

Supporting Information

Two-electron redox-active tricyano iron(II) complex with
2,4,6-tris(2-pyrimidyl)-1,3,5-triazine as a building block for
coordination polymers

Takuya Shiga,* Haruka Miyamoto,
Graham N. Newton and Hiroki Oshio*

Prof. H. Oshio
Graduate School of Pure and Applied Sciences,
University of Tsukuba
Tennodai 1-1-1, Tsukuba, Ibaraki 305-8571 (Japan)
FAX: (+81)29-852-5923
E-mail: oshio@chem.tsukuba.ac.jp

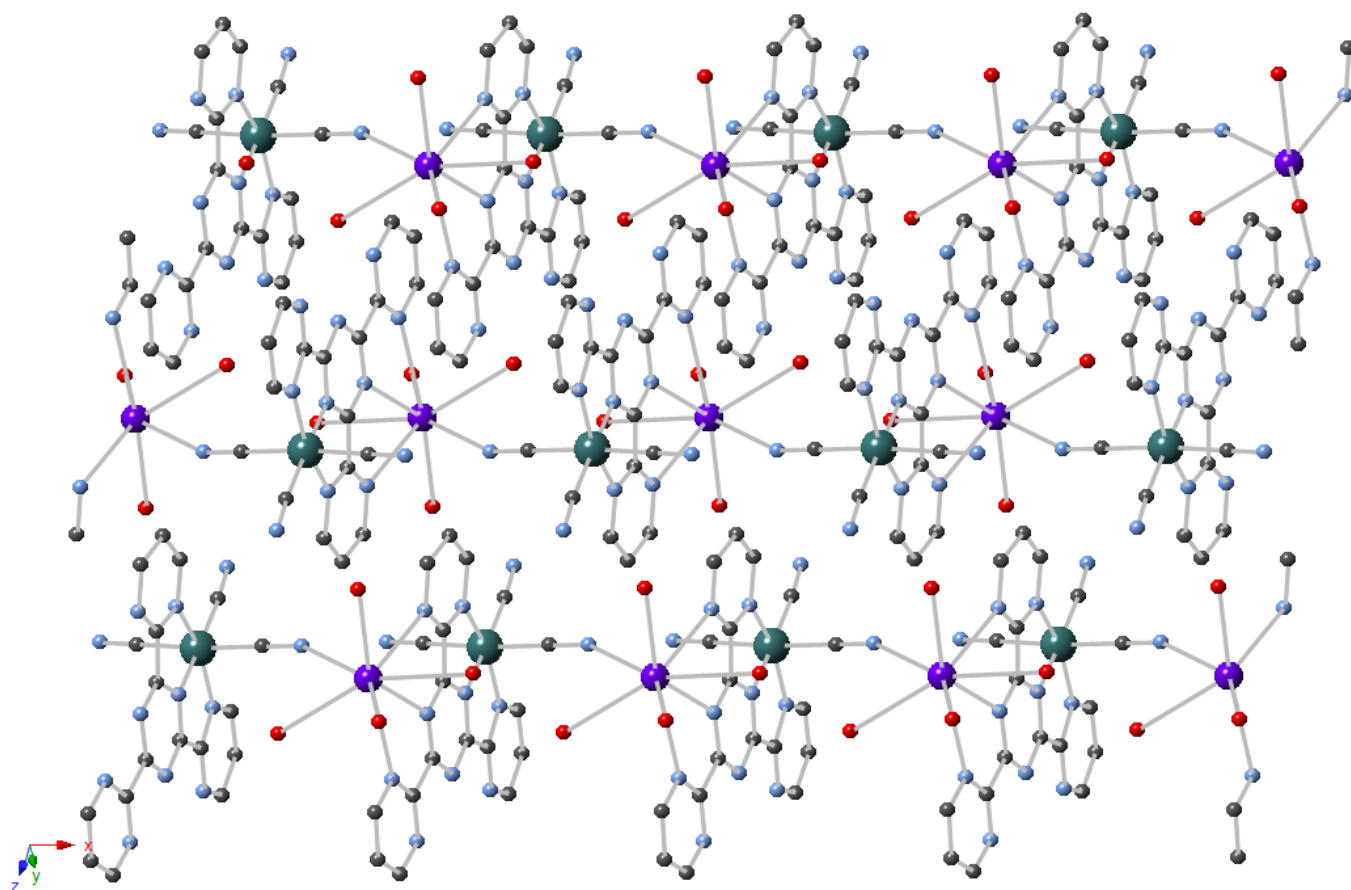


Figure S1. Packing structure of 1. Solvent molecules were omitted for clarity.

