O(1)#1-Mn(1)-N(1)	103.74(14)
N(2)#2-Mn(1)-N(1)	86.73(16)
N(2)#3-Mn(1)-N(1)	93.27(16)
N(1)#1-Mn(1)-N(1)	180.0
C(7)-O(1)-Mn(1)	117.5(3)
C(2)-N(1)-C(6)	119.5(4)
C(2)-N(1)-Mn(1)	130.8(3)
C(6)-N(1)-Mn(1)	109.1(3)
C(13)-N(2)-Mn(1)#4	127.2(4)
C(14)-N(2)-Mn(1)#4	117.9(3)

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

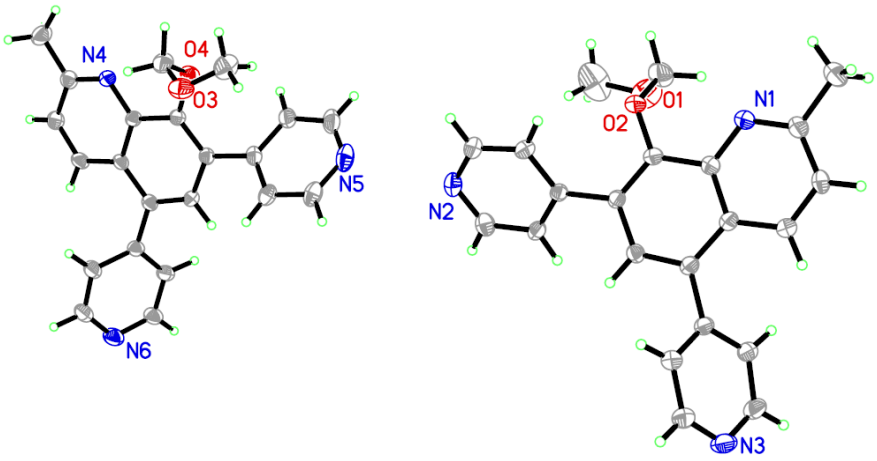
4. Table S4. Selected Bond lengths [Å] and angles [º] for **3**.

Mn(1)-O(1)	2.065(4)
Mn(1)-O(2)	2.069(4)
Mn(1)-N(3)#1	2.291(5)
Mn(1)-N(1)	2.295(6)
Mn(1)-N(5)#2	2.296(5)
Mn(1)-N(4)	2.301(6)
N(3)-Mn(1)#3	2.291(5)
N(5)-Mn(1)#4	2.296(5)
O(1)-Mn(1)-O(2)	179.72(19)
O(1)-Mn(1)-N(3)#1	90.88(18)
O(2)-Mn(1)-N(3)#1	89.11(19)
O(1)-Mn(1)-N(1)	76.21(17)
O(2)-Mn(1)-N(1)	103.51(17)
N(3)#1-Mn(1)-N(1)	90.9(2)
O(1)-Mn(1)-N(5)#2	89.68(18)
O(2)-Mn(1)-N(5)#2	90.33(18)
N(3)#1-Mn(1)-N(5)#2	178.9(2)
N(1)-Mn(1)-N(5)#2	88.3(2)
O(1)-Mn(1)-N(4)	104.33(17)
O(2)-Mn(1)-N(4)	75.94(17)

