Supporting Information

# Cyanide-Bridged Mn(III)-Fe(III) Bimetallic Complexes Based on the Pentacyano(1-methylimidazole)ferrate(III) Building Block: Structure and Magnetic Characterizations

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**Table S1.** Selected Bond Distances (Å) and Angles (deg) of Complex **3**.

| | | | |
|---|---|---|---|
| Fe(1)-C(1) | 1.946(6) | Fe(1)-C(2) | 1.920(6) |
| Fe(1)-C(3) | 1.921(7) | Fe(1)-C(4) | 1.944(6) |
| Fe(1)-C(5) | 1.945(7) | Fe(1)-N(6) | 2.010(6) |
| Fe(2)-C(43) | 1.921(7) | Fe(2)-C(44) | 1.937(6) |
| Fe(2)-C(45) | 1.969(6) | Fe(2)-C(46) | 1.956(6) |
| Fe(2)-C(47) | 1.947(6) | Fe(2)-N(16) | 1.990(5) |
| Mn(1)-N(1) | 2.221(5) | Mn(1)-O(1W) | 2.246(4) |
| Mn(1)-O(1) | 1.908(4) | Mn(1)-N(8) | 2.098(5) |
| Mn(1)-O(2) | 1.907(4) | Mn(1)-N(9) | 2.042(5) |
| Mn(2)-N(2) | 2.249(5) | Mn(2)-O(2W) | 2.233(4) |
| Mn(2)-O(3) | 1.883(4) | Mn(2)-N(10) | 2.051(5) |
| Mn(2)-O(4) | 1.918(4) | Mn(2)-N(11) | 2.059(5) |
| Mn(3)-N(13) | 2.229(5) | Mn(3)-O(3W) | 2.234(4) |
| Mn(3)-O(5) | 1.907(4) | Mn(3)-N(18) | 2.049(5) |
| Mn(3)-O(6) | 1.907(4) | Mn(3)-N(19) | 2.070(5) |
| Mn(4)-N(12) | 2.298(5) | Mn(4)-O(4W) | 2.222(4) |
| Mn(4)-O(7) | 1.875(4) | Mn(4)-N(20) | 2.029(5) |
| Mn(4)-O(8) | 1.892(4) | Mn(4)-N(21) | 2.050(5) |
| | | | |
| Mn(1)-N(1)-C(1) | 165.2(6) | N(1)-C(1)-Fe(1) | 176.8(6) |
| Mn(2)-N(2)-C(2) | 156.9(5) | N(2)-C(2)-Fe(1) | 174.8(6) |
| Mn(3)-N(13)-C(46) | 152.8(5) | N(13)-C(46)-Fe(2) | 174.5(6) |
| Mn(4)-N(12)-C(44) | 147.8(5) | N(12)-C(44)-Fe(2) | 177.1(6) |