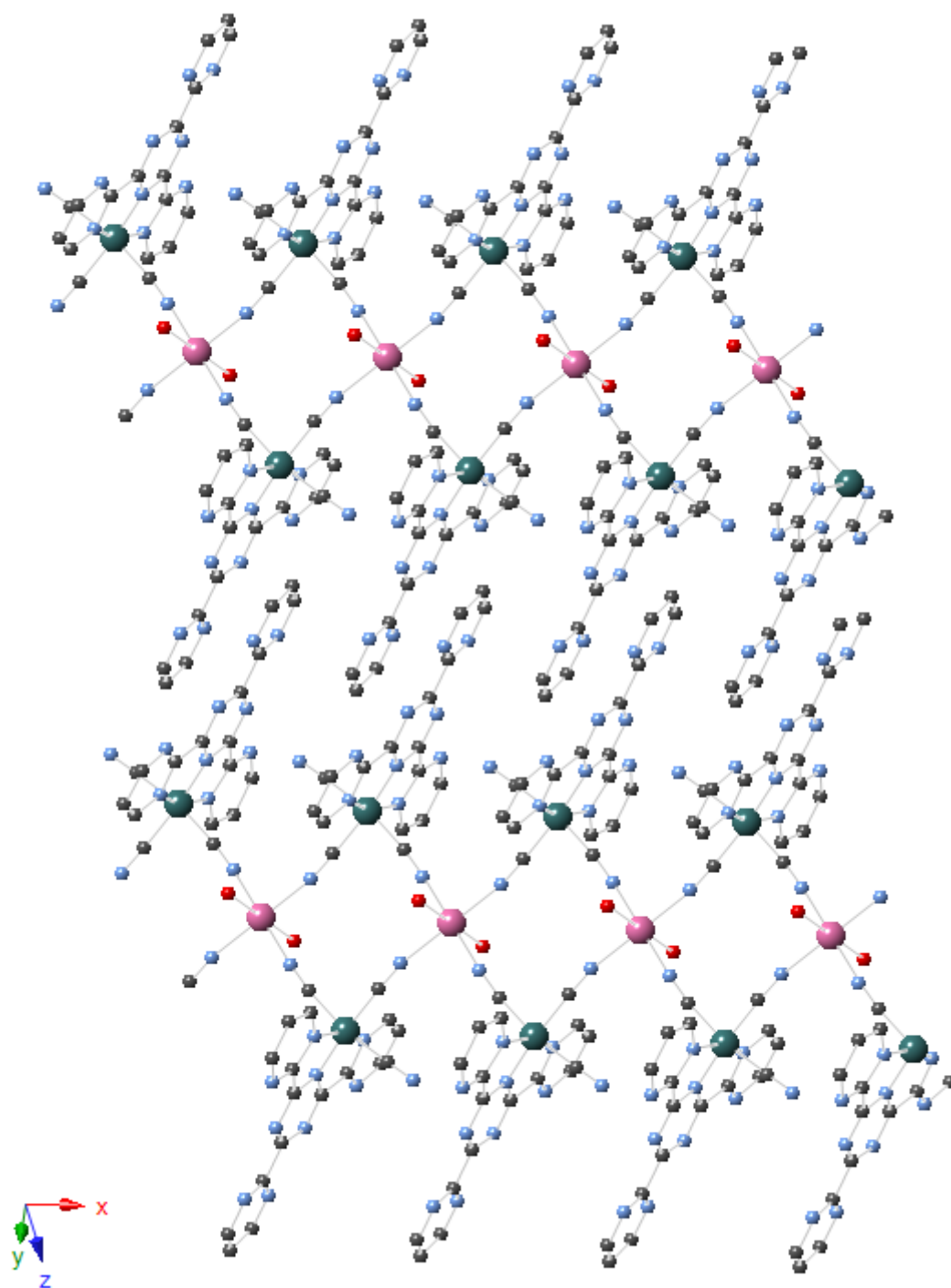


Figure S2. Packing structure of **3**. Solvent molecules were omitted for clarity.

