

Construction of Fe₆, Fe₈ and Mn₈ Metallamacrocyclic Complexes and Magnetic Properties

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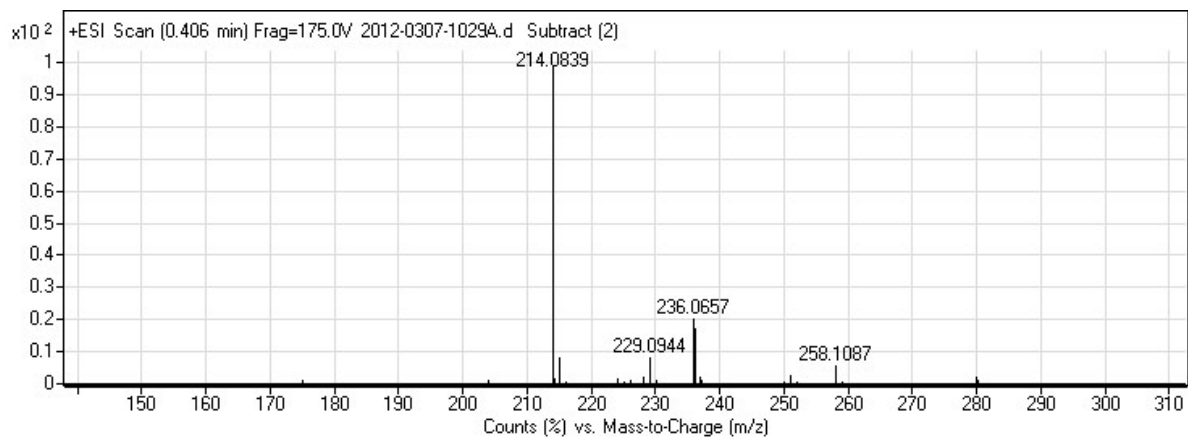
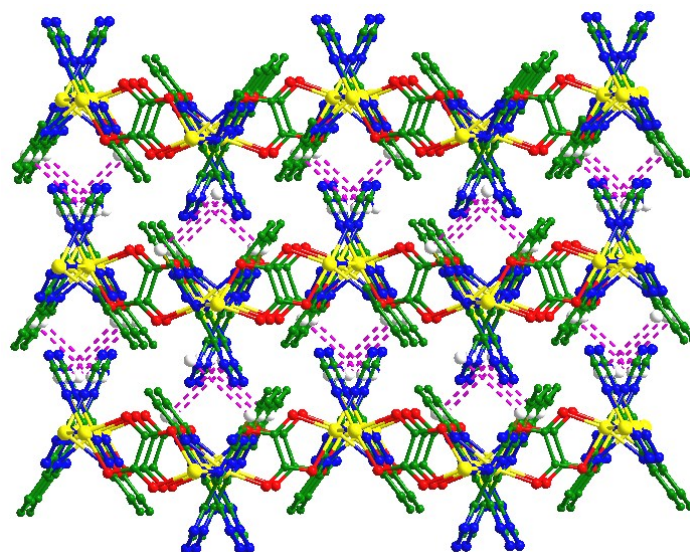
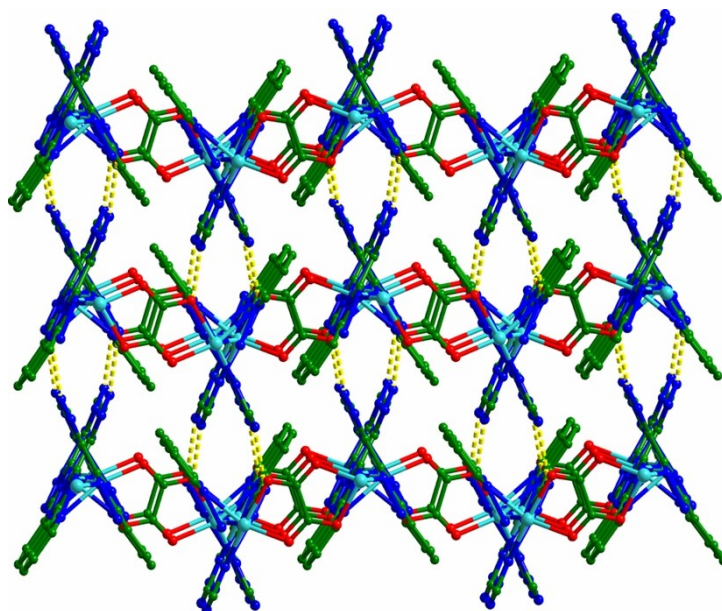


Figure S1: The MS spectra of H₂L.



a



b

Figure S2. The three-dimensional supermolecular structure formed by $\pi \cdots \pi$ (a) and hydrogen-bonding interactions (b).

