

Supplementary Material for:

Spin crossover in mixed ligand iron(III) complexes

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Supporting Figures

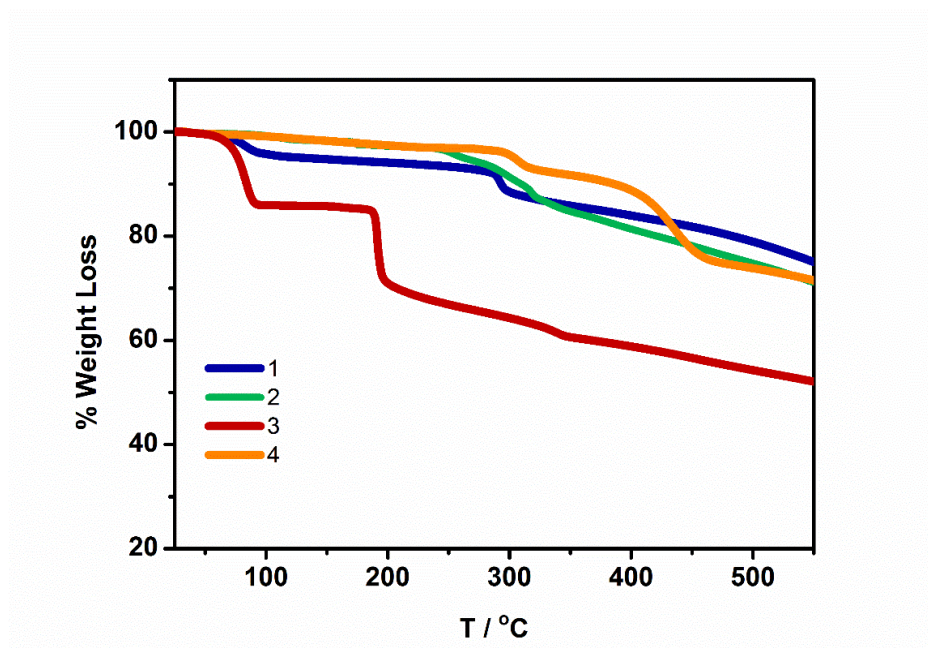


Figure S1 TGA studies of $[\text{Fe}(\text{qsal-Cl})(\text{qsal-Br})\text{Y}]$ ($\text{Y} = \text{NCS}$ **1**, PF_6 **2**, BPh_4 **3** and OTf **4**).

