Structural diversity and magnetic properties of six ferrocenyl monocarboxylate Mn(II), Ni(II) and Co(II) complexes with 1D aqua, carboxyl or dinuclear hydroxyl bridge

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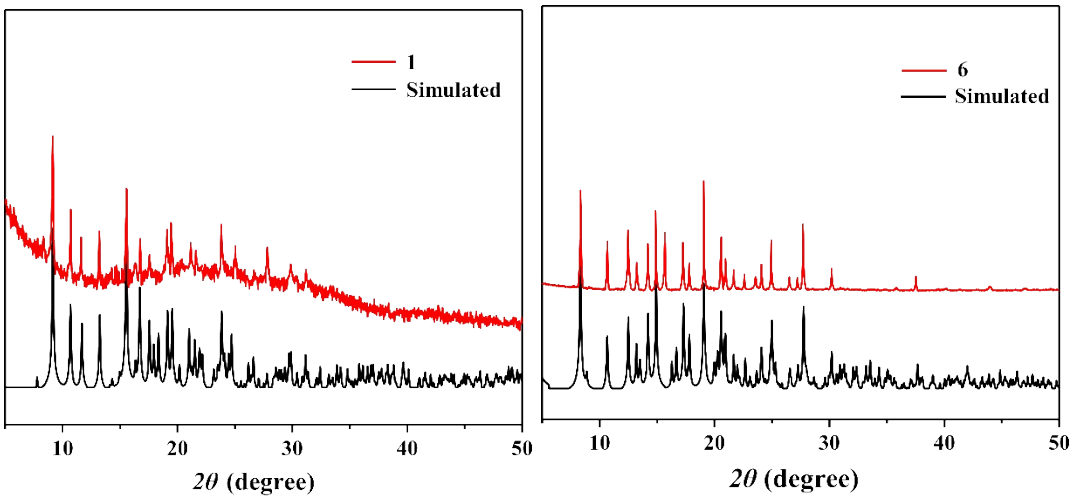

Figure S1. (a) Simulated PXRD pattern from the single crystal structure of **1** (black), observed PXRD pattern of **1** at room temperature (red). (b) Simulated PXRD pattern from the single crystal of **6** (black), observed PXRD pattern of **6** at room temperature (red).

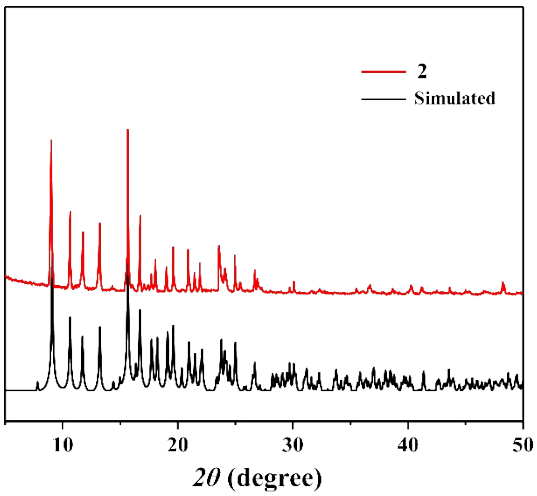

Figure S2. (a) Simulated PXRD pattern from the single crystal structure of **2** (black), observed PXRD pattern of **2** at room temperature (red).

