Electronic Supplementary Material (ESI) for Dalton Transactions.


## Support Information

# Synthesis, Crystal Structures and Magnetic Properties of *mer*-Cyanideiron(III)-Based 1D Heterobimetallic Cyanide-Bridged Chiral Coordination Polymers

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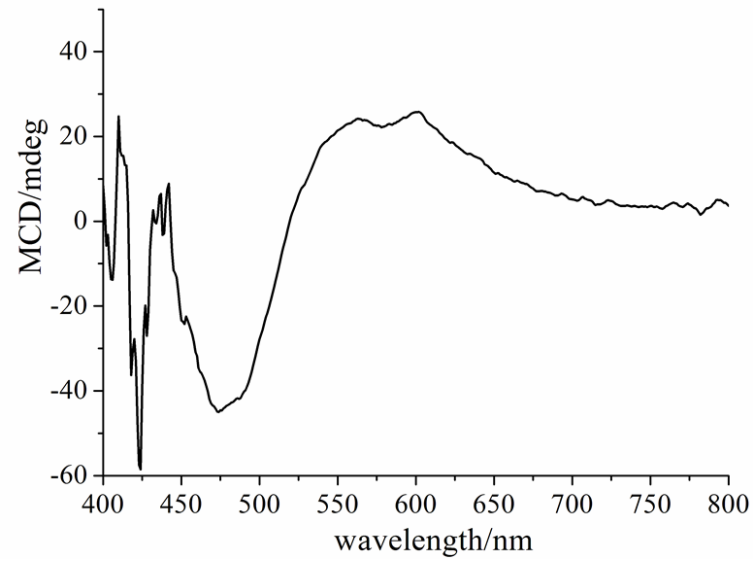


Figure S1. The MCD spectra of complex **1**.

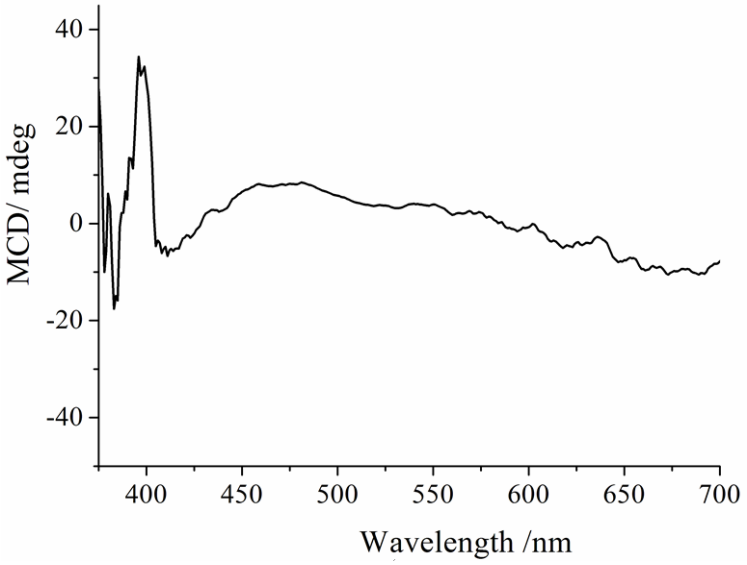


Figure S2. The MCD spectra of complex **3**.

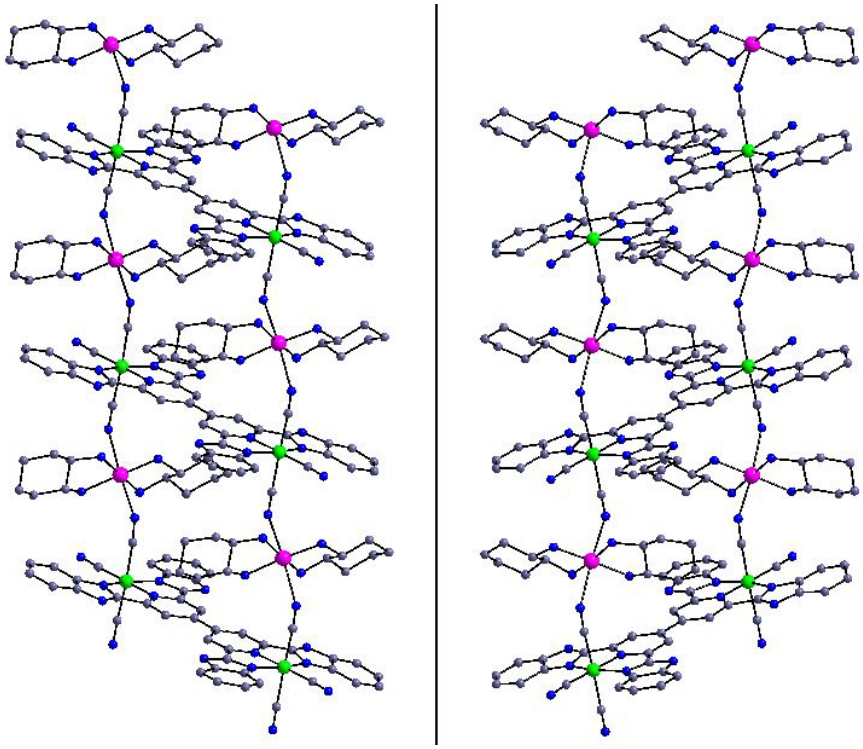

Figure S3. Perspective view of ladder-like double infinite chains of **3** (S,S isomer, left) and **4** (R,R isomer, right), respectively.

