Two Polynuclear Manganese(II) Complexes Based on multidentate N-heterocyclic aromatic ligand and V-shaped polycarboxylate ligand: Synthesis, Crystal Structure Analysis and Magnetic Properties

Huarui Wang *, Jianhua Qin

Henan Key Laboratory of Function-Oriented Porous Materials, College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang 471934, China; jh_q128105@126.com

* Correspondence: whr@lynu.edu.cn; Tel.: +86-379-6861-8321

Table S1. Selected bond lengths /Å and angles /°for **1**-**2**

Complex **1**			
Mn(1)-O(8)	2.127(4)	Mn(3)-O(7)	2.102(4)
Mn(1)-O(2)#1	2.143(4)	Mn(3)-O(1)	2.107(4)
Mn(1)-O(13)	2.196(4)	Mn(3)-N(14)#4	2.161(4)
Mn(1)-N(15)	2.281(4)	Mn(3)-N(19)	2.184(4)
Mn(1)-N(18)	2.316(4)	Mn(3)-N(13)#4	2.431(4)
Mn(1)-N(17)	2.354(4)	Mn(3)-N(21)	2.483(5)
Mn(2)-O(11)#2	2.081(4)	Mn(4)-O(12)	2.088(4)
Mn(2)-O(6)#3	2.123(4)	Mn(4)-O(5)#3	2.131(4)
Mn(2)-O(14)	2.258(4)	Mn(4)-N(8)#5	2.189(4)
Mn(2)-N(4)	2.273(5)	Mn(4)-N(3)	2.196(4)
Mn(2)-N(7)	2.284(4)	Mn(4)-N(10)#5	2.373(5)
Mn(2)-N(6)	2.315(4)	Mn(4)-N(2)	2.469(5)
O(8)-Mn(1)-O(2)#1	89.29(16)	O(7)-Mn(3)-O(1)	91.99(16)
O(8)-Mn(1)-O(13)	166.96(16)	O(7)-Mn(3)-N(14)#4	103.58(16)
O(2)#1-Mn(1)-O(13)	84.96(15)	O(1)-Mn(3)-N(14)#4	88.14(16)
O(8)-Mn(1)-N(15)	93.66(16)	O(7)-Mn(3)-N(19)	87.66(16)
Complex **2**			
Mn(1)-O(7)#1	2.048(4)	Mn(2)-O(9)	2.198(4)
Mn(1)-O(6)#2	2.079(4)	Mn(2)-N(7)	2.233(4)
Mn(1)-O(4)	2.114(4)	Mn(2)-N(4)	2.248(4)
Mn(1)-N(8)	2.158(4)	Mn(2)-N(6)	2.305(4)
Mn(1)-N(10)	2.423(5)	Mn(3)-O(1)#3	2.147(4)
Mn(2)-O(3)	2.060(4)	Mn(3)-N(3)	2.182(4)
Mn(2)-O(8)	2.185(4)	Mn(3)-O(1)	2.260(4)
Mn(3)-Br(1)	2.4963(13)	Mn(3)-N(1)	2.356(5)
O(7)#1-Mn(1)-O(6)#2	125.1(2)	Mn(3)-O(2)	2.435(4)
O(7)#1-Mn(1)-O(4)	96.30(19)	N(3)-Mn(3)-O(1)	108.64(16)
O(6)#2-Mn(1)-O(4)	93.90(19)	N(3)-Mn(3)-N(1)	72.23(16)
O(7)#1-Mn(1)-N(8)	109.42(18)	O(1)-Mn(3)-N(1)	164.41(16)
O(6)#2-Mn(1)-N(8)	121.27(18)	O(1)-Mn(3)-O(2)	54.79(14)
O(4)-Mn(1)-N(8)	100.70(16)	O(1)#3-Mn(3)-Br(1)	110.80(12)
O(4)-Mn(1)-N(10)	170.38(16)	N(3)-Mn(3)-Br(1)	142.45(12)
N(8)-Mn(1)-N(10)	70.66(15)	O(1)-Mn(3)-Br(1)	98.55(11)
O(3)-Mn(2)-O(8)	84.04(16)	Mn(3)#3-O(1)-Mn(3)	104.88(15)
O(3)-Mn(2)-O(9)	93.25(16)	N(7)-N(8)-Mn(1)	132.9(3)
O(8)-Mn(2)-O(9)	176.43(15)	N(8)-N(7)-Mn(2)	134.4(3)

