Supplementary Material (ESI) for Dalton Transactions


# Thermal and Light-Induced Spin-Transitions in Iron(II) Complexes of 2,6-*Bis*(4-halopyrazolyl)pyridines – the Influence of Polymorphism on a Spin-Crossover Compound

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## Electronic Supplementary Information

**Figure S1** Partial packing diagram of $L^2$.

**Figure S2** Alternative partial packing diagram of $L^2$.

**Figure S3** Variable temperature magnetic behaviour of **3**.

**Figure S4** Powder diffraction data for dried **3**.

**Figure S5** DSC data for α-**1** and **2**.

**Figure S6** DSC and TGA data for β-**1**.

**Figure S7** DSC and TGA data for **3**.

**Figure S8** Solution-phase magnetic data in $CD_3NO_2$ for **1** and **2**.

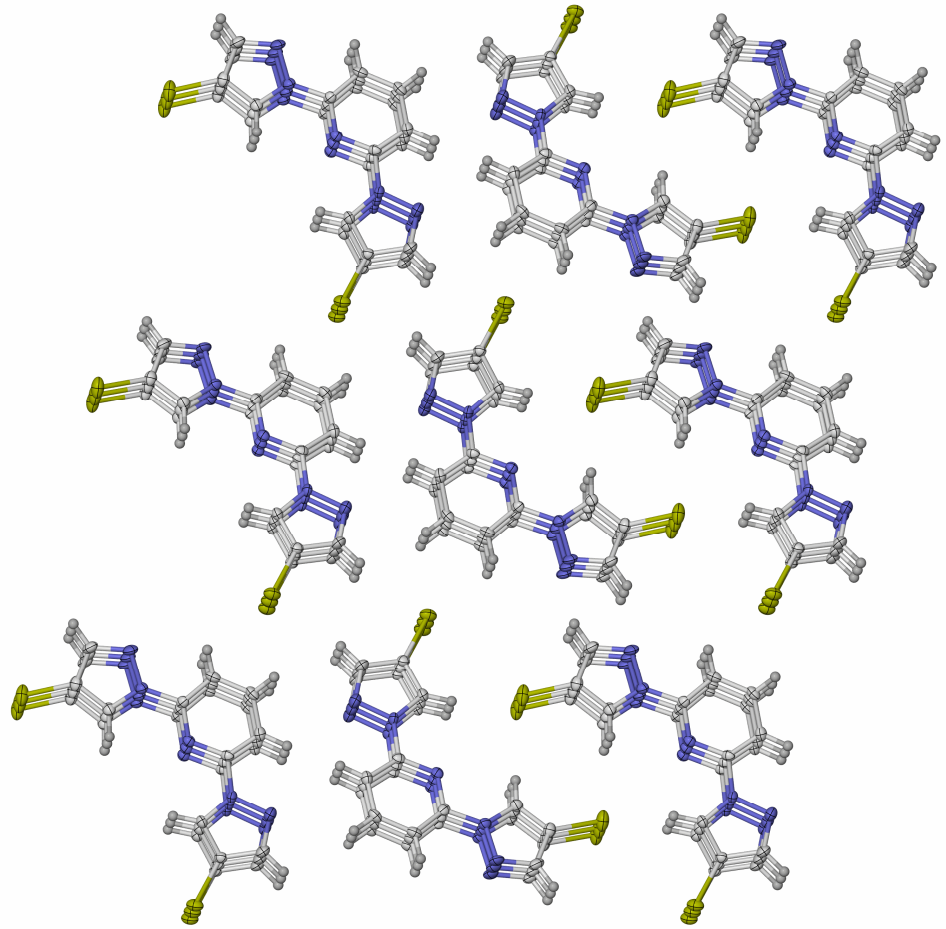


**Figure S1** Partial packing diagram of $L^2$. The view is almost parallel to the (010) crystal plane with [100] horizontal. Crystals of $L^1$ are isostructural with $L^2$, and give a visually indistinguishable molecular structure and packing. Neighbouring molecules in each stack are related by *x*, 1+*y*, *z*, are coplanar by symmetry and are 3.455(9) Å apart [3.422(9) Å in $L^1$]. Colour code: C, white; H, grey; Br, yellow; N, blue.