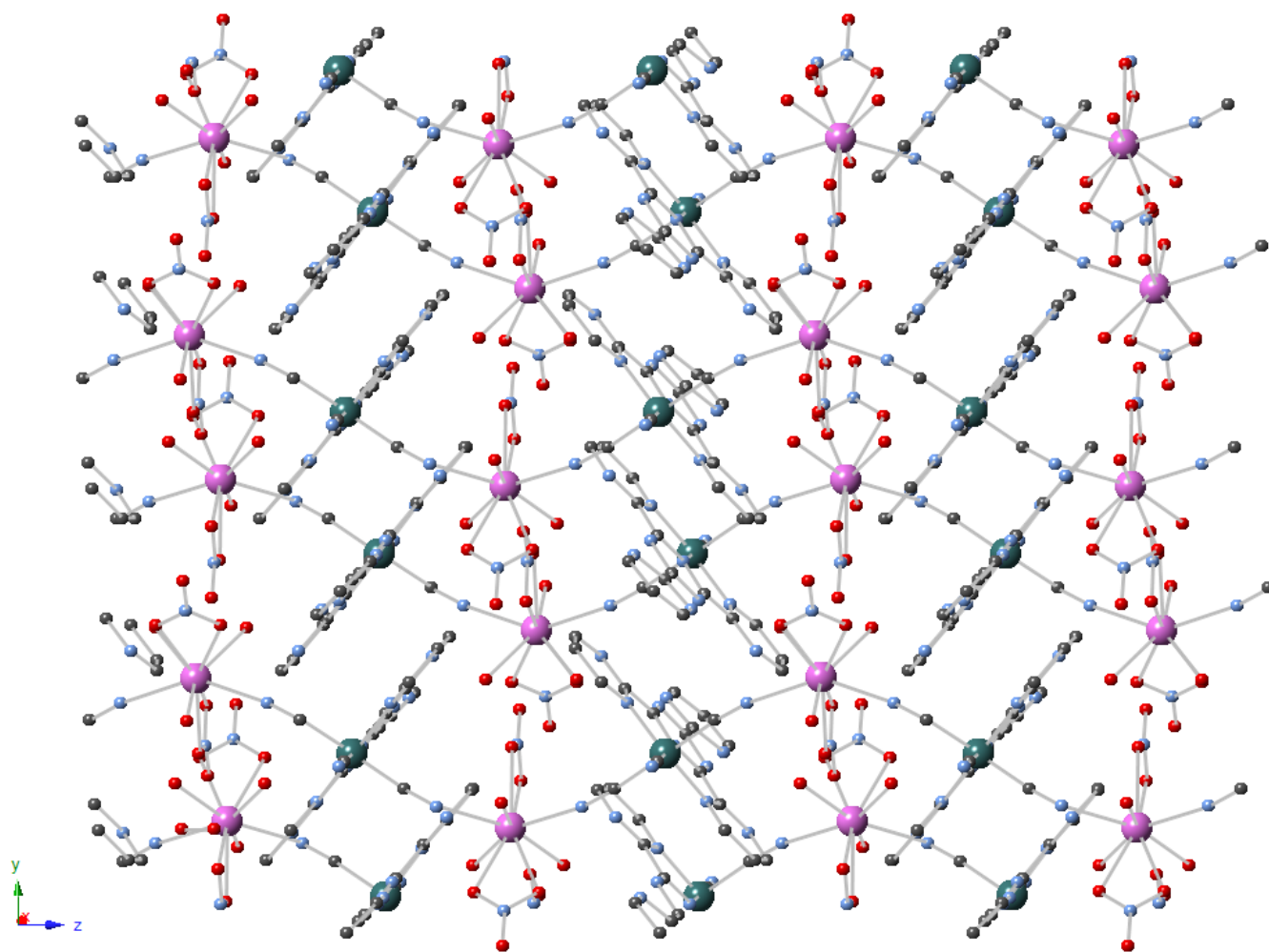


Figure S3. Packing structure of **4**. Solvent molecules were omitted for clarity.

