Supporting Information

An electrical conducting molecular crystal composed of a magnetic iron (III) complex (S = 1/2) with a large aromatic ligand, 1,2-naphthlalocyanine (C_{4h} isomer): towards the development of molecular spintronics

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Contents

Fig. S1 shows the infrared (IR) spectra of Fe(1,2-Nc) (a), $K[Fe^{III}(1,2\text{-Nc})(CN)_2]$ (b), and the $Ph_4P[Fe^{III}(1,2\text{-Nc})(CN)_2]_2$ crystals that grown on the anode by the electrocrystallization (c). All of them are almost identical to each other, and also to those of Co(1,2-Nc) and $K[Co^{III}(1,2\text{-Nc})(CN)_2]$.[1)]

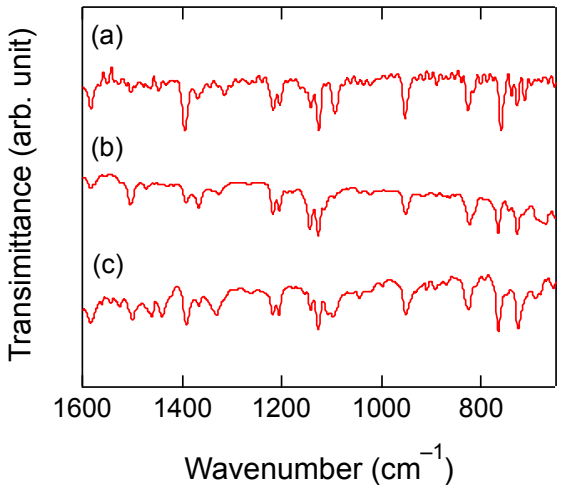

Fig. S1 IR spectra of Fe(1,2-Nc) (a), $K[Fe^{III}(1,2\text{-Nc})(CN)_2]$ (b), and $Ph_4P[Fe^{III}(1,2\text{-Nc})(CN)_2]_2$ (c).

Fig. S2 shows the X-ray diffraction (XRD) pattern of $Ph_4P[Fe^{III}(1,2\text{-Nc})(CN)_2]_2$ polycrystals used in the static magnetic susceptibility measurement (a), along with that simulated from crystallographic data of $Ph_4P[Fe^{III}(1,2\text{-Nc})(CN)_2]_2$ (b).

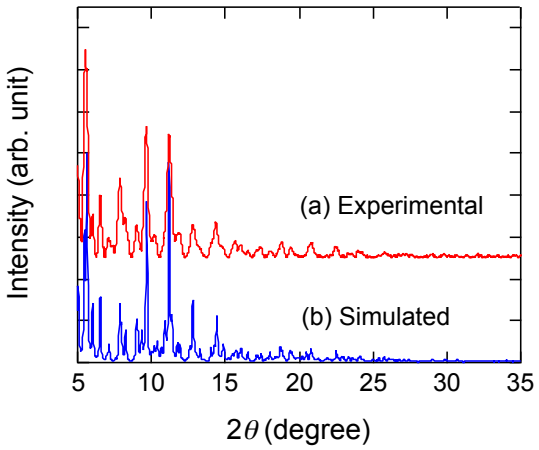

Fig. S2 (a) XRD pattern of polycrystals of $Ph_4P[Fe^{III}(1,2\text{-Nc})(CN)_2]_2$. (b) XRD pattern simulated from crystallographic data of $Ph_4P[Fe^{III}(1,2\text{-Nc})(CN)_2]_2$.

Experimental section

IR spectra were recorded on a Jasco FT/IR-4600 spectrometer as KBr pellets. XRD measurement was performed by Rigaku SuperNova system with monochromated Mo-Kα radiation (λ = 0.71073 Å).

References

1) E. H. Gacho, H. Imai, R. Tsunashima, T. Naito, T. Inabe, and N. Kobayashi, *Inorg. Chem.*, 2006, **45**, 4170–4176.