Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Optical Recognition of Alkyl Nitrile by Homochiral Iron(II) Spin Crossover Host

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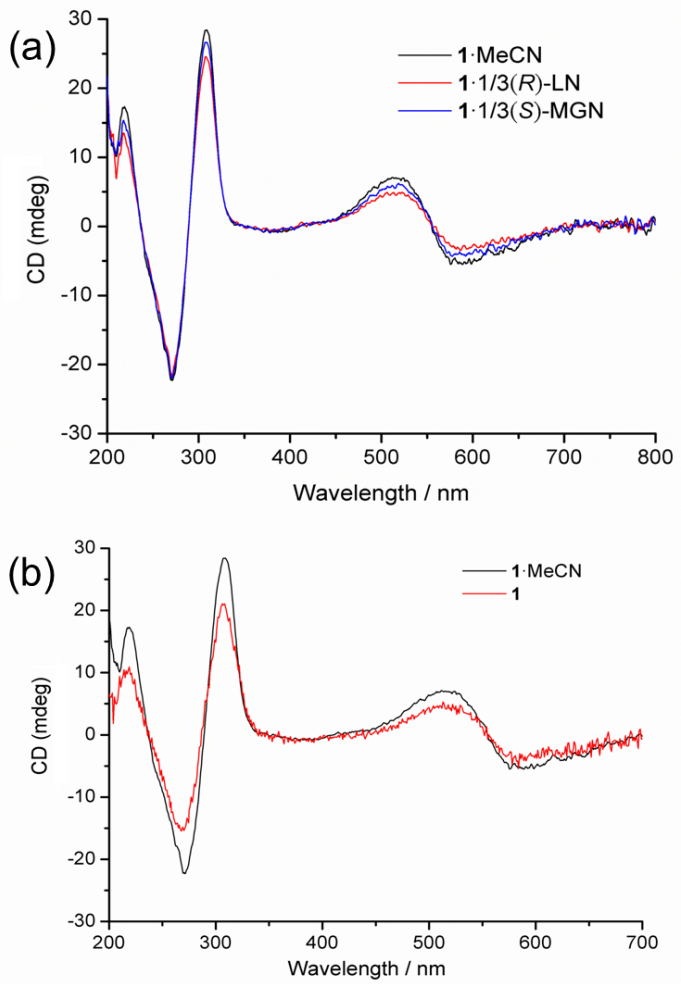


Fig. S1 (a) Circular dichroism (CD) spectra of chiral complexes **1**·MeCN (black), **1**·1/3(*R*)-LN (red)

and **1**·1/3(*S*)-MGN (blue) in acetonitrile. **(b)** CD spectra of **1**·MeCN in solution (black) and desolvated complex **1** in KBr pellets (red). **1** is obtained by placing **1**·MeCN in thermostatic vacuum drier for 12 h under 80 °C.