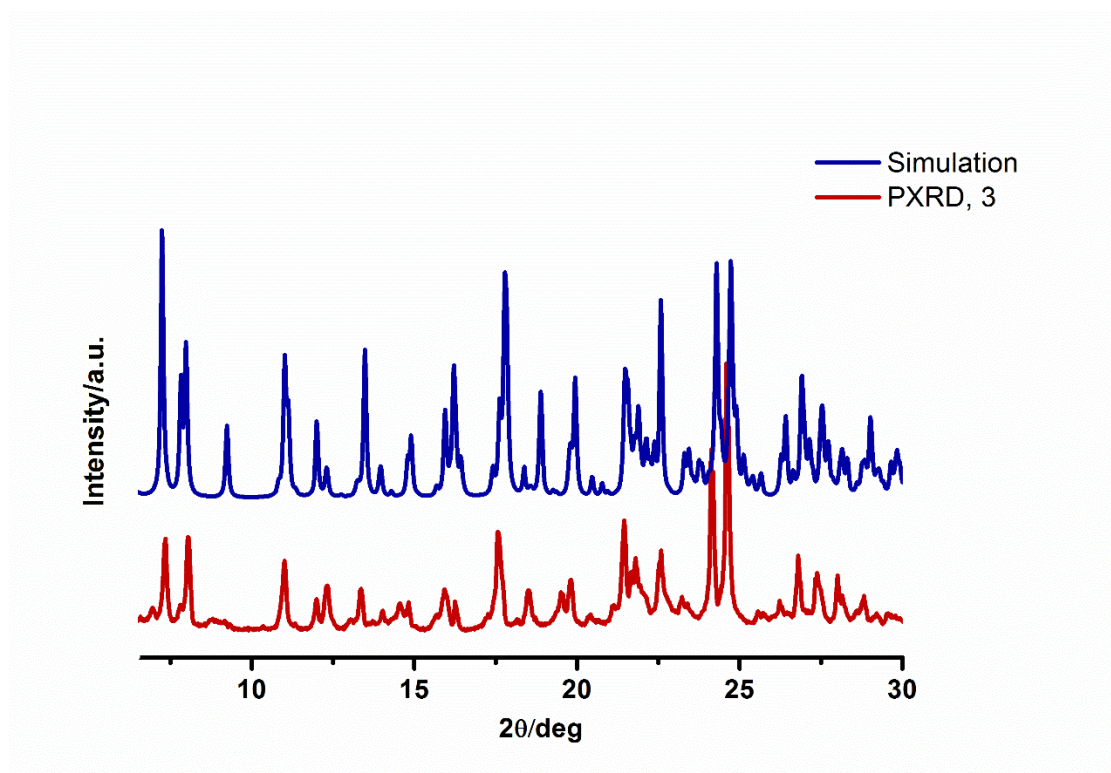


Figure S2 PXRD of $[\text{Fe}(\text{qsal-Cl})(\text{qsal-Br})\text{BPh}_4 \cdot 2\text{CH}_2\text{Cl}_2]$ **3**.

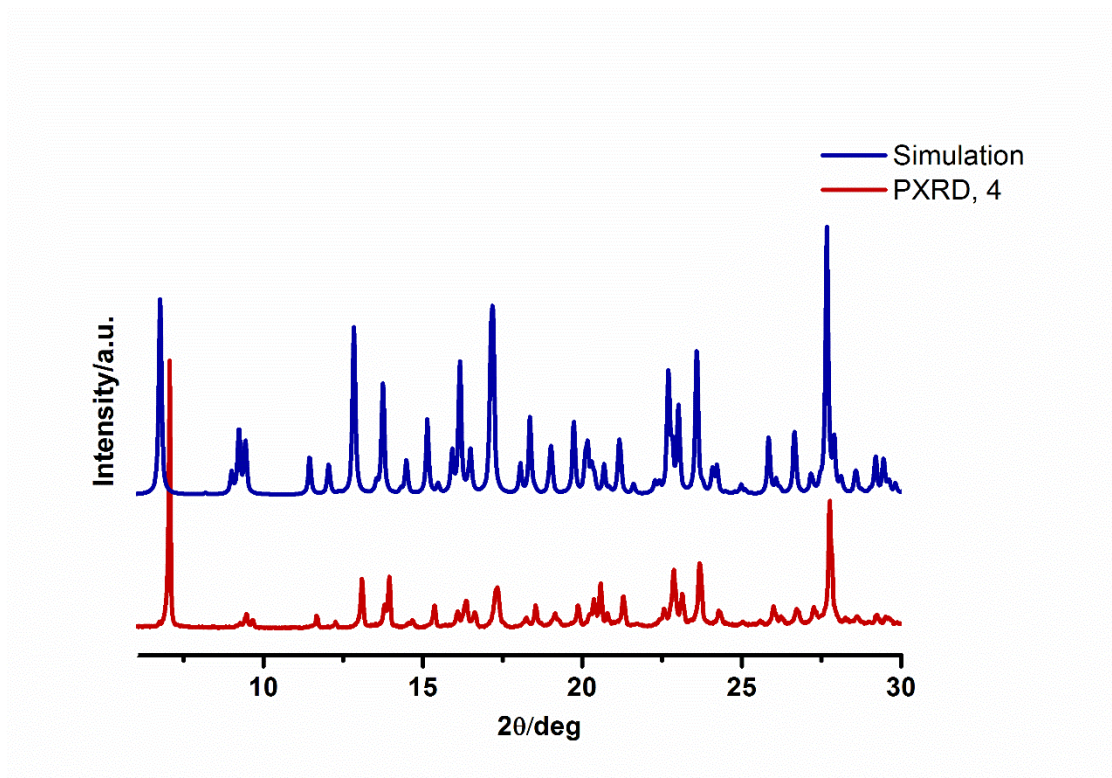


Figure S3 PXR D of $[\text{Fe}(\text{qsal-Cl})(\text{qsal-Br})]\text{OTf}\cdot 0.5\text{MeOH}$ 4.

