Supplementary Material (ESI) for Dalton Transactions

Electronic Supporting Information （ESI）

3D Mn^{II} Coordination Polymer with Alternating Azide/Azide/Formate/Formate bridged Chains: Synthesis, Structure, and Magnetic Properties

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Table S1. The selected bond lengths [Å] and angles [deg] for complex **1**.

Mn(1)-O(3)	2.123(5)	Mn(2)-O(4)#3	2.169(5)
Mn(1)-O(5)#1	2.146(5)	Mn(2)-O(6)	2.176(5)
Mn(1)-O(6)	2.156(5)	Mn(2)-O(6)#3	2.176(5)
Mn(1)-O(7)#2	2.159(5)	Mn(3)-O(8)#2	2.112(5)
Mn(1)-N(1)	2.225(6)	Mn(3)-O(8)#4	2.112(5)
Mn(1)-O(1)	2.250(5)	Mn(3)-O(1)#5	2.192(5)
Mn(2)-O(2)#3	2.133(6)	Mn(3)-O(1)	2.192(5)
Mn(2)-O(2)	2.133(6)	Mn(3)-N(1)	2.253(7)
Mn(2)-O(4)	2.169(5)	Mn(3)-N(1)#5	2.253(7)
O(3)-Mn(1)-O(5)#1	95.4(2)	O(2)-Mn(2)-O(6)	90.5(2)
O(3)-Mn(1)-O(6)	89.5(2)	O(4)-Mn(2)-O(6)	91.4(2)
O(5)#1-Mn(1)-O(6)	87.3(2)	O(4)#3-Mn(2)-O(6)	88.6(2)

O(3)-Mn(1)-O(7)#2	173.3(2)	O(2)#3-Mn(2)-O(6)#3	90.5(2)
O(5)#1-Mn(1)-O(7)#2	91.2(2)	O(2)-Mn(2)-O(6)#3	89.5(2)
O(6)-Mn(1)-O(7)#2	89.9(2)	O(4)-Mn(2)-O(6)#3	88.6(2)
O(3)-Mn(1)-N(1)	88.4(2)	O(4)#3-Mn(2)-O(6)#3	91.4(2)
O(5)#1-Mn(1)-N(1)	99.5(2)	O(6)-Mn(2)-O(6)#3	180.0(2)
O(6)-Mn(1)-N(1)	173.0(2)	O(8)#2-Mn(3)-O(8)#4	180.000(1)
O(7)#2-Mn(1)-N(1)	91.5(2)	O(8)#2-Mn(3)-O(1)#5	93.7(2)
O(3)-Mn(1)-O(1)	87.8(2)	O(8)#4-Mn(3)-O(1)#5	86.3(2)
O(5)#1-Mn(1)-O(1)	176.36(19)	O(8)#2-Mn(3)-O(1)	86.3(2)
O(6)-Mn(1)-O(1)	91.08(19)	O(8)#4-Mn(3)-O(1)	93.7(2)
O(7)#2-Mn(1)-O(1)	85.6(2)	O(1)#5-Mn(3)-O(1)	180.000(1)
N(1)-Mn(1)-O(1)	82.2(2)	O(8)#2-Mn(3)-N(1)	90.1(2)
O(2)#3-Mn(2)-O(2)	180.0(2)	O(8)#4-Mn(3)-N(1)	89.9(2)
O(2)#3-Mn(2)-O(4)	92.6(3)	O(1)#5-Mn(3)-N(1)	97.1(2)
O(2)-Mn(2)-O(4)	87.4(3)	O(1)-Mn(3)-N(1)	82.9(2)
O(2)#3-Mn(2)-O(4)#3	87.4(3)	O(8)#2-Mn(3)-N(1)#5	89.9(2)
O(2)-Mn(2)-O(4)#3	92.6(3)	O(8)#4-Mn(3)-N(1)#5	90.1(2)
O(4)-Mn(2)-O(4)#3	180.000(1)	O(1)#5-Mn(3)-N(1)#5	82.9(2)
O(2)#3-Mn(2)-O(6)	89.5(2)	O(1)-Mn(3)-N(1)#5	97.1(2)
N(1)-Mn(3)-N(1)#5	180.000(1)		

