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Supplementary Information

Soft X-ray Absorption Spectroscopy Study of Spin Crossover Fe-compounds: Persistent High Spin Configurations under Soft X-ray Irradiation

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1. FT-IR

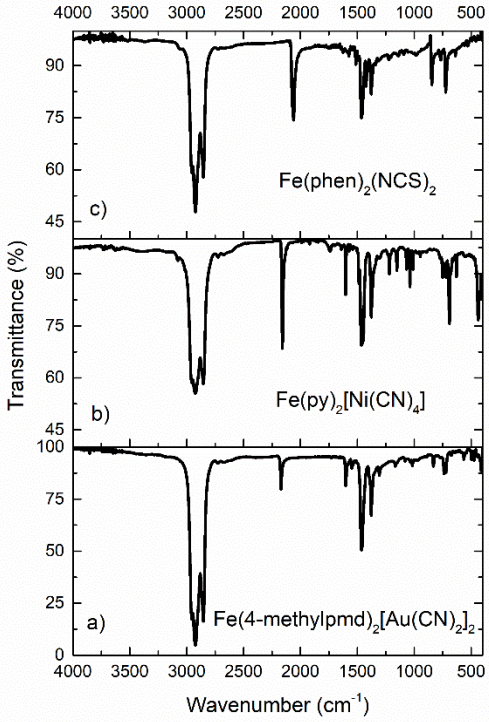

Figure S1. FT-IR spectroscopy analysis of (**a**) Fe(4-methylpmd)$_2$[Au(CN)$_2$]$_2$, (**b**) Fe(py)$_2$[Ni(CN)$_4$], and (**c**) Fe(phen)$_2$(NCS)$_2$.

IR spectra were obtained by the Nujol mull method using JASCO FTIR-4100 spectrometer (JASCO Corp., Hachioji, Tokyo, Japan). (a) $Fe(4\text{-methylpmd})_2[Au(CN)_2]_2$: ν_{max}/cm^{-1} = 2170, 1619, 1599, 1556, 1492, 1325, 1014 and 845; (b) $Fe(py)_2[Ni(CN)_4]$: ν_{max}/cm^{-1} = 2158, 1603, 1573, 1218, 1152, 1038, 1011, 751, 690, 626, 437 and 419; (c) $Fe(phen)_2(NCS)_2$: ν_{max}/cm^{-1} = 2072 and 2060.

2. XRD- $Fe(4\text{-methylpmd})_2[Au(CN)_2]_2$

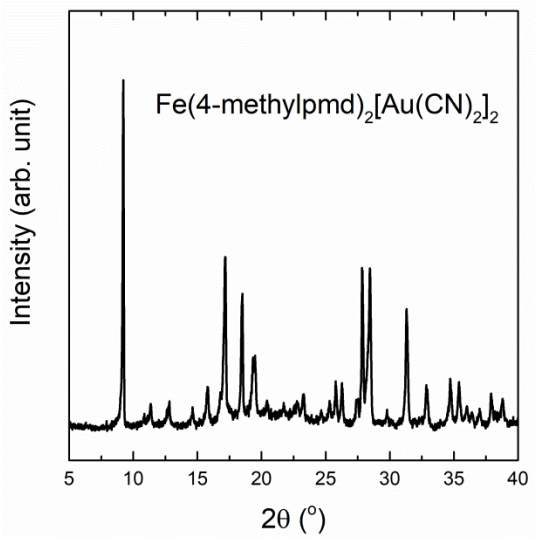

Figure S2. Powder XRD pattern of $Fe(4\text{-methylpmd})_2[Au(CN)_2]_2$.

Powder X-ray diffraction pattern of $Fe(4\text{-methylpmd})_2[Au(CN)_2]_2$ was measured by using a Rigaku RINT2500 diffractometer (Rigaku Corp., Akishima, Tokyo, Japan) with graphite-monochromated Cu Kα radiation (λ= 1.5406 Å). It is similar to that of the reported $Fe(4\text{-methylpy})_2[Au(CN)_2]_2$. (Kosone, T.; Tomori, I.; Kanadani, C.; Saito, T.; Mochida, T.; Kitazawa, T. Unprecedented three-step spin-crossover transition in new 2-dimensional coordination polymer $\{Fe^{II}(4\text{-methylpyridine})_2[Au^{I}(CN)_2]_2\}$. Dalton Trans, **2010**. 39(7): p. 1719-21, DOI: 10.1039/b914330k).

3. TGA- $Fe(4\text{-methylpmd})_2[Au(CN)_2]_2$

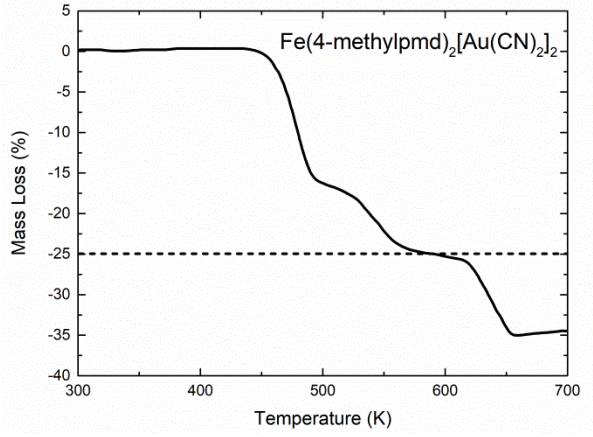

Figure S3. Thermogravimetric analysis (TGA) of $Fe(4\text{-methylpmd})_2[Au(CN)_2]_2$.

The thermal decomposition was investigated on TG/DTA6200 (SII Nano Technology, Makuhari, Chiba, Japan) under a dry N_2 gas flow by recording the thermogravimetric (TG) curve. The 25.4 % weight loss at the plateau between 577–617 K indicates the thermal decomposition of $Fe(4\text{-methylpmd})_2[Au(CN)_2]_2$ into $Fe[Au(CN)_2]_2$.