X-ray Crystallography

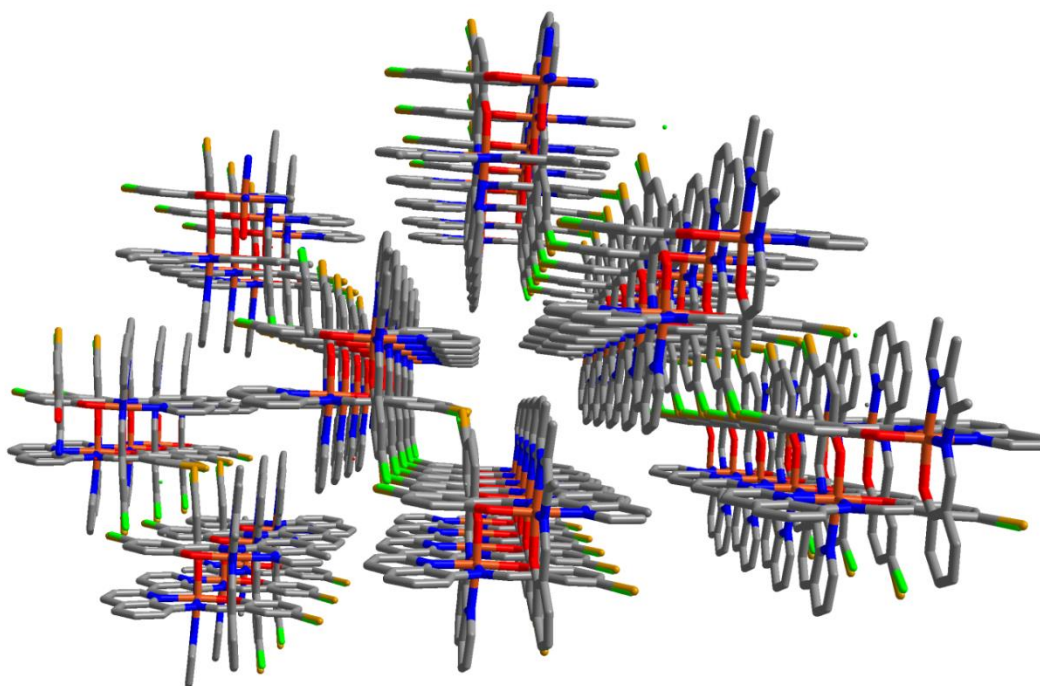


Figure S4 View of the 1D π - π chains in $[\text{Fe}(\text{qsal-Cl})(\text{qsal-Br})]\text{NCS}\cdot\text{MeOH}$ 1.

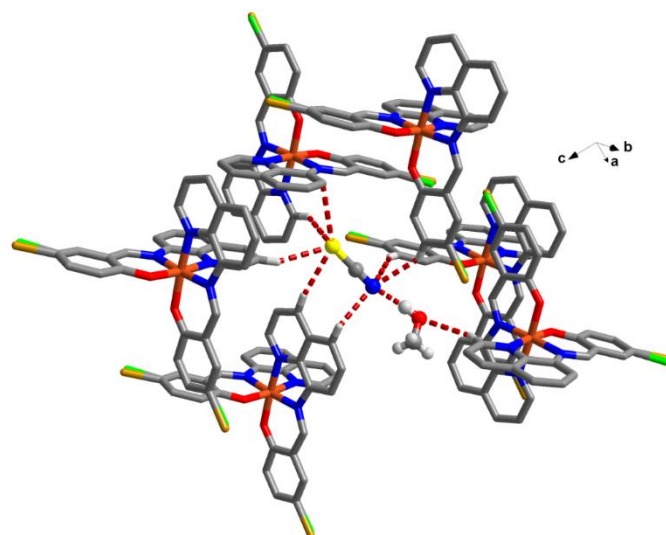


Figure S5 View of the interactions between the thiocyanate and the $[\text{Fe}(\text{qsal-Cl})(\text{qsal-Br})]^+$ cations in $[\text{Fe}(\text{qsal-Cl})(\text{qsal-Br})]\text{NCS}\cdot\text{MeOH}$ **1**.