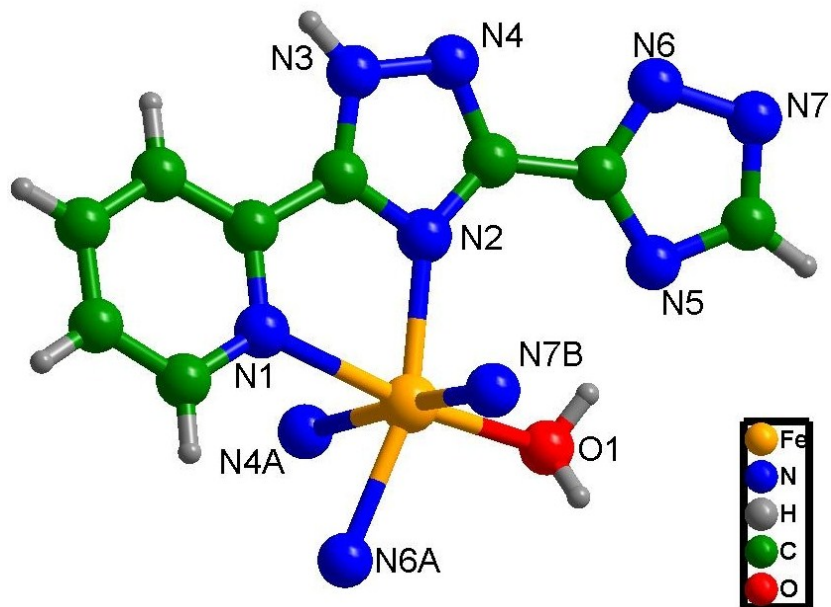
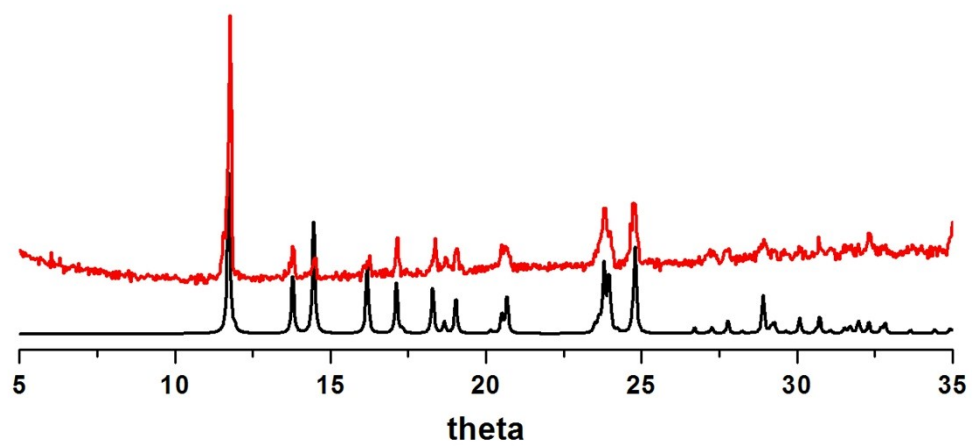
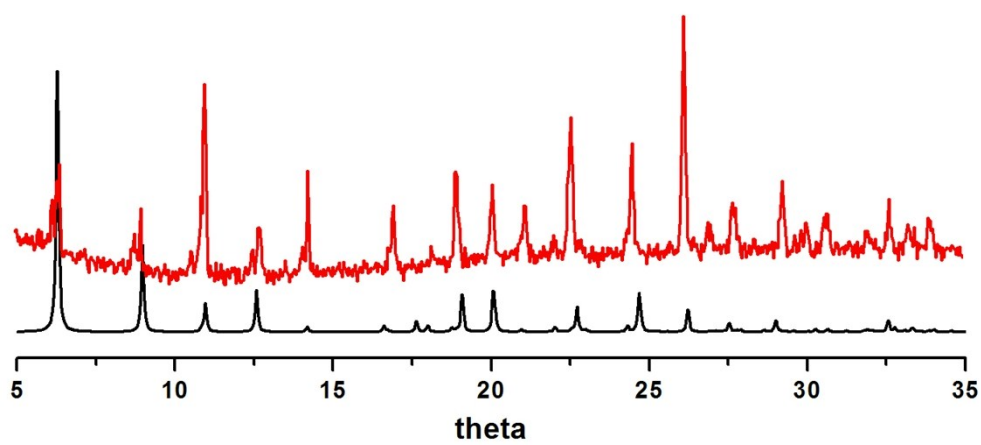