#1 -x+1,-y+1,-z+1 #2 -x,-y+1,-z #3 -x+1,-y+1,-z

#4 x+1,y+1,z+1 #5 -x+1,-y+2,-z+1

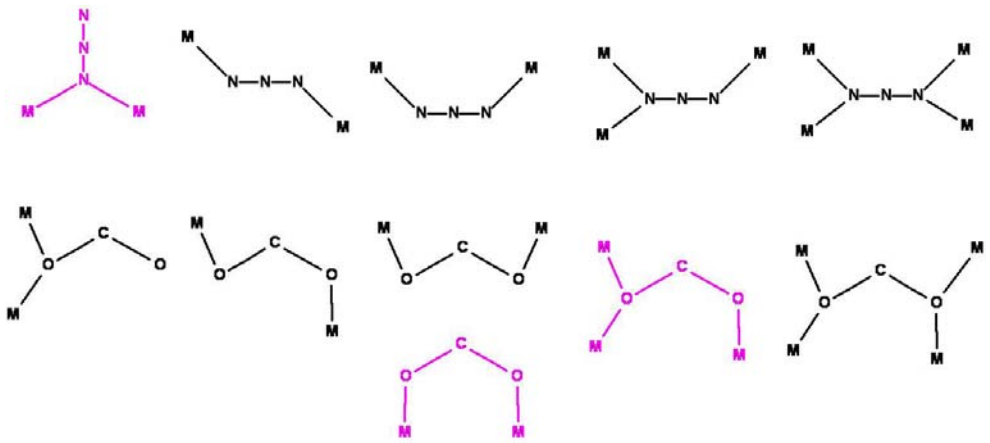


Chart 1. The frequent coordination modes of the ligands azide carboxylate (including formate). The modes in pink color were those presented in complex **1**.

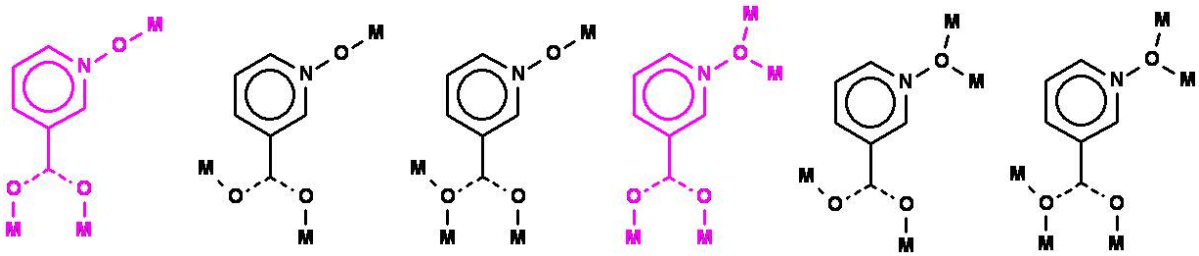


Chart 2. The frequent coordination modes of nicotinate N-oxide.

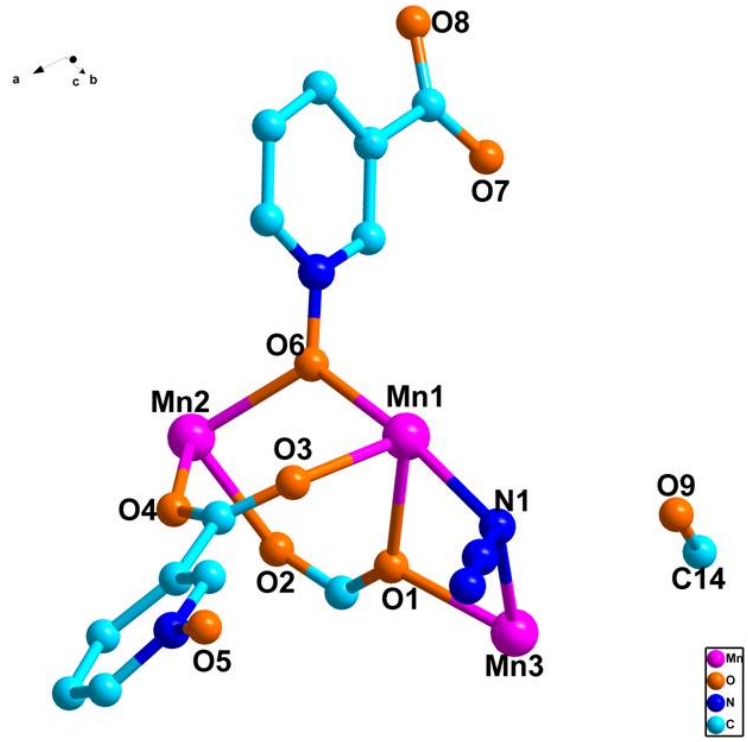


Figure S1. The asymmetry unit of complex **1**.