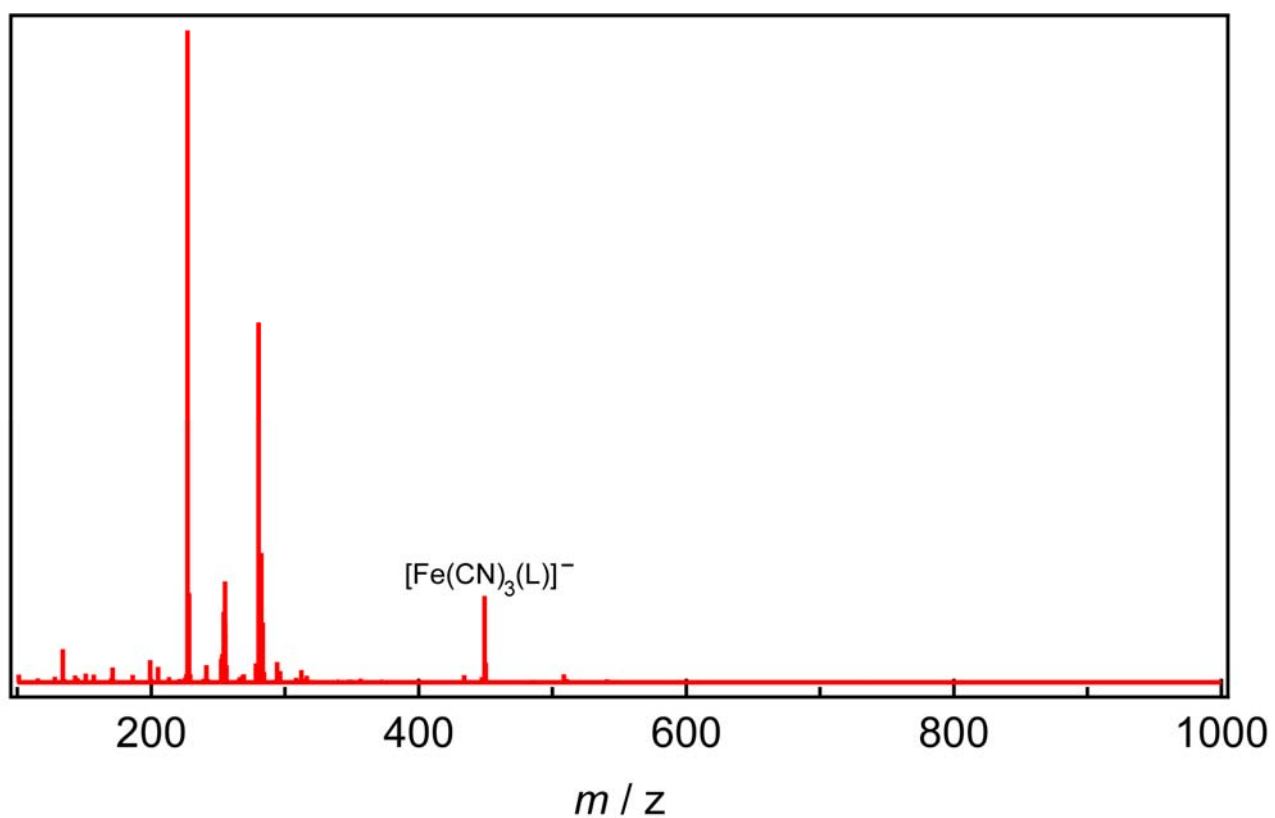


Figure S4. ESI-MS data of 1. Observed peak at $m/z = 449.2$ is assigned as $[\text{Fe}(\text{CN})_3(\text{L})]^-$ (calcd. $m/z = 449.0$)