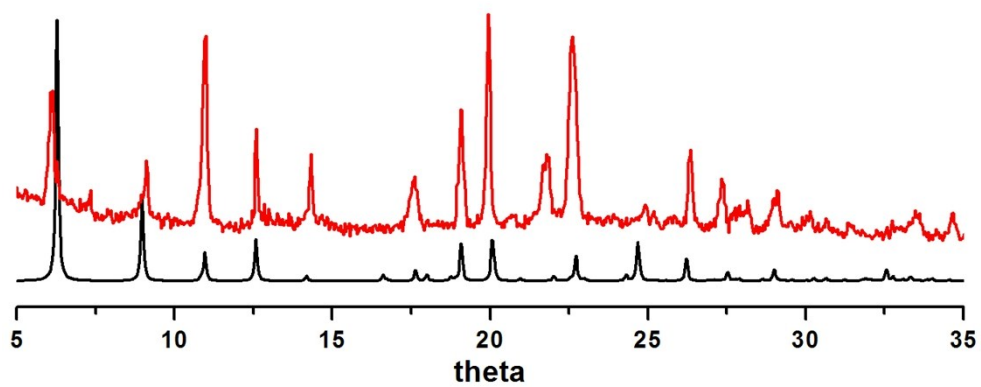
Figure S3: The coordination environment of Fe^{2+} in polymer 2.



1



2



3

Figure S4. The PXR D patterns of polymers 1-3.

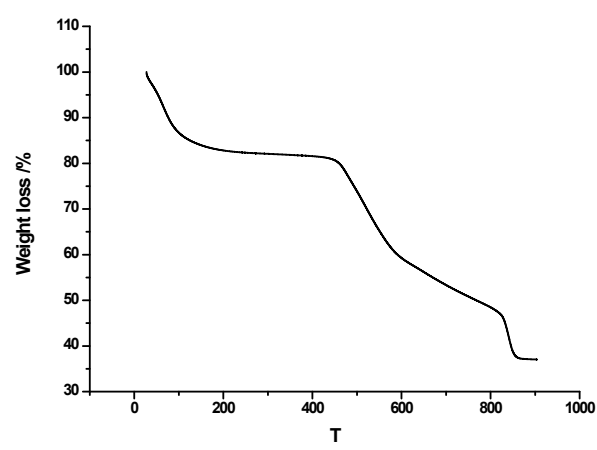
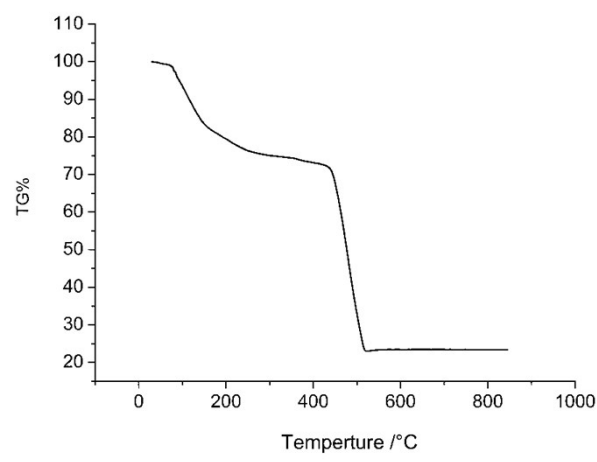
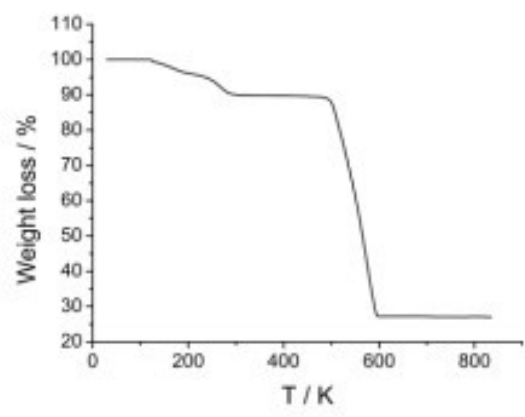


Figure S5. The TG curves of complexes 1-3.