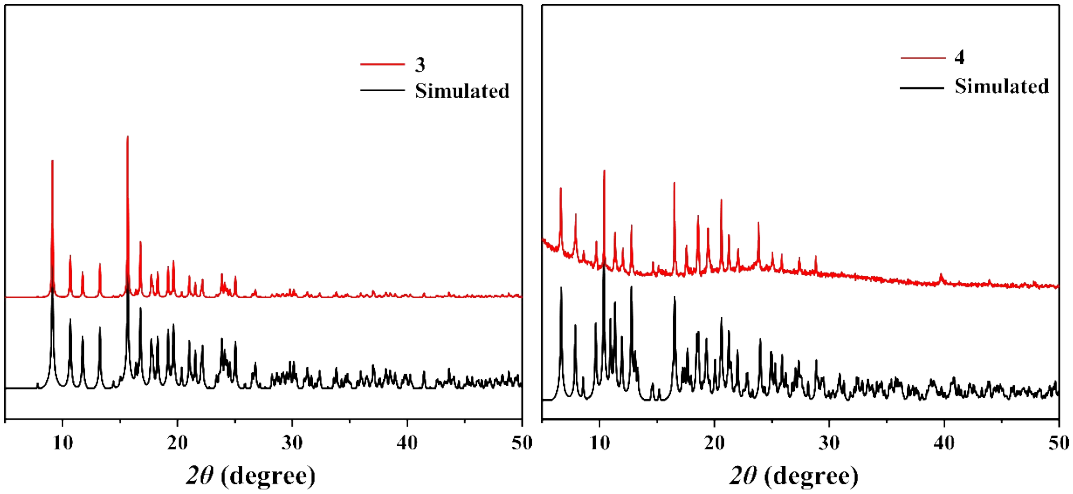

Figure S3. (a) Simulated PXRD pattern from the single crystal structure of **3** (black), observed PXRD pattern of **3** at room temperature (red). (b) Simulated PXRD pattern from the single crystal of **4** (black), observed PXRD pattern of **4** at room temperature (red).

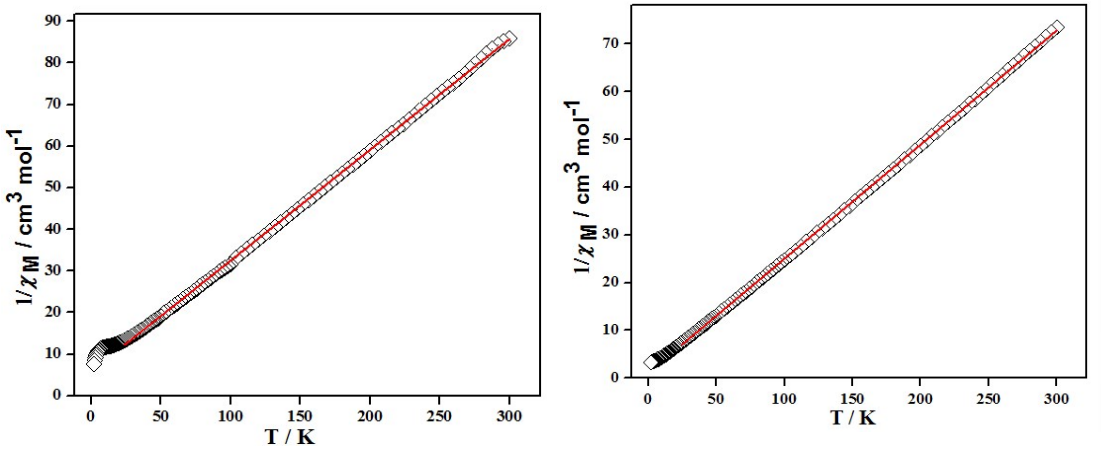

Figure S4. (a) Plot of χ_M^{-1} *vs* T for **1.** (b) Plot of χ_M^{-1} *vs* T for **6.**