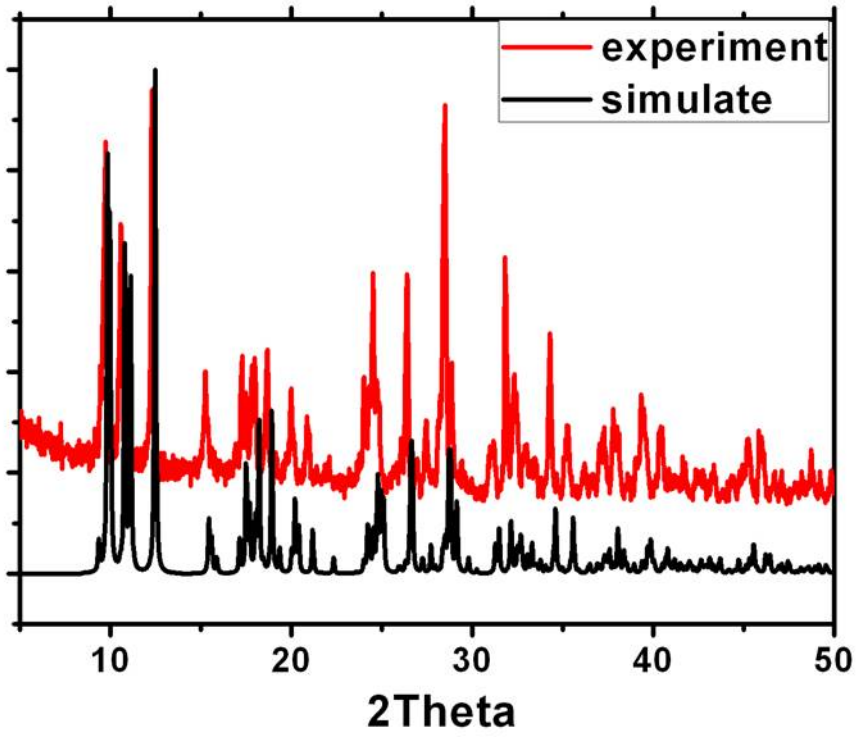


Figure S2. The XRPD diagram of complex **1**.

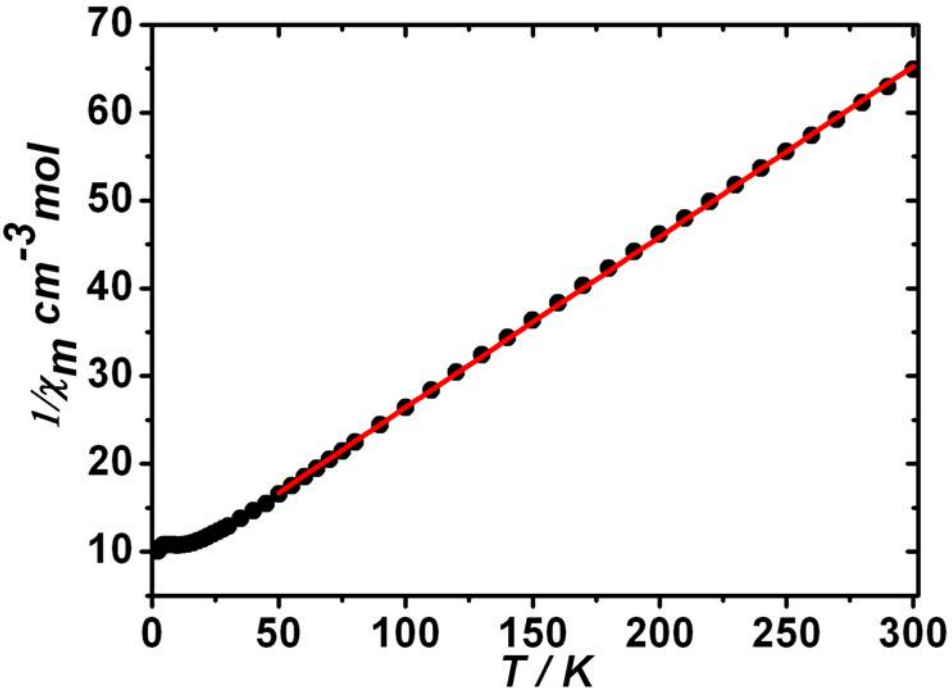


Figure S3. Curie plot for complex **1**. The solid line is the best fit to the Curie-Weiss law.