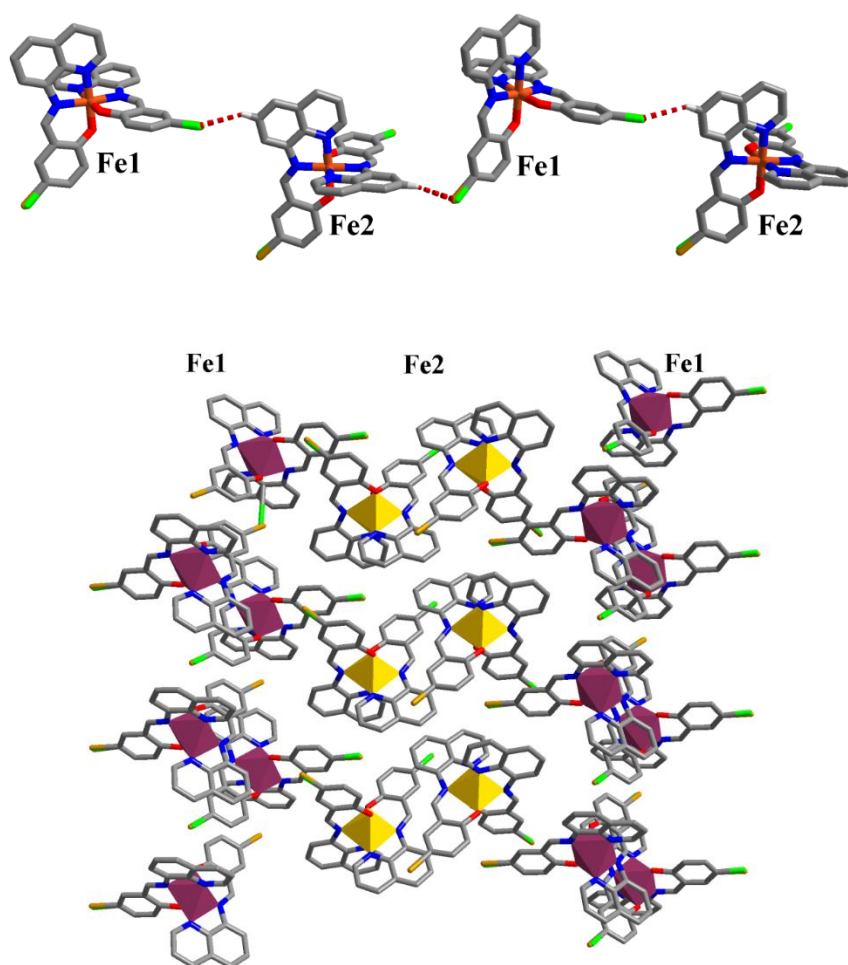


Figure S6 View of the $\text{C-H}\cdots\text{Cl/Br}$ interactions that link the $[\text{Fe}(\text{qsal-Cl})(\text{qsal-Br})]^+$ cations in $[\text{Fe}(\text{qsal-Cl})(\text{qsal-Br})]\text{PF}_6$ **2**.

