Electronic Supplementary Material for CrystEngComm

Supplementary Information

Fe (II) Spincrossover Complex of [1,2,5]thiadiazolo[3,4-*f*][1,10]phenanthroline

Yoshiaki Shuku, Rie Suizu, Kunio Awaga, and Osamu Sato

Table S1 Crystallographic data summary for **1**·CH_2Cl_2, and **2**.

	1·CH_2Cl_2	**3**
Formula	$C_{27}H_{14}Cl_2FeN_{10}S_4$	$C_{38}H_{18}FeN_{14}S_5$
Formula weight	733.47	886.80
Temperature / K	173	173
Crystal system	Monoclinic	Triclinic
Space group	$P2_1/n$	P-1
a / Å	11.802(3)	12.174(2)
b / Å	18.533(5)	12.264(2)
c / Å	13.233(3)	12.350(2)
α / °	90	73.543(4)
β / °	100.485(4)	88.616(7)
γ / °	90	83.507(6)
V / Å^3	2846.1(12)	1756.9(5)
Z	4	2
D_{calc} / g cm^{-3}	1.712	1.676
μ(Mo Kα) / cm^{-1}	10.517	7.819
F(000)	1480.00	900.00
$2\theta_{max}$ / °	55.0	55.0
Reflections collected	22714	14139
Unique reflections (R_{int})	6513 (0.145)	7721 (0.073)
Number of parameters	398	521
Final R_1 [$I > 2\sigma(I)$][a]	0.1194	0.0559
wR_2[b]	0.3421	0.1415
Goodness-of-fit	1.103	1.074

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR_2 = [\Sigma\{w(F_o^2 - F_c^2)^2\}/\Sigma w(F_o^2)^2]^{1/2}$

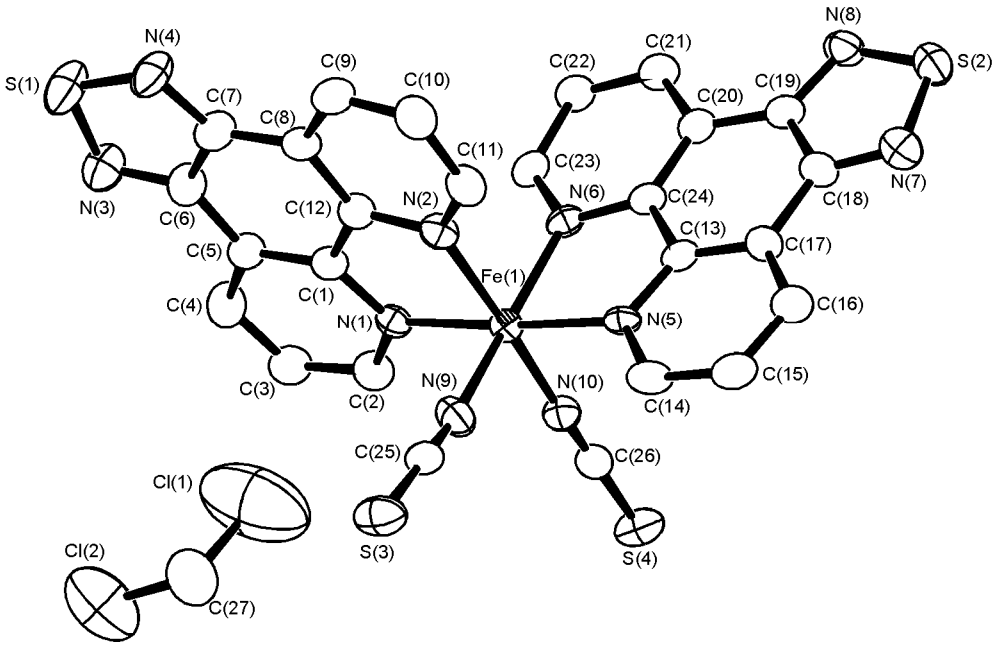

Fig. S1. The molecularstructure of **1**·CH_2Cl_2 with displacement ellipsoids at the 50% probability level. Hydrogen atoms and were omitted for clarity. The crystalline solvent (CH_2Cl_2) in **1**·CH_2Cl_2 is considerably disordered over several positions and assigned tentatively.

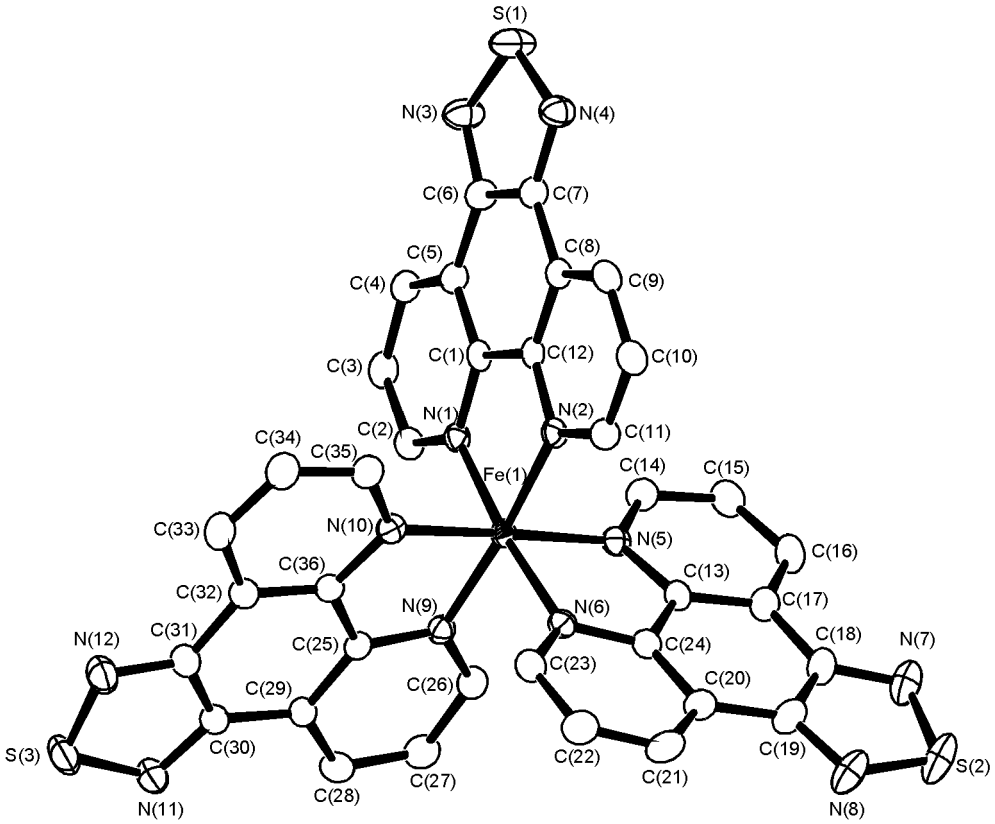

Fig. S2. The molecular structure of **3** with displacement ellipsoids at the 50% probability level. Hydrogen atoms and NCS anion were omitted for clarity. Isothiocyanate anion in **3** is disordered two positions with 50:50 occupancy.