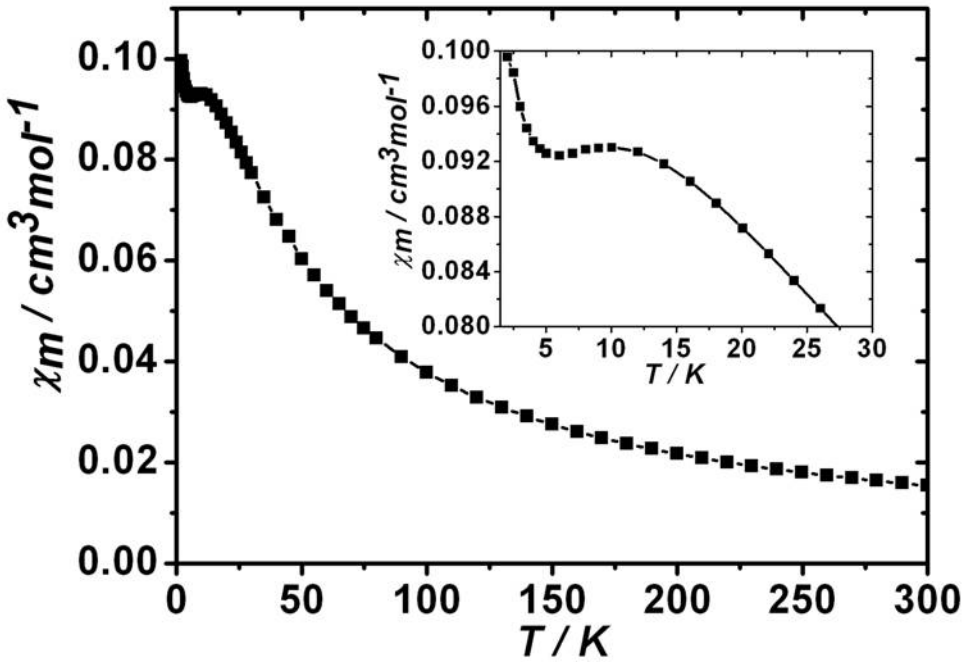
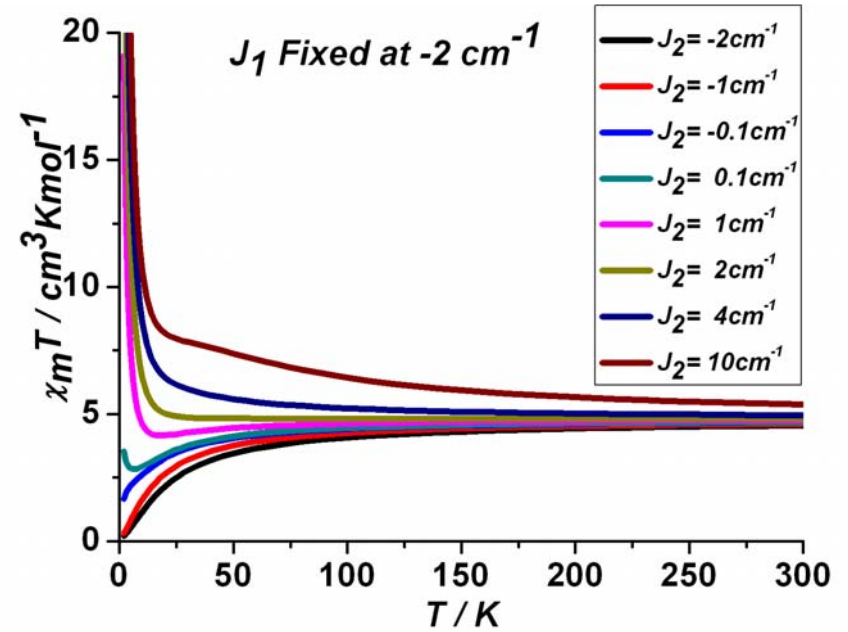
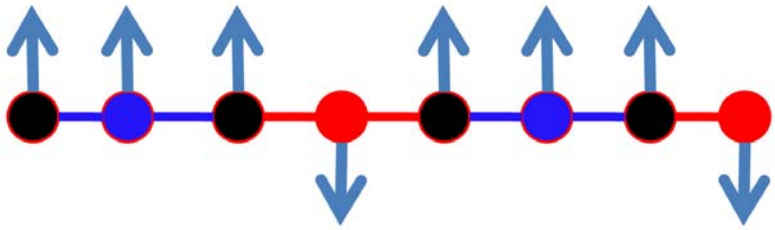


Figure S4. The χ_m *VS*. T plot for complex **1**.



(a)



(b)

Figure S5. (a) Simulation of the magnetic behavior of a $J_1/J_1/J_2/J_2$ 1D system for a set of the $J_2/|J_1|$ ratio between -1 and 5.0. A constant value of J_1 = -2 cm^{-1} has been assumed in the simulations. (b) Proposed schematic representation of the spin alignment in the $J_1/J_1/J_2/J_2$ 1D system for the J_1 and J_2 signing opposite.