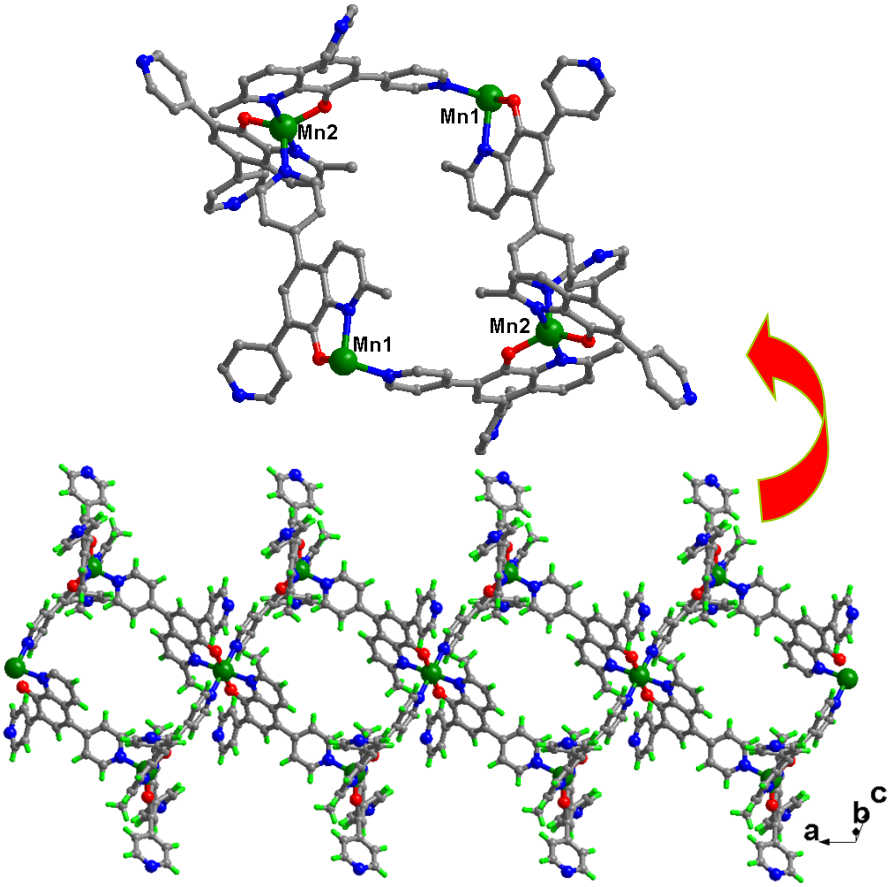
N(3)#1-Mn(1)-N(4)	90.2(2)
N(1)-Mn(1)-N(4)	178.8(2)
N(5)#2-Mn(1)-N(4)	90.6(2)
C(7)-O(1)-Mn(1)	117.6(4)
C(2)-N(1)-Mn(1)	131.1(5)
C(6)-N(1)-Mn(1)	109.5(4)
C(30)-O(2)-Mn(1)	118.3(4)
C(18)-N(3)-Mn(1)#3	121.5(4)
C(19)-N(3)-Mn(1)#3	121.1(5)
C(22)-N(4)-Mn(1)	132.2(5)
C(26)-N(4)-Mn(1)	109.4(4)
C(34)-N(5)-Mn(1)#4	123.5(4)
C(33)-N(5)-Mn(1)#4	120.7(4)

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

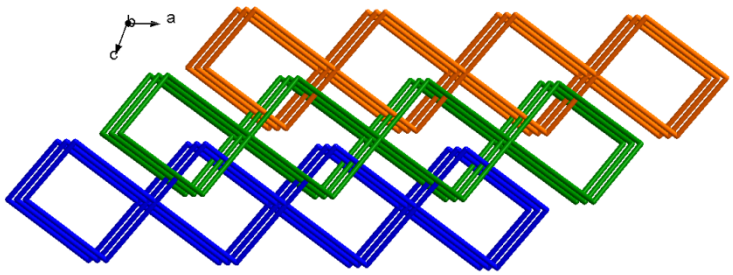
5. Fig. S1. Crystal structures of ligands L-MOM, 30% thermal ellipsoids.



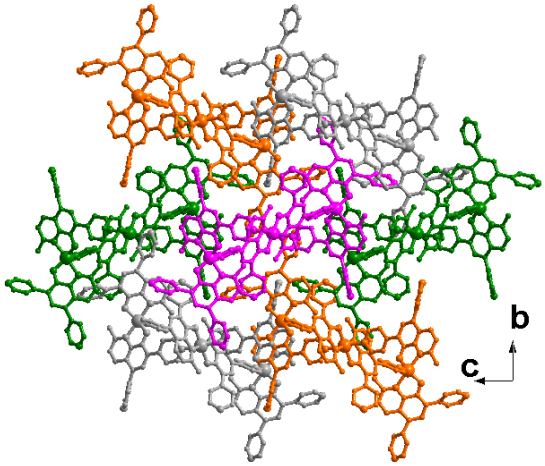
6.1. Fig. S2. View of a 1D infinite chain fabricated by cyclic tetramers Mn_4L_6 in complex **1** along *a* axis.