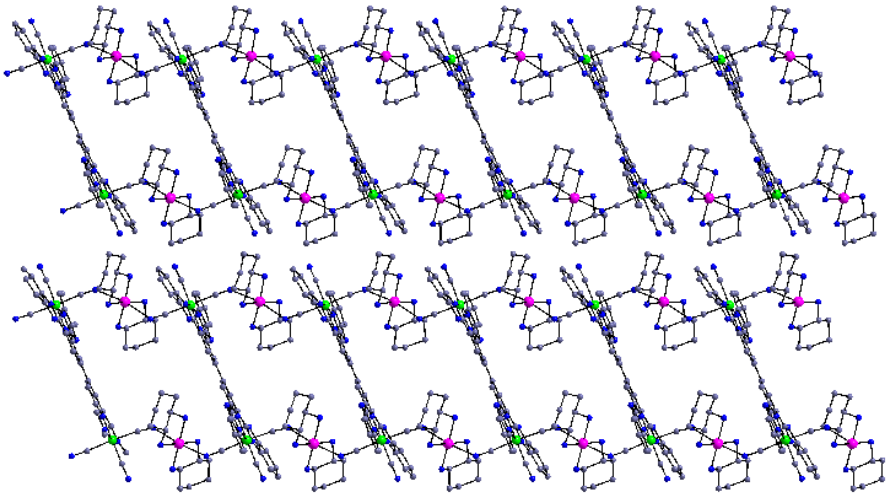

Figure S4. The cell packing diagram along *a* axis for complexes **3** and **4**. All the H atoms and the solvent molecules have been omitted for clarity.

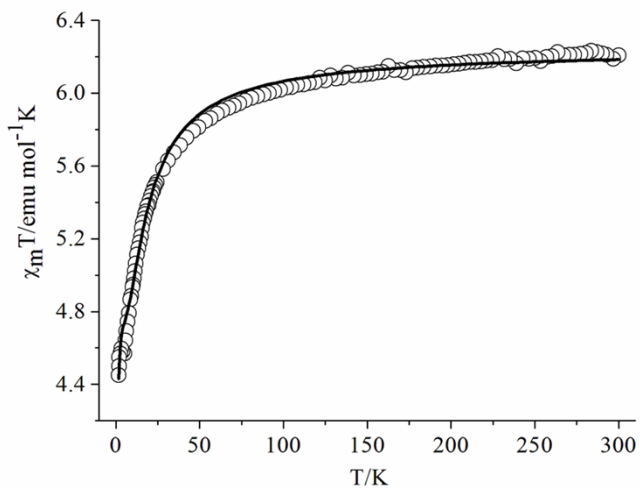


Figure S5. Temperature dependence of $\chi_M T$ for complex **2**. The fitting results are $J$ = -7.44 cm$^{-1}$, D = -1.51 cm$^{-1}$, g = 1.99, $R$ = 1.61×10$^{-5}$ (**2**).

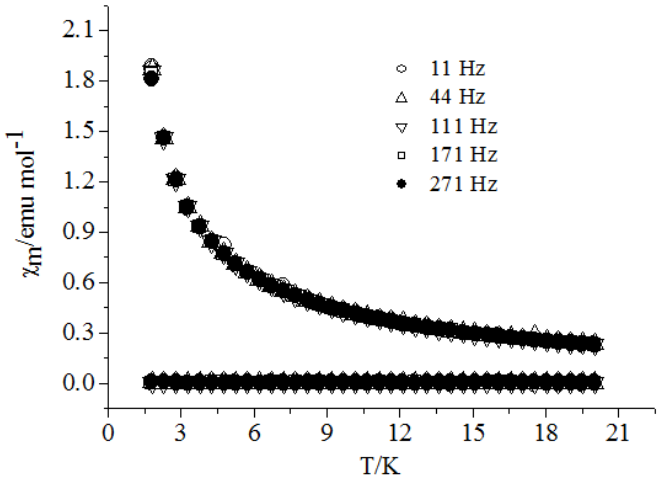


Figure S6. Temperature dependence of ac magnetization of complex **1** in a zero-static field and an ac field of 2 Oe at frequencies of 11, 44, 111, 171 and 271 Hz.