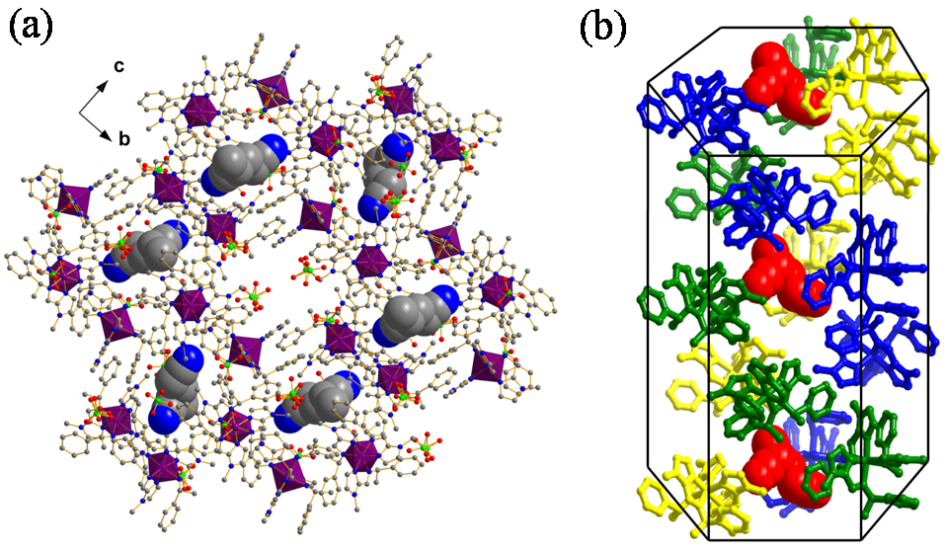


Fig. S2 (a) Crystal-packing diagram of **1**·1/3(*S*)-MGN, viewed along the crystallographic *a* axis. (*S*)-MGN molecules in space-filling mode are enclosed in the middle of pseudo-hexagonal column; (b) Side view of **1**·1/3(*S*)-MGN column in the crystal-packing diagram. The cations are stacked into left-handed triple helix with (*S*)-MGN captured in the channel. (*S*)-MGN is highlighted by red molecules and the anions are omitted for clarity.

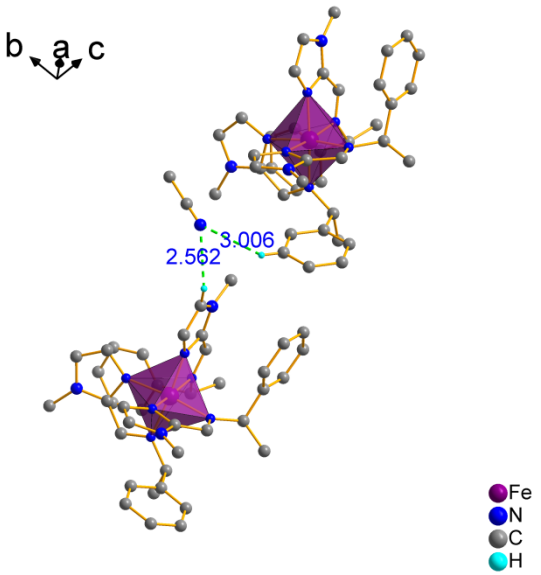


Fig. S3 The N···H–C hydrogen bonds between acetonitrile molecule and cations in the complex **1**·MeCN. Dashed light green lines represent interactions. Each acetonitrile molecule is interactive with two metal cations.

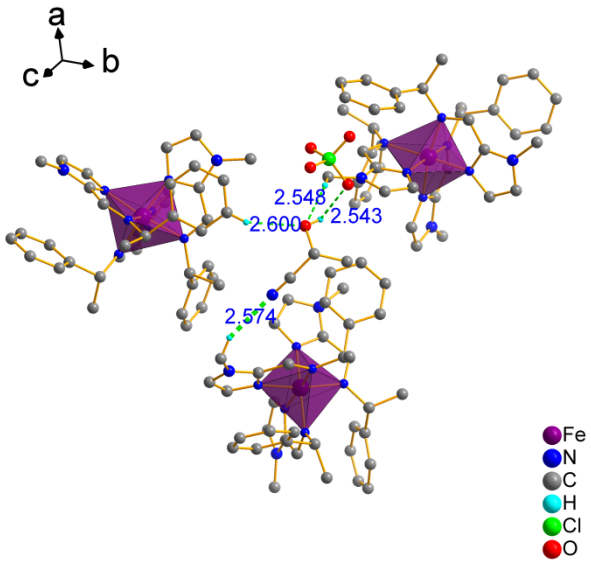


Fig. S4 The hydrogen bonds between (*R*)-lactonitrile and metal cations in complex **1**·1/3(*R*)-LN. Dashed light green lines represent interactions. Each (*R*)-LN is interactive with three metal cations. The nitrogen atom of LN is N···H-C hydrogen bonded to one cation, while the oxygen atom of LN is O···H-C bonded to two cations. Meanwhile the oxygen atom is additionally O···H-O hydrogen bonded to the oxygen atom of a perchlorate ion.