Symmetry transformations used to generate equivalent atoms in (**1**): #1 -x+1, y-1/2, -z+3/2; #2 -x+2, y+1/2, -z+3/2; #3 x+1, y, z; #4 -x+1, y+1/2, -z+3/2; #5 -x+2,y-1/2,-z+3/2.; (**2**): #1 x,y+1,z #2 -x+2,-y,-z+1 #3 -x+1,-y,-z.

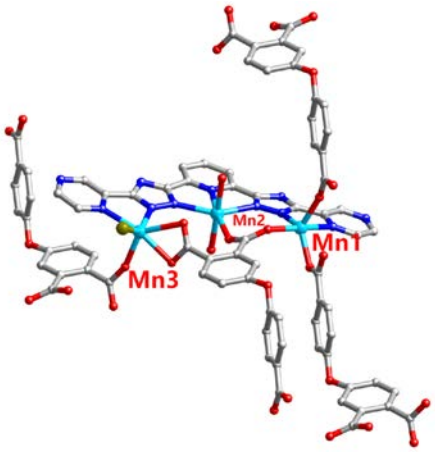

Figure S1. The 4-connected network and tri-nucleated Mn(II) cluster of complex **2**.

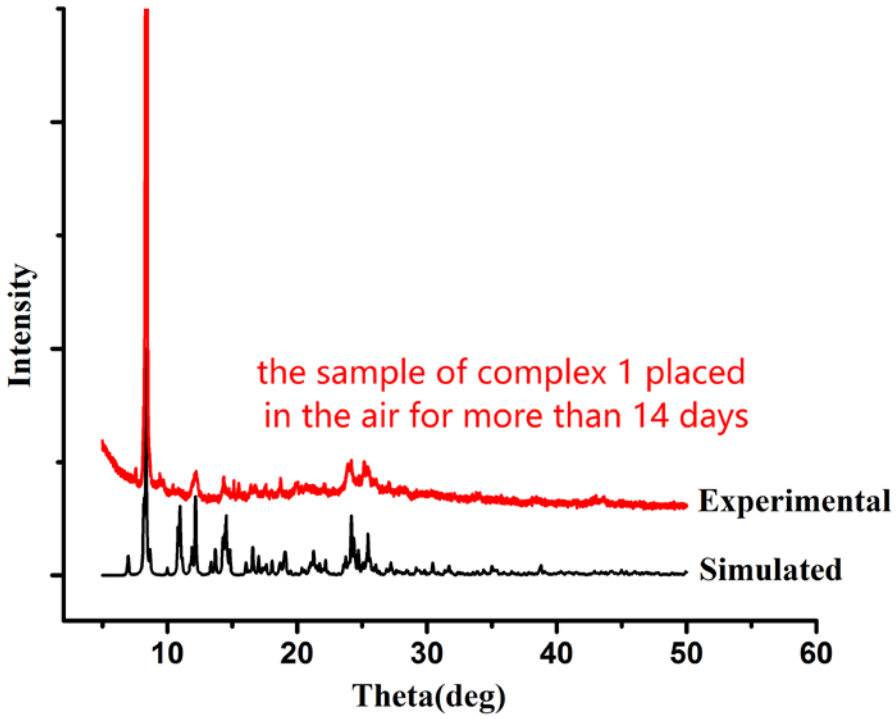

Figure S2. Simulated and experimental PXRD pattern of **1** placed in the air for more than 14 days.