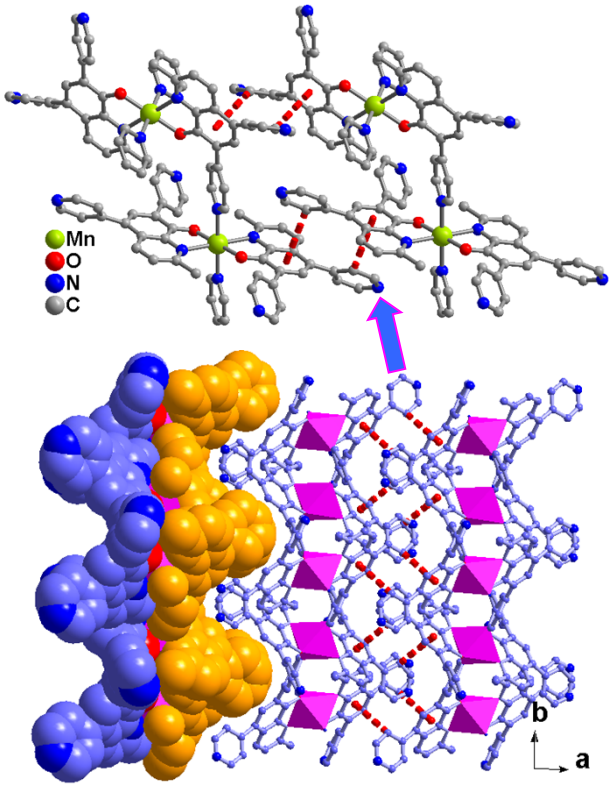
6.2. Fig. S3. Schematic representation of 3-fold interpenetrated architecture in **1**.



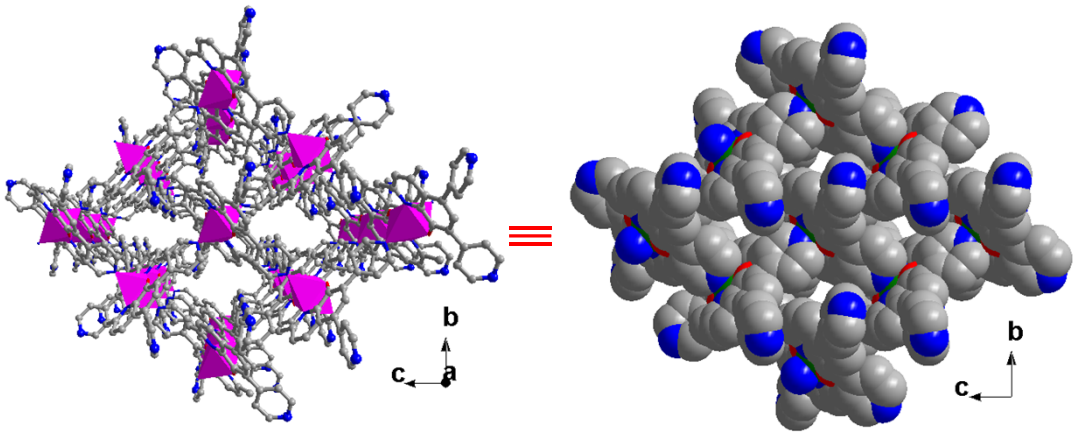
6.3. Fig. S4. View of the 3D architecture of complex **1**.