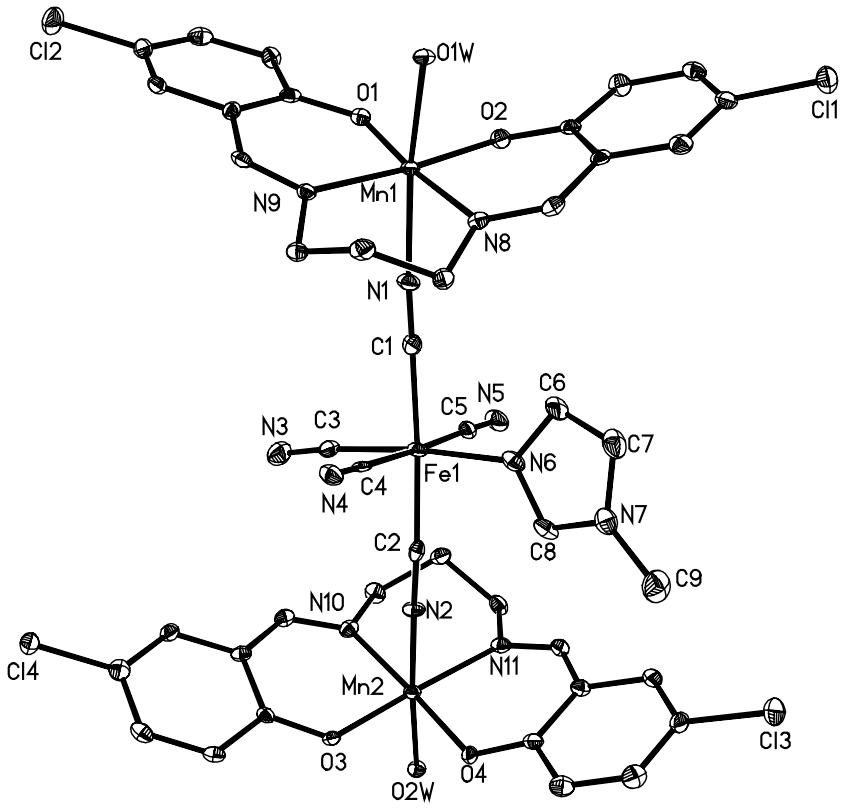



**Figure S1.** One of the two independent *trans*-trinuclear units in complex **3** with atom labeling scheme showing 30% probability thermal ellipsoids (hydrogen atoms are omitted for clarity).

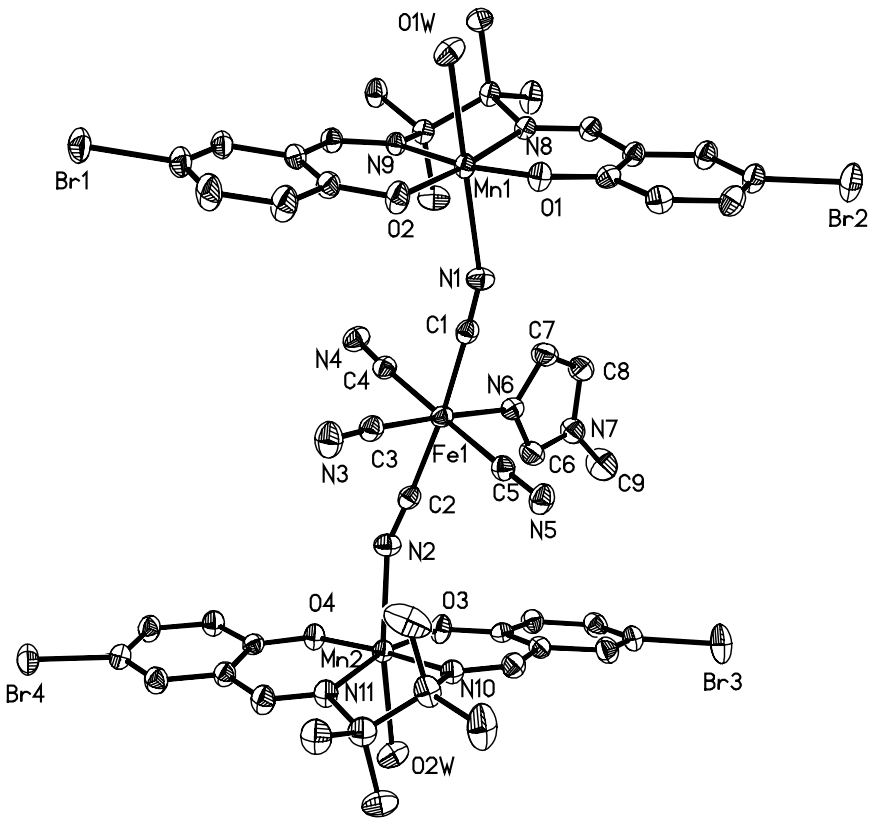



**Figure S2.** Trinuclear structure of complex **5** with atom labeling scheme showing 30% probability thermal ellipsoids (hydrogen atoms and crystallized methanol molecules are omitted for clarity).