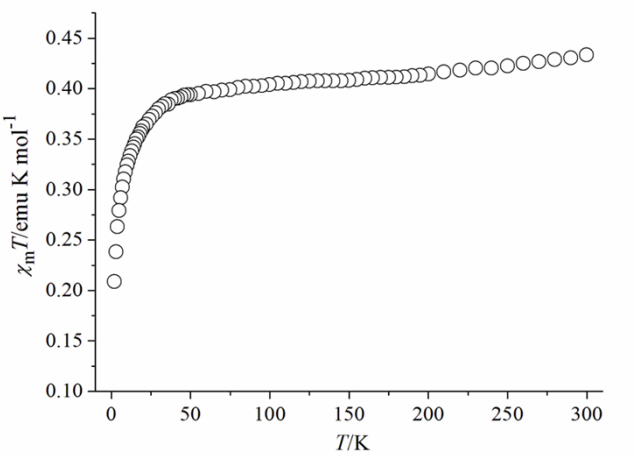


Figure S7. Temperature dependence of $\chi_M T$ of $K_4[Fe_2(tbbp)(CN)_6]$.

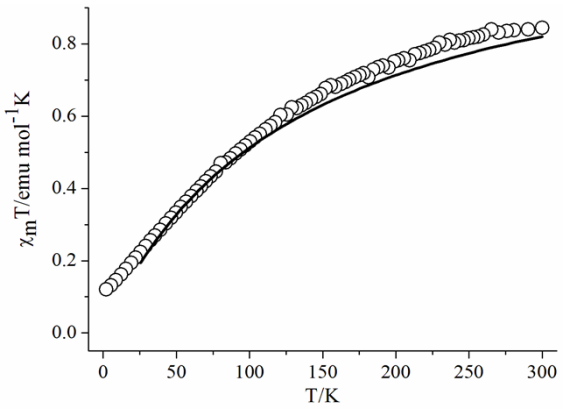


Figure S8. Temperature dependence of $\chi_M T$ of **4**. The magnetic fitting results are $J$ = -4.29 $cm^{-1}$, g = 2.08, $R = 2.65\times10^{-4}$ (**4**).

**Table S1**. Selected bond lengths (Å) and angles (°) for complexes **1**-**2**.

| | **1** | **2** |
|---|---|---|
| Mn1-N1 | 2.319(3) | 2.277(7) |
| Mn1-N9 | 1.996(3) | 2.019(7) |
| Mn1-N10 | 2.001(3) | 1.998(6) |
| Mn1-N15 | 2.263(3) | 2.280(7) |
| Mn1- O3 | 1.870(2) | 1.879(5) |
| Mn1-O4 | 1.888(2) | 1.886(6) |
| Fe1-C1 | 1.961(3) | 1.962(8) |
| Fe1-C2 | 1.958(3) | 1.962(9) |
| Fe1-C3 | 1.920(3) | 1.903(8) |
| Fe1-N4 | 1.940(3) | 1.962(7) |
| Fe1-N6 | 1.952(3) | 1.918(7) |
| Fe1-N8 | 1.944(3) | 1.934(8) |
| N15-Mn1-N1 | 169.44(11) | 168.8(3) |
| Mn1-N1-C1 | 151.5(3) | 153.9(7) |
| Mn1-N15-C64#1 | 157.1(3) | 157.4(7) |
| Fe1-C1-N1 | 177.7(3) | 178.1(7) |
| Fe1-C2-N2 | 178.5(3) | 175.5(8) |

#1: x+1, y, z

**Table S2**. Selected bond lengths (Å) and angles (°) for complexes **3**-**4**.

| | **3** | **4** |
|---|---|---|
| Cu1-N1 | 2.502(12) | 2.550(10) |
| Cu1-N17 | 1.943(12) | 2.028(11) |
| Cu1-N18 | 1.997(9) | 1.997(11) |
| Cu1-N19 | 1.976(12) | 2.008(9) |
| Cu1-N20 | 1.942(13) | 2.010(10) |
| Cu2-N5 | 2.572(10) | 2.528(10) |
| Cu2-N21 | 1.975(14) | 2.052(9) |
| Cu2-N22 | 2.040(10) | 2.028(10) |
| Cu2-N23 | 2.099(11) | 2.014(10) |
| Cu2-N24 | 2.036(9) | 2.022(9) |
| Fe1-C1 | 1.974(15) | 1.977(13) |
| Fe1-C2 | 2.005(13) | 1.974(14) |
| Fe1-C3 | 1.932(11) | 1.953(14) |
| Fe1-N7 | 1.939(9) | 1.966(9) |
| Fe1-N9 | 1.967(9) | 1.947(9) |
| Fe1-N11 | 1.948(9) | 1.951(8) |
| Fe2-C5 | 1.900(14) | 1.986(11) |
| Fe2-C4 | 1.934(12) | 1.905(11) |
| Fe2-C6 | 1.957(13) | 1.948(14) |
| Fe2-N12 | 1.935(8) | 1.913(9) |
| Fe2-N14 | 1.919(9) | 1.960(8) |
| Fe2-N16 | 1.956(8) | 1.956(9) |
| | | |
| C1-N1-Cu1 | 140.8(9) | 138.2(9) |
| C5-N5-Cu2 | 131.7(10) | 134.2(10) |
| C1-Fe1-C2 | 176.3(5) | 176.9(5) |
| C5-Fe2-C4 | 176.0(5) | 179.5(4) |