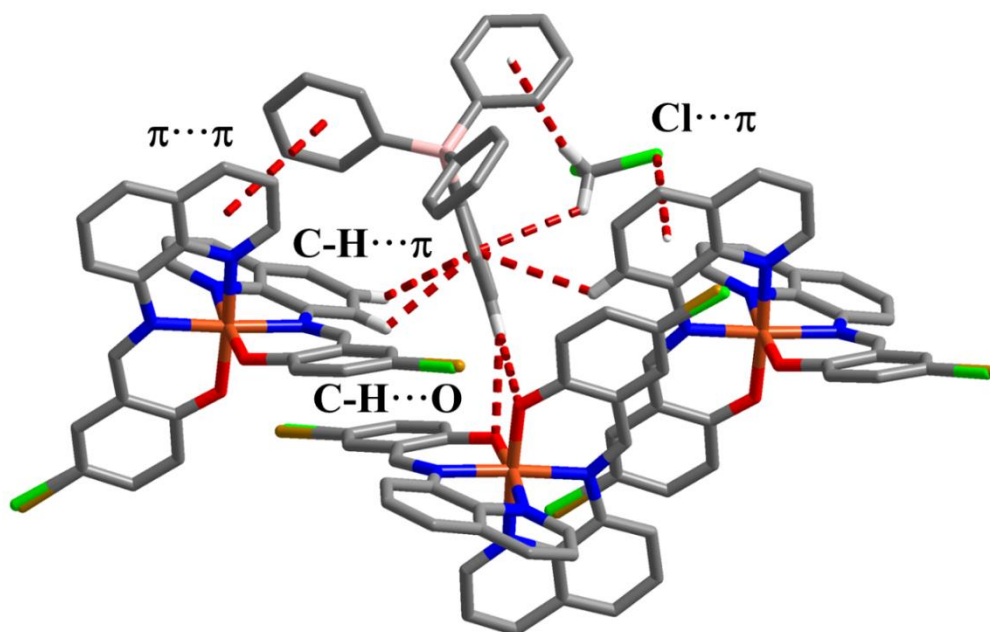


Figure S7 View of the supramolecular connectivity of $[\text{Fe}(\text{qsal-Cl})(\text{qsal-Br})]^+$ cation to the BPh_4^- anion and the CH_2Cl_2 molecule in $[\text{Fe}(\text{qsal-Cl})(\text{qsal-Br})]\text{BPh}_4 \cdot 2\text{CH}_2\text{Cl}_2$ **3**.

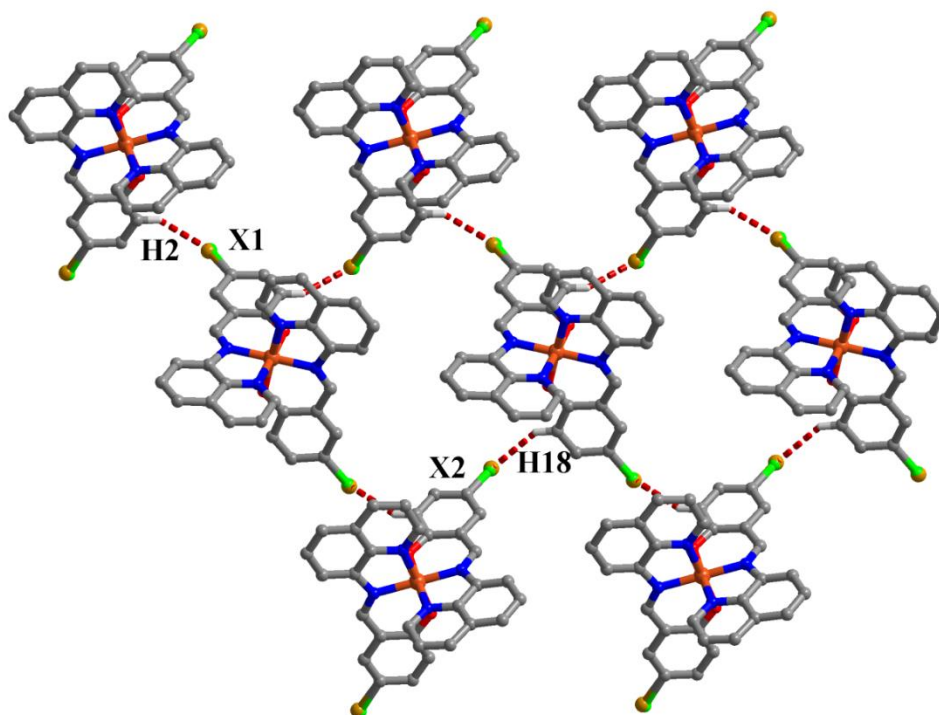


Figure S8 View of the $\text{C-H}\cdots\text{Cl/Br}$ interactions that link the $[\text{Fe}(\text{qsal-Cl})(\text{qsal-Br})]^+$ cations in $[\text{Fe}(\text{qsal-Cl})(\text{qsal-Br})]\text{OTf} \cdot 0.5\text{MeOH}$ **4**.