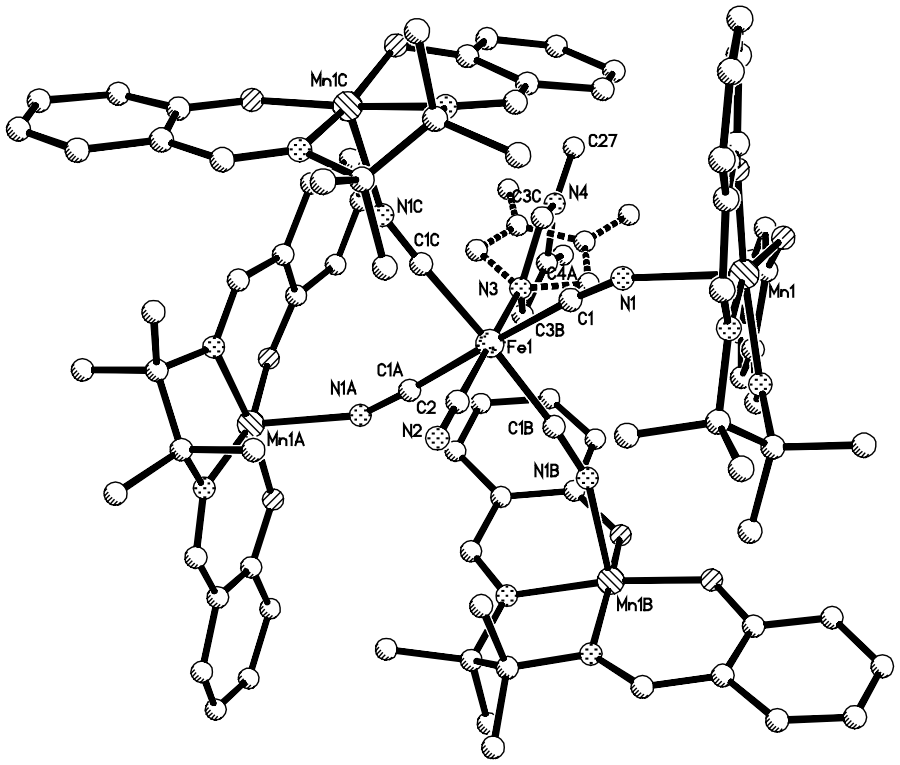



**Figure S3.** Structure of complex **7** (hydrogen atoms, perchlorate ions and water molecules are omitted for clarity). Dashed lines represent the disordered 1-methylimidazole groups. Selected bond distances (Å) and angles (deg): Fe(1)-C(1) 1.936(8); Fe(1)-C(2) 1.935(14); Fe(1)-N(3) 1.961(13); Mn(1)-N(1) 2.197(8); Mn(1)-O(1) 1.871(5); Mn(1)-O(2) 1.863(6); Mn(1)-N(5) 1.984(8); Mn(1)-N(6) 1.969(7); Fe(1)-C(1)-N(1) 176.0(7); C(1)-N(1)-Mn(1) 157.3(7).

Eq. 1:

$$\chi_t = \frac{Ng^2\beta^2}{kT}[\frac{A}{B}] \qquad (1)$$

in which A = 165 + 84exp(-9$J$/$kT$) + 84exp(-$J$/$kT$) + 35exp(-8$J$/$kT$) + 35exp(-2$J$/$kT$) + 10exp(-7$J$/$kT$) + 10exp(-3$J$/$kT$) + exp(-6$J$/$kT$) + exp(-4$J$/$kT$) and B = 20 + 16exp(-9$J$/$kT$) + 16exp(-$J$/$kT$) + 12exp(-8$J$/$kT$) + 12exp(-2$J$/$kT$) + 8exp(-7$J$/$kT$) + 8exp(-3$J$/$kT$) + 4exp(-6$J$/$kT$) + 4exp(-4$J$/$kT$).