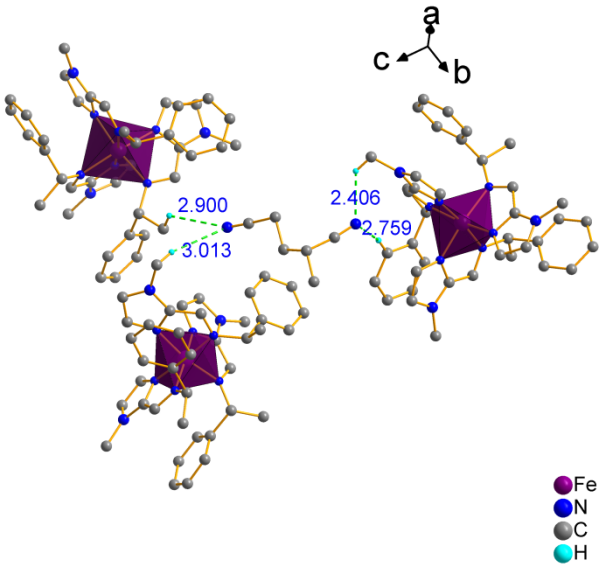
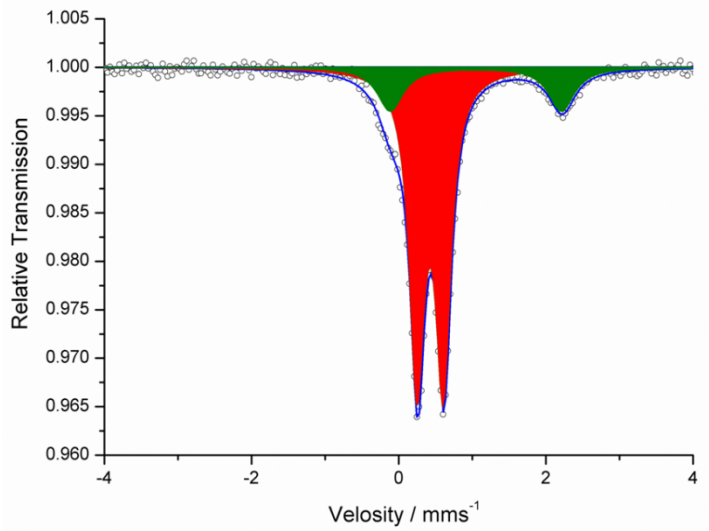


Fig. S5 The N···H-C hydrogen bonds between (*S*)-methylglutaronitrile and metal cations in complex **1**·1/3(*S*)-MGN. Dashed light green lines represent interactions. Each (*S*)-MGN is interactive with three metal cations. One nitrogen atom of MGN was linked to one cation, while the other nitrogen atom of MGN was linked to two cations with N···H-C hydrogen bonds.



I.S.	Q.S.	fwhm	d[%]	rel_I. [%]
0.44	0.36	0.25	3.17	78.82
1.06	2.33	0.43	0.46	21.18

Fig. S6 Mössbauer spectrum of desolvated **1**·MeCN at 100 K. Mössbauer experiment was carried out using a ^{57}Co/Pd source in a constant acceleration transmission spectrometer. The spectrometer was calibrated using a standard R-Fe foil, and the reported isomer shifts are relative to the center of the R-Fe spectrum. The MossWinn program was used to determine the Mössbauer parameters.