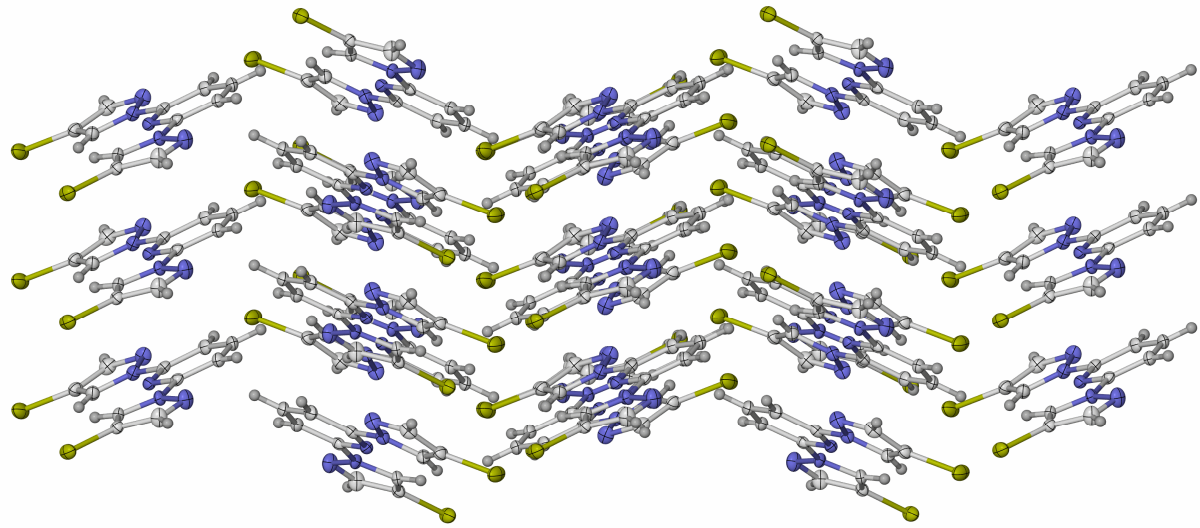


**Figure S2** Alternative partial packing diagram of $L^2$, showing the relative orientations of the stacks of molecules in the lattice. The view is almost parallel to the (102) crystal plane with [010] vertical. Other details as in Fig. S1.

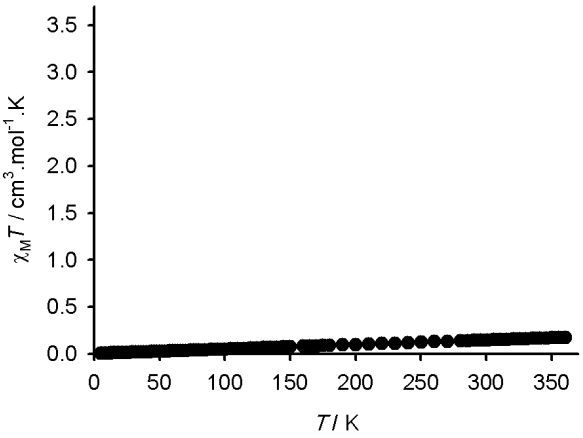



**Figure S3** Variable temperature magnetic behaviour of solid **3**.

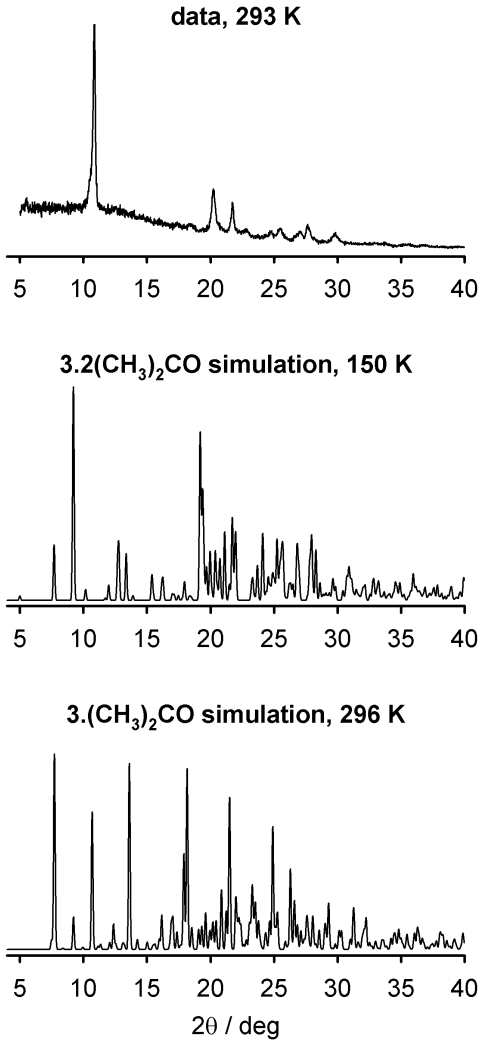
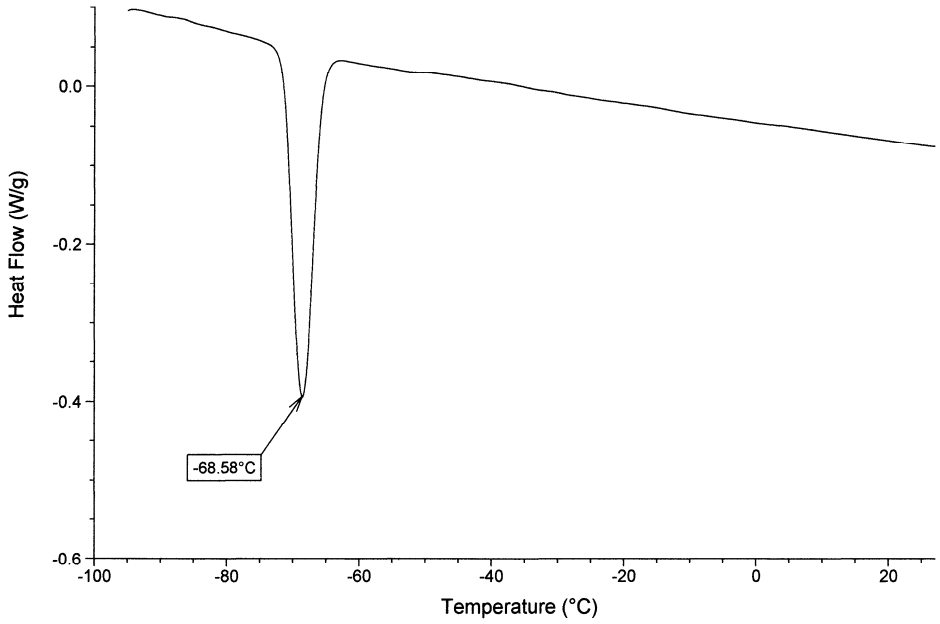