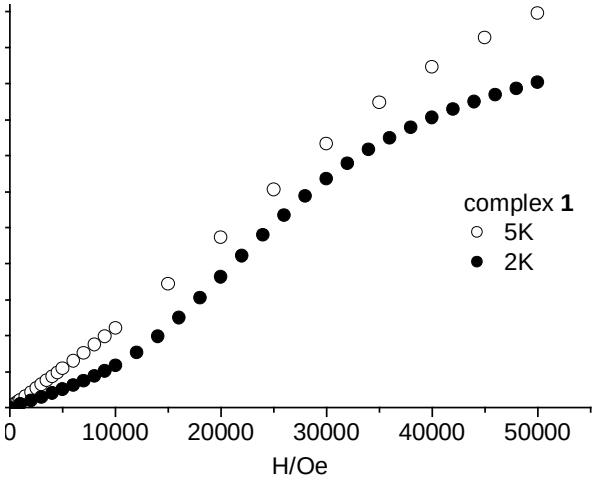
Eq. 2:

$$\chi_m = \frac{\chi_t}{1-\chi_t(2zJ'/Ng^2\beta^2)} \qquad (2)$$

Eq. 3:

$$\chi_m = \frac{Ng^2\beta^2}{kT}[\frac{A}{B}] \qquad (3)$$

in which A = 1 + 9exp(2$D$/$kT$) + 25exp(6$D$/$kT$) + 49exp(12$D$/$kT$) + 81exp(20$D$/$kT$) + 84exp(-9$J$/$kT$) + 84exp(-$J$/$kT$) + 35exp(-8$J$/$kT$) + 35exp(-2$J$/$kT$) + 10exp(-7$J$/$kT$) + 10exp(-3$J$/$kT$) + exp(-6$J$/$kT$) + exp(-4$J$/$kT$) and B = 4 + 4exp(2$D$/$kT$) + 4exp(6$D$/$kT$) + 4exp(12$D$/$kT$) + 4exp(20$D$/$kT$) + 16exp(-9$J$/$kT$) + 16exp(-$J$/$kT$) + 12exp(-8$J$/$kT$) + 12exp(-2$J$/$kT$) + 8exp(-7$J$/$kT$) + 8exp(-3$J$/$kT$) + 4exp(-6$J$/$kT$) + 4exp(-4$J$/$kT$).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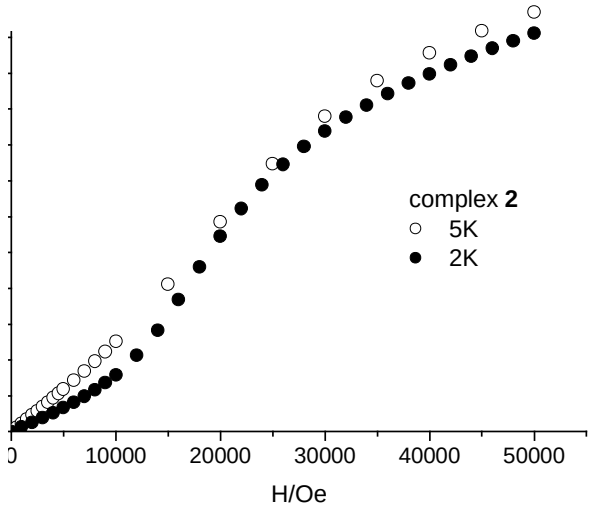
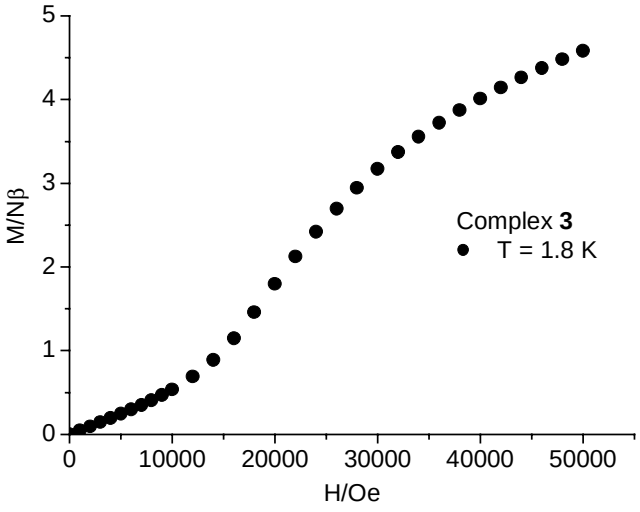
2K
0
10000
20000
30000
40000
50000
H/Oe