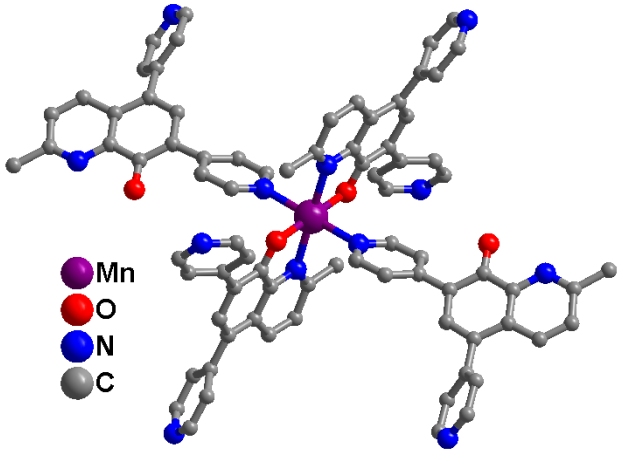
7.1. Fig. S5. 2D grids are further linked by the C–H···π (between C-H group of pyridine and phenolato ring of adjacent ligand) interactions along the *a* axis to form a 3D framework structure in **2**.



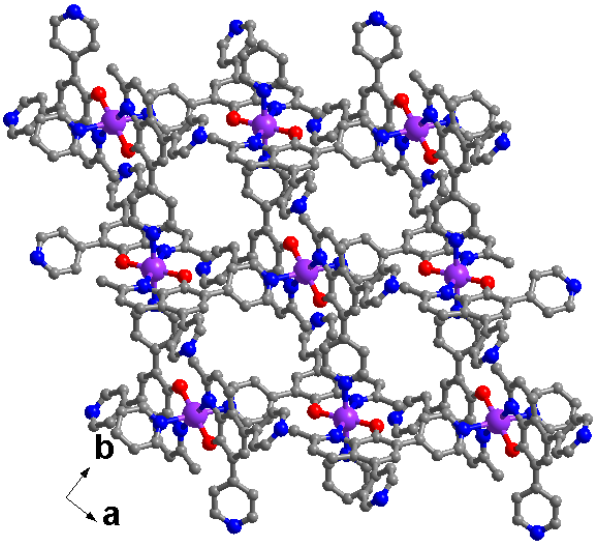
7.2. Fig. S6. View of 3D framework structure in **2**.



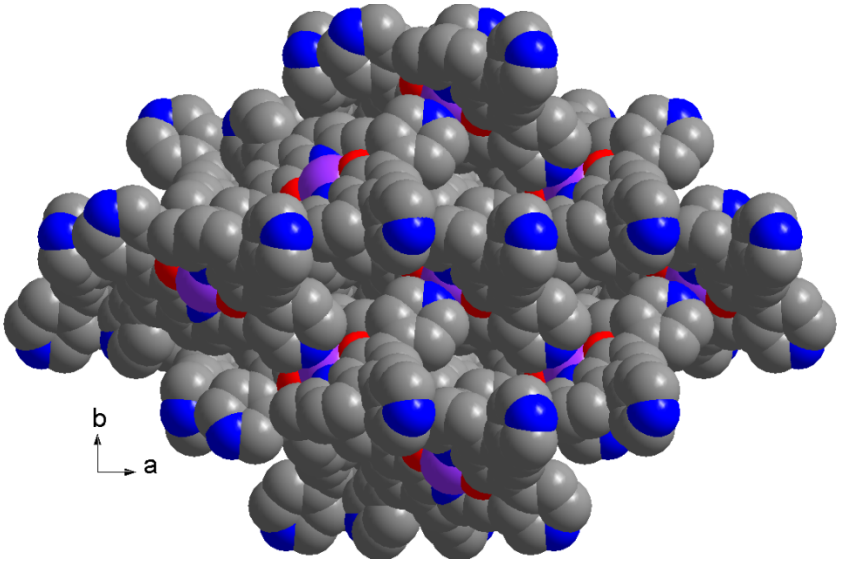
8.1. Fig. S7. Views of the coordination geometries of Mn(II) atoms in **3**.



8.2. Fig. S8. 2D rhombohedral grid structure of complex **3** in the *ab* plane



8.2. Fig. S9. Space-filling mode of 3D structure in **3**.



9. Fig. S10. Emission spectrum of the ligand L-MOM.