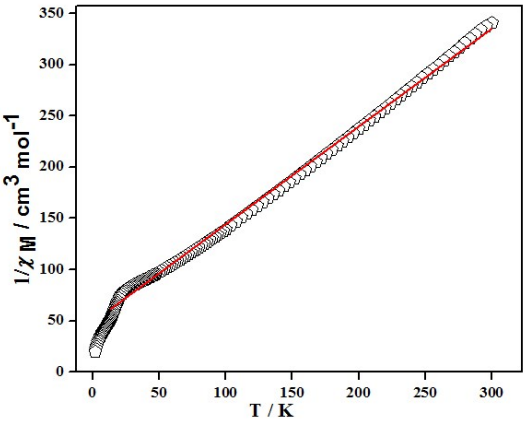

Figure S5. Plot of χ_M^{-1} *vs* T for **2.**

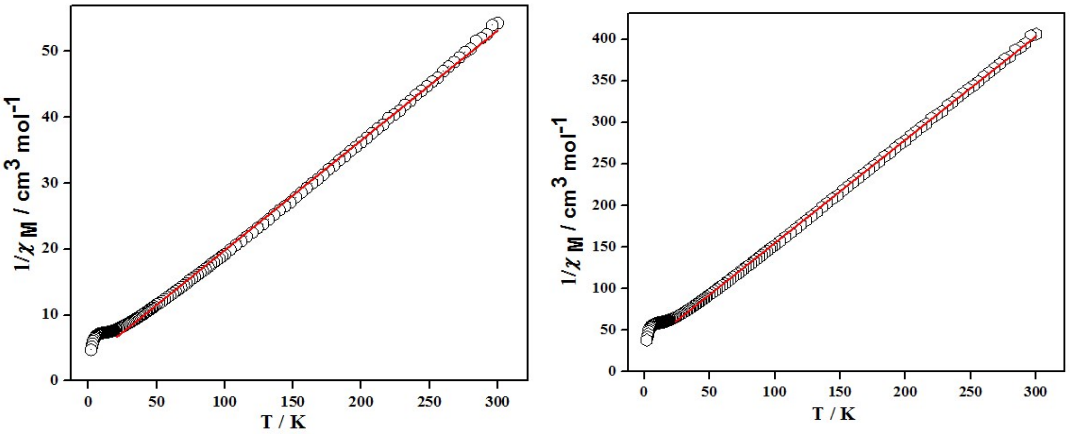

Figure S6. (a) Plot of χ_M^{-1} *vs* T for **3**. (b) Plot of χ_M^{-1} *vs* T for **4.**