complex **2**
5K
2K
0
10000
20000
30000
40000
50000
H/Oe


M/Nβ
0
1
2
3
4
5
Complex **3**
T = 1.8 K
0
10000
20000
30000
40000
50000
H/Oe

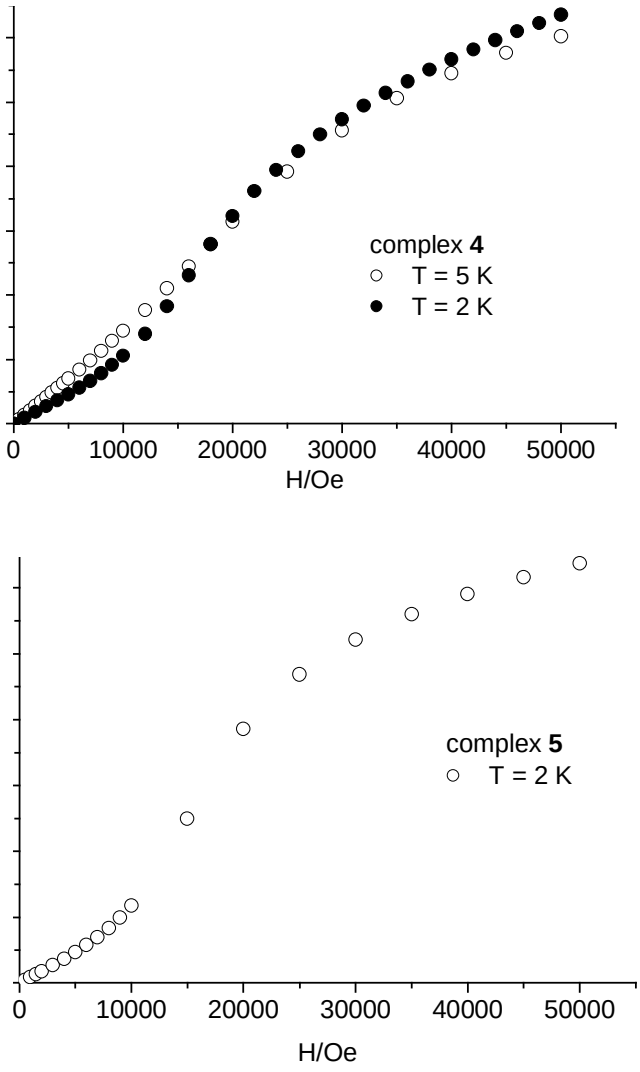



**Figure S4.** Field dependence of magnetization for the trinuclear complexes.

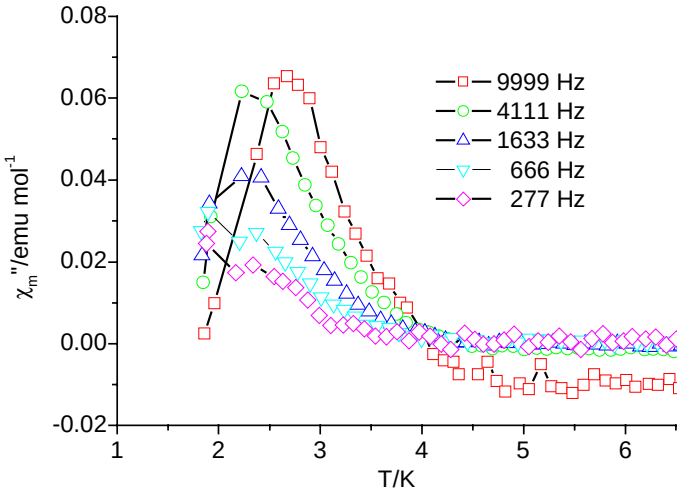



**Figure S5.** Out-of-phase component of the zero-static ($H_{DC}$ = 0) AC susceptibility at different frequencies for **5**.