Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information for:

Structure and magnetic properties of an unusual homoleptic iron(III) thiocyanate dimer

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Table 1. Crystallographic Data for **2.**

Empirical formula	C78 H48 Fe2 N14 S22	
Formula weight	1998.32	
Temperature	147(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 11.6864(4) Å	α= 90°.
	b = 29.2257(9) Å	β= 108.8590(17)°.
	c = 13.0996(4) Å	γ = 90°.
Volume	4233.9(2) $Å^3$	
Z	2	
Density (calculated)	1.567 Mg/m^3	
Absorption coefficient	8.257 mm^{-1}	
F(000)	2036	
Crystal size	0.360 x 0.130 x 0.040 mm^3	
Theta range for data collection	3.024 to 67.183°.	
Index ranges	-13<=h<=12, -34<=k<=34, -15<=l<=15	
Reflections collected	84784	
Independent reflections	14940 [R(int) = 0.0652]	
Completeness to theta = 67.679°	98.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7529 and 0.4615	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14940 / 787 / 1141	
Goodness-of-fit on F^2	1.028	
Final R indices [I>2sigma(I)]	R1 = 0.0471, wR2 = 0.1062	
R indices (all data)	R1 = 0.0520, wR2 = 0.1095	
Absolute structure parameter	0.3782(19)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.598 and -0.457 $e.Å^{-3}$	

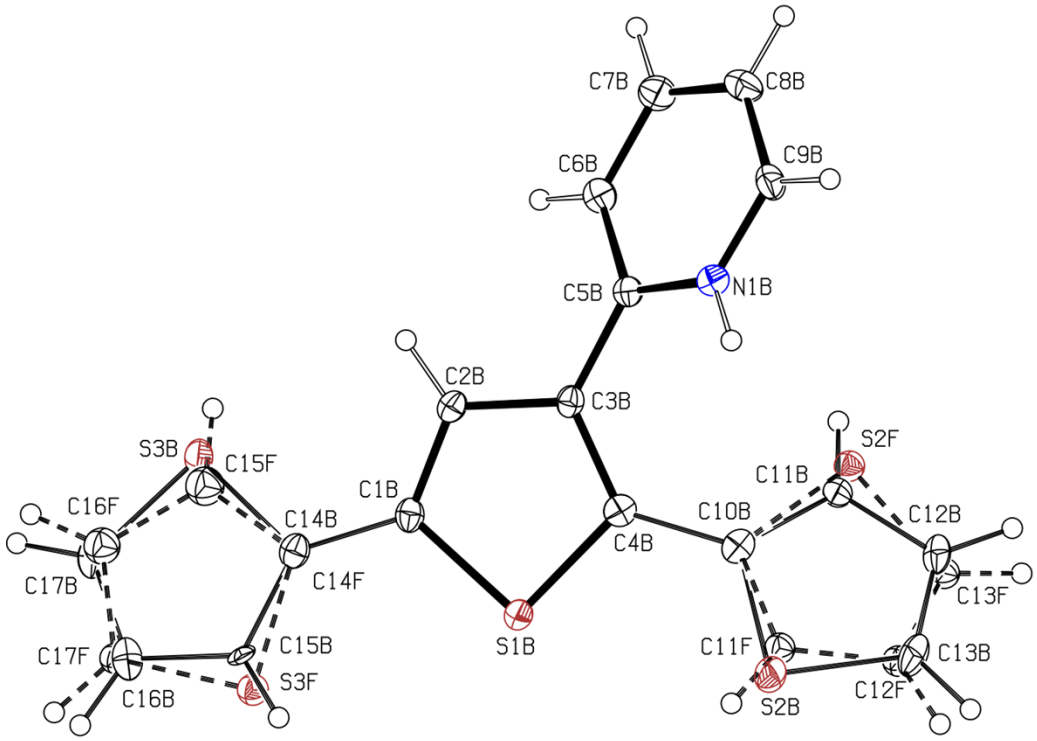

Figure S1. Displacement ellipsoid plot of the molecular structure of **2**. Single cation shown for clarity. Displacement ellipsoids at 30%.