Table S1. Selected bond lengths (Å) and angles (°) for **1**-**6.**

Complex **1**					
Mn(1)-O(3)	2.123(3)	Mn(1)-O(1)	2.269(3)	O(3)-Mn(1)-O(3)#1	180.0
Mn(1)-O(2)	2.148(4)	Co(2)-N(4)	2.035(3)	O(3)-Mn(1)-O(2)#1	88.7(17)
O(3)-Mn(1)-O(2)	91.32(17)	O(3)-Mn(1)-O(1)#1	90.17(13)	O(2)-Mn(1)-O(1)	93.14(16)
O(3)#1-Mn(1)-O(2)	180.0	O(3)#1-Mn(1)-O(1)#1	89.93(13)	O(1)#1-Mn(1)-O(1)	180.0
Mn(1)#2-O(1)-Mn(1)	128.0(3)				
Complex **2**					
Ni(1)-O(1)	2.055c(3)	Ni(1)-O(4)	2.075(3)	Ni(1)-O(3)	2.22(17)
O(1)-Ni(1)-O(1)#1	180.0	O(1)-Ni(1)-O(4)#1	89.22(14)	O(1)-Ni(1)-O(4)	90.78(14)
O(4)#1-Ni(1)-O(4)	180.0	O(1)-Ni(1)-O(3)#1	88.20(10)	O(1)-Ni(1)-O(3)	91.80(10)
O(4)-Ni(1)-O(3)	93.02(12)	Ni(1)-O(3)-Ni(1)#2	130.6(2)		
Complex **3**					
Co(1)-O(2)	2.048(4)	Co(1)-O(3)	2.212(2)	O(2)#1-Co(1)-O(2)	180.0
Co(1)-O(4)	2.089(4)	O(2)#1-Co(1)-O(4)	89.11 (18)	O(2)-Co(1)-O(4)	90.90(18)
O(4)-Co(1)-O(4)#1	180.0	O(2)#1-Co(1)-O(3)	91.75(14)	O(2)-Co(1)-O(3)	88.25()
O(4)-Co(1)-O(3)	86.55(16)	O(4)#1-Co(1)-O(3)	93.45(16)	O(3)-Co(1)-O(3)#1	180.0
Co(1)#2-O(3)-Co(1)	1301.0(3)				
Complex **4**					
Co(1)-O(5)	1.996(3)	Co(1)-O(5)#1	2.105(3)	Co(1)-N(4)#1	2.134(4)
Co(1)-N(1)	2.141(4)	Co(1)-O(1)	2.177(3)	Co(1)-O(2)	2.197(3)
O(5)-Co(1)-O(5)#1	79.64(13)	O(5)-Co(1)-N(4)#1	106.8(14)	O(5)#1-Co(1)-N(4)#1	84.11(14)
O(5)-Co(1)-O(1)	96.02(12)	O(5)#1-Co(1)-N(1)	167.85(1)	N(4)#1-Co(1)-N(1)	95.50(15)
O(5)#1-Co(1)-O(1)	94.93(12)	N(4)#1-Co(1)-O(1)	156.5(14)	N(1)-Co(1)-O(1)	90.22(14)
O(5)-Co(1)-O(2)	154.8(12)	O(5)#1-Co(1)-O(2)	93.32(12)	N(4)#1-Co(1)-O(2)	96.37(14)
N(1)-Co(1)-O(2)	98.78(14)	O(1)-Co(1)-O(2)	60.23(12)	Co(1)-O(5)-Co(1)#1	100.36(13)
Complex **5**					
N(1)-Ni(1)	2.072(3)	N(4)-Ni(1)#1	2.077(3)	Ni(1)-O(3)	2.099(2)
Ni(1)-O(3)#1	2.036(2)	Ni(1)-O(2)	2.120(2)	Ni(1)-O(1)	2.127(3)
N(5)-N(4)-Ni(1)#1	117.5 (2)	O(3)-Ni(1)-O(3)#1	80.7(9)	O(3)-Ni(1)-N(1)	88.91(10)
O(3)#1-Ni(1)-N(1)	169.01(10)	O(3)-Ni(1)-N(4)#1	100.69(1)	O(3)#1-Ni(1)-N(4)#1	85. 29(10)
N(1)-Ni(1)-N(4)#1	93.39(12)	O(3)-Ni(1)-O(2)	159.3(10)	O(3)#1-Ni(1)-O(2)	95.16(9)
N(1)-Ni(1)-O(2)	95.74(10)	N(4)#1-Ni(1)-O(2)	99.06(11)	O(3)-Ni(1)-O(1)	97.94(10)
O(3)#1-Ni(1)-O(1)	92.23(9)	N(1)-Ni(1)-O(1)	91.64(11)	N(4)#1-Ni(1)-O(1)	160.5(10)
O(2)-Ni(1)-O(1)	61.85(10)	Ni(1)-O(3)-Ni(1)#1	99.64(9)		
Complex **6**					
Mn(1)-O(1)	2.120(4)	Mn(1)-O(2)#2	2.204(4)	Mn(1)-N(1)	2.292(8)
O(2)-Mn(1)#3	2.204(4)	O(1)#1-Mn(1)-O(1)	92.0(2)	O(1)#1-Mn(1)-O(2)#2	104.31(17)
O(1)-Mn(1)-O(2)#2	88.20 (16)	O(2)#2-Mn(1)-O(2)#3	162.1(3)	O(1)#1-Mn(1)-N(1)	97.2(3)
O(1)-Mn(1)-N(1)	170.1(3)	O(2)#2-Mn(1)-N(1)	86.2(2)	O(2)#3-Mn(1)-N(1)	79.5(2)
O(1)#1-Mn(1)-N(1)#1	170.1(12)	N(1)-Mn(1)-N(1)#1	73.8(6)		

Symmetry transformations used to generate equivalent atoms:

For **1**: #1 -x,-y+1,-z+1; #2 -x,y,-z+3/2.

For **2**: #1 -x+2,-y+1,-z; #2 -x+2,y,-z-1/2.

For **3**: #1 -x,-y+1,-z+2; #2 -x,y,-z+3/2.

For **4**: #1 -x+1,-y+1,-z.

For **5**: #1 -x,-y,-z+1.

For **6**: #1 -x,y,-z+1/2; #2 x,-y+2,z-1/2; #3 -x,-y+2,-z+1.