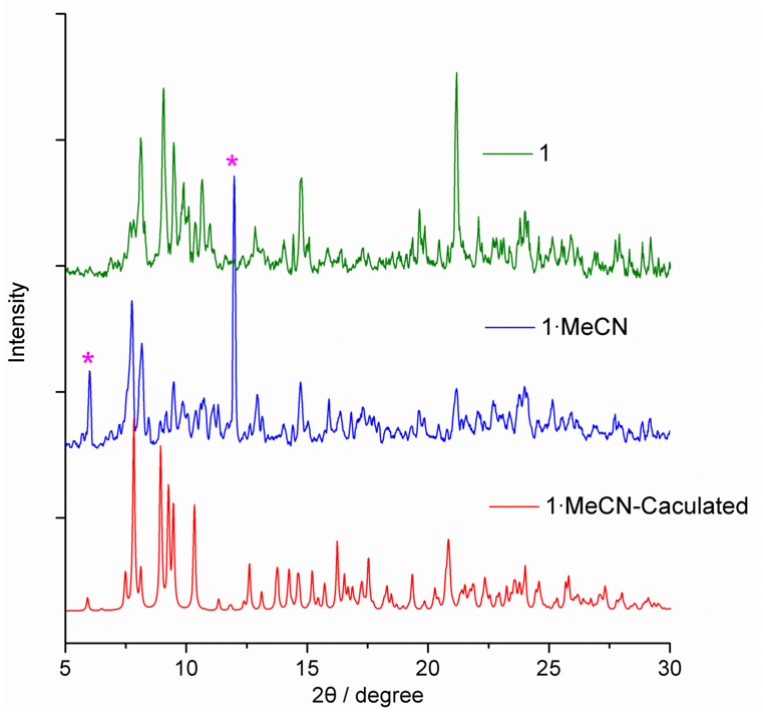


Fig. S7 X-ray power diffraction profiles of **1**·MeCN (blue), desovated **1**·MeCN (green) and calculated pattern (red). **1** is obtained by placing **1**·MeCN in thermostatic vacuum drier for 12 h under 80 °C. Main peaks of **1**·MeCN are maintained in **1**, except the marked peaks of solvent at 6° and 12° vanish in the pattern of **1**. This suggests the stability of crystal structure of the iron(II) complex after removing the solvent molecules.

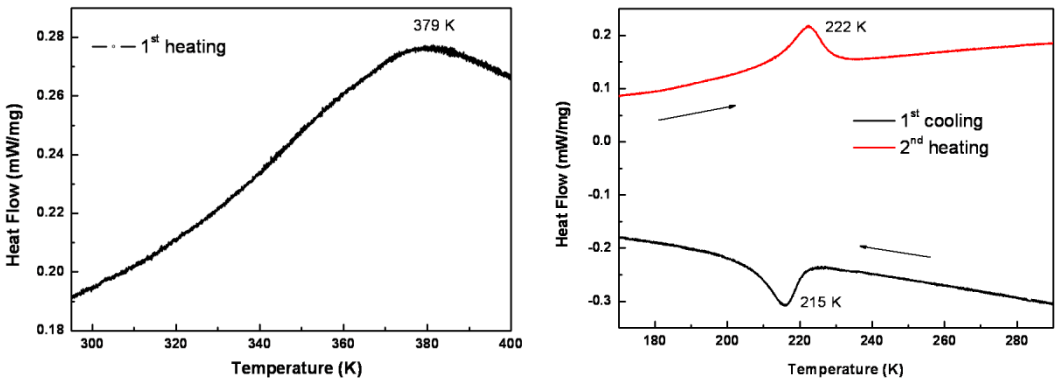


Fig. S8 Differential scanning calorimeter (DSC) curves of **1**·MeCN. Phase transition temperatures in the first heating mode is 379 K, while the phase transition temperatures first cooling mode and second heating mode comes to 215 K and 222 K, respectively.

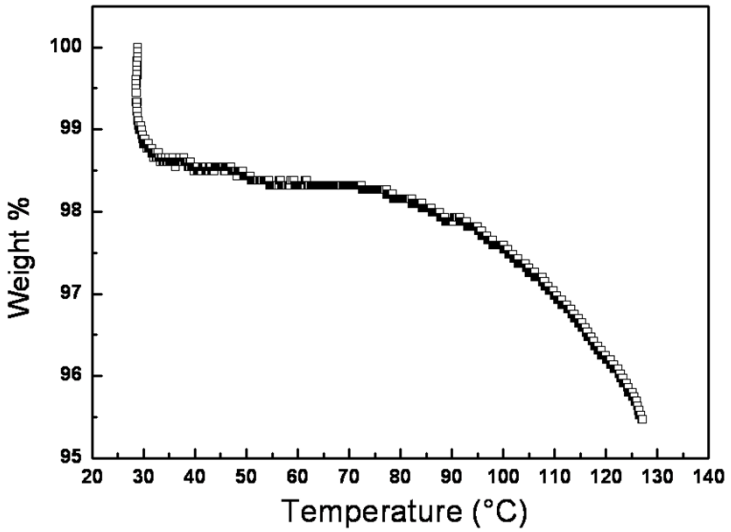


Fig. S9 The thermogravimetric (TG) curve of **1**·MeCN with a temperature range of 25-127 °C. The obvious weight loss around room temperature is likely attributed to the rapid loss of solvent. At 35 °C, about 1.4 % weight has lost. And further weight loss presents upon the following heating. At 127 °C (400 K), 4.5 percent of weight loss in the curve is roughly consistent with the theoretical percentage of acetonitrile molecules (4.4 %).