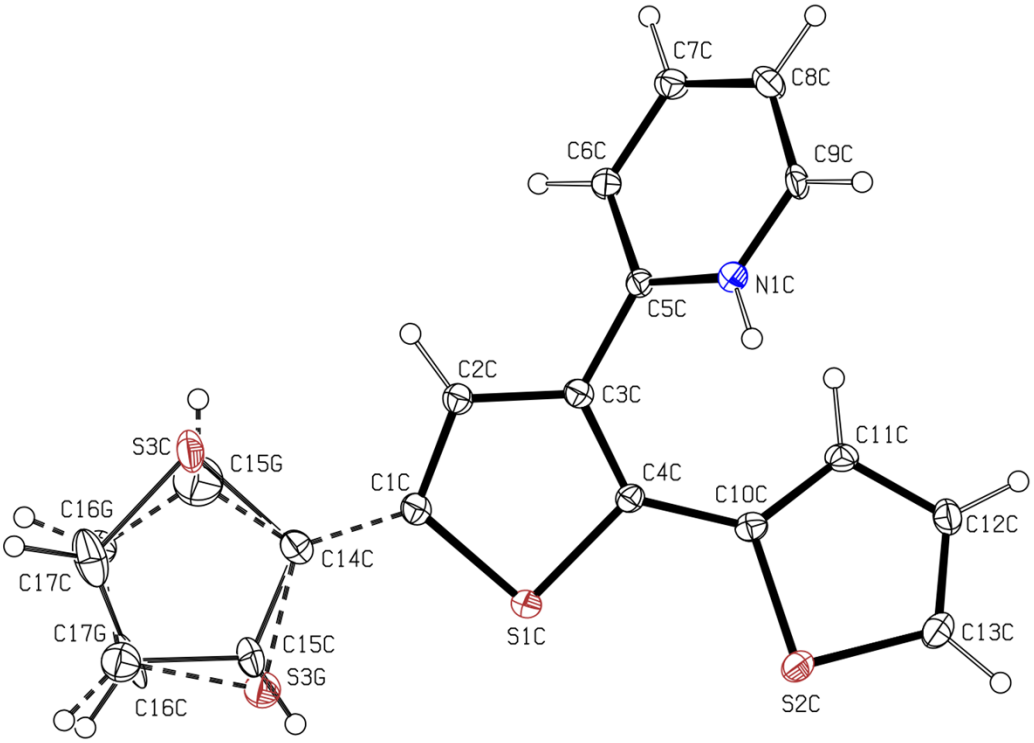

Figure S2. Displacement ellipsoid plot of the molecular structure of **2**. Single cation shown for clarity. Displacement ellipsoids at 30%.

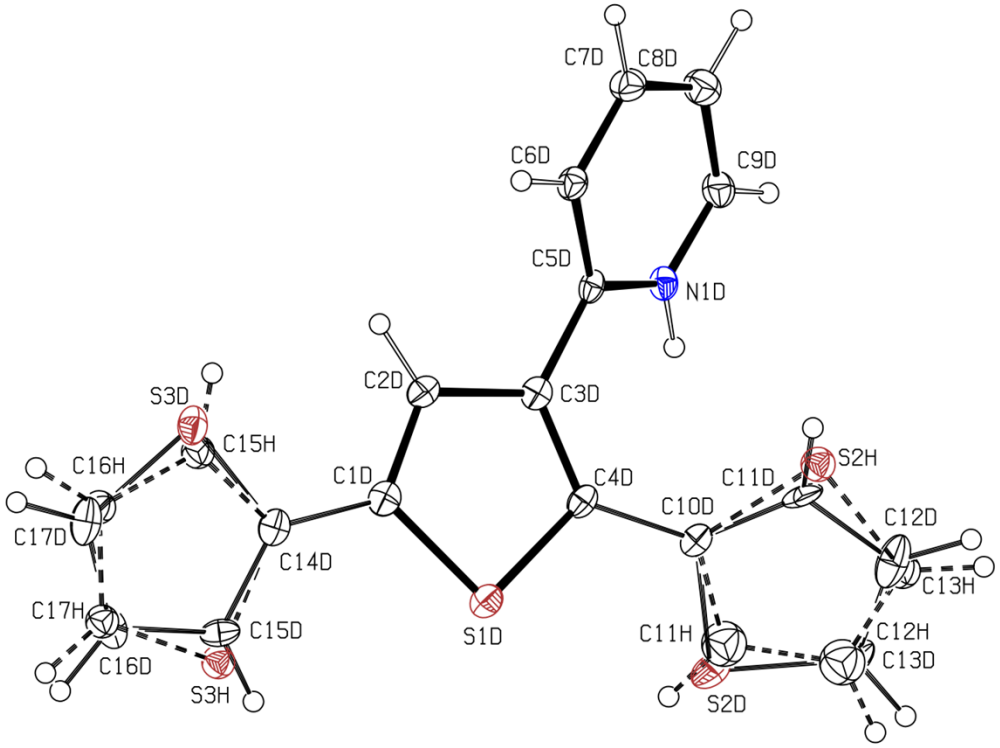

Figure S3. Displacement ellipsoid plot of the molecular structure of **2**. Single cation shown for clarity. Displacement ellipsoids at 30%.

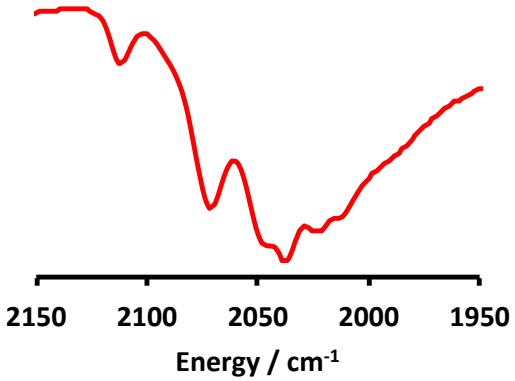

Figure S4. FT-IR spectrum of **2** recorded as a KBr pellet (y-axis not shown is in units of percent transmittance).

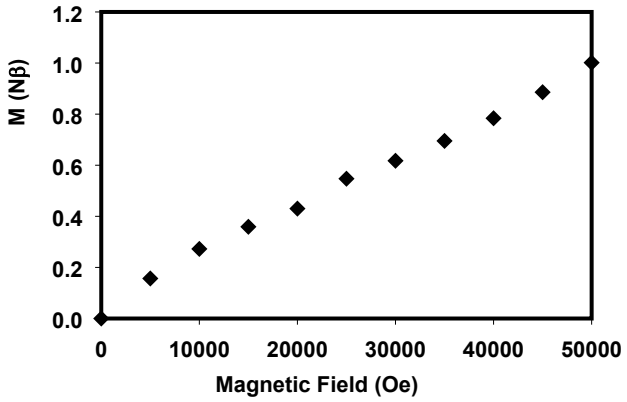

Figure S5. Magnetization versus field plot for **2** at a temperature of 2 K.