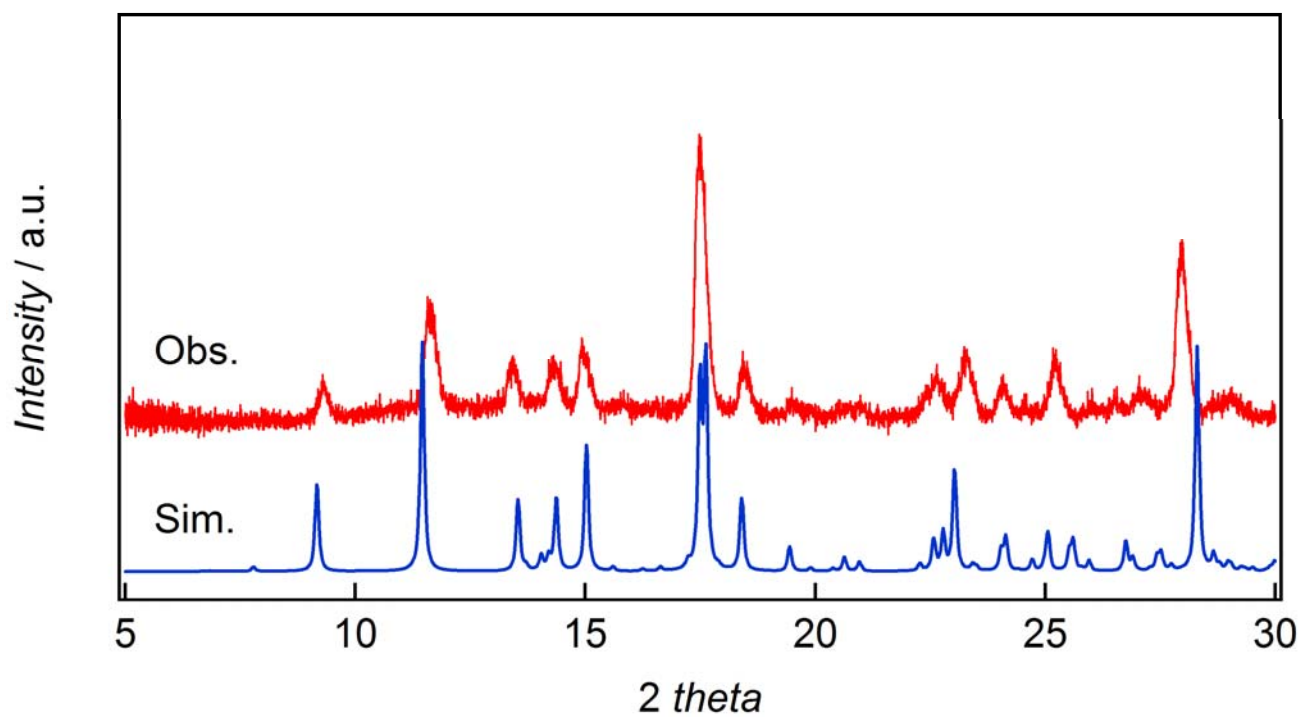


Figure S5. PXRD data of 2.

Table S1. Crystal parameters of 1–4.

	Comp. 1	Comp. 2	Comp. 3	Comp. 4
Formula	C ₁₈ H ₂₃ N ₁₂	C ₁₈ H ₁₇ N ₁₂	C ₁₈ H ₁₇ N ₁₂	C ₂₀ H ₂₅ N ₁₄
	O ₇ KFe	O ₄ Fe _{1.5}	O ₄ FeMn _{0.5}	O _{11.5} FeGd
M / g mol ⁻¹	614.43	549.21	548.75	858.64
Temp. / K	100(2)	100(2)	100(2)	100(2)
Crystal system	Triclinic	Triclinic	Triclinic	Orthorhombic
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$Pbcm$
$a / \text{\AA}$	8.3483(11)	7.036(3)	7.096(2)	15.142(3)
$b / \text{\AA}$	12.6991(16)	12.005(4)	12.045(4)	10.635(2)
$c / \text{\AA}$	12.8859(16)	13.309(5)	13.365(5)	19.470(4)
$\alpha / ^\circ$	110.674(2)	76.130(4)	75.886(4)	-
$\beta / ^\circ$	91.693(2)	83.693(4)	83.782(5)	-
$\gamma / ^\circ$	97.884(2)	75.671(5)	75.639(4)	-
$V / \text{\AA}^3$	1261.6(3)	1055.9(7)	1071.8(6)	3135.4(11)
Z	2	2	2	4
$d / \text{g cm}^{-3}$	1.617	1.727	1.700	1.819
μ / mm^{-1}	0.828	1.102	1.042	2.639
F(000)	632	560	559	1700
Reflections				
collected / unique	7294 / 5562	5911 / 4538	6137 / 4653	17194 / 3706
R_{int}	0.0194	0.0358	0.0305	0.0821
GOF	1.039	0.953	1.022	1.101
$R1 (I > 2\sigma(I))$	0.0586	0.0438	0.0587	0.0559
$R_w2 (I > 2\sigma(I))$	0.1620	0.1229	0.1122	0.1277
$\Delta\rho_{\text{max}} / \text{e \AA}^{-3}$	2.019	1.019	0.788	2.055
$\Delta\rho_{\text{min}} / \text{e \AA}^{-3}$	-2.064	-0.668	-0.508	-1.890
CCDC No.	1847517	1847518	1847519	1847520