Table S1. Selected bond lengths /Å and angles /° for **1-3**

Complex 1			
Fe(1)-O(2)#1	2.092(2)	Fe(1)-N(3)#2	2.149(3)
Fe(1)-N(2)	2.173(3)	Fe(1)-O(1)	2.189(2)
Fe(1)-N(5)#2	2.195(3)	Fe(1)-N(1)	2.239(3)
O(2)#1-Fe(1)-N(3)#2	95.44(10)	O(2)#1-Fe(1)-N(2)	102.36(10)
N(3)#2-Fe(1)-N(2)	162.09(10)	O(2)#1-Fe(1)-O(1)	77.36(9)
N(3)#2-Fe(1)-O(1)	92.79(10)	N(2)-Fe(1)-O(1)	89.18(10)
O(2)#1-Fe(1)-N(5)#2	100.83(9)	N(3)#2-Fe(1)-N(5)#2	76.06(10)
N(2)-Fe(1)-N(5)#2	102.22(10)	O(1)-Fe(1)-N(5)#2	168.55(10)
O(2)#1-Fe(1)-N(1)	160.88(9)	N(3)#2-Fe(1)-N(1)	86.66(10)
N(2)-Fe(1)-N(1)	75.87(9)	O(1)-Fe(1)-N(1)	83.57(9)
Complex 2			
O(1)-Fe(1)-N(7)#1	93.12(14)	Fe(1)-N(6)#2	2.171(3)
O(1)-Fe(1)-N(2)	96.33(11)	Fe(1)-N(4)#2	2.204(3)
N(7)#1-Fe(1)-N(2)	91.11(12)	Fe(1)-N(1)	2.285(3)
O(1)-Fe(1)-N(6)#2	98.58(12)	N(2)-Fe(1)-N(4)#2	94.84(12)
N(7)#1-Fe(1)-N(6)#2	96.15(11)	N(6)#2-Fe(1)-N(4)#2	76.37(11)
N(2)-Fe(1)-N(6)#2	163.01(12)	O(1)-Fe(1)-N(1)	170.93(12)
O(1)-Fe(1)-N(4)#2	92.87(13)	N(7)#1-Fe(1)-N(1)	90.13(14)
N(7)#1-Fe(1)-N(4)#2	171.05(12)	N(2)-Fe(1)-N(1)	75.12(11)
O(1)-Fe(1)-N(7)#1	93.12(14)	N(6)#2-Fe(1)-N(1)	89.48(12)
O(1)-Fe(1)-N(2)	96.33(11)	N(4)#2-Fe(1)-N(1)	84.94(13)
N(7)#1-Fe(1)-N(2)	91.11(12)		
Complex 3			
O(1)-Mn(1)-N(6)#1	92.85(15)	Mn(1)-N(6)#1	2.212(4)
O(1)-Mn(1)-N(4)#2	95.77(14)	Mn(1)-N(5)	2.241(4)
N(6)#1-Mn(1)-N(4)#2	91.42(15)	Mn(1)-N(2)	2.311(4)
O(1)-Mn(1)-N(5)	95.70(14)	N(4)#2-Mn(1)-N(1)#2	74.28(15)
N(6)#1-Mn(1)-N(5)	97.28(14)	N(5)-Mn(1)-N(1)#2	93.44(15)
N(4)#2-Mn(1)-N(5)	165.22(14)	O(1)-Mn(1)-N(2)	92.80(15)
O(1)-Mn(1)-N(1)#2	169.08(15)	N(6)#1-Mn(1)-N(2)	169.70(15)
N(6)#1-Mn(1)-N(1)#2	91.91(16)	N(4)#2-Mn(1)-N(2)	96.58(15)
O(1)-Mn(1)-N(6)#1	92.85(15)	N(5)-Mn(1)-N(2)	73.59(14)
O(1)-Mn(1)-N(4)#2	95.77(14)	N(1)#2-Mn(1)-N(2)	84.06(16)
N(6)#1-Mn(1)-N(4)#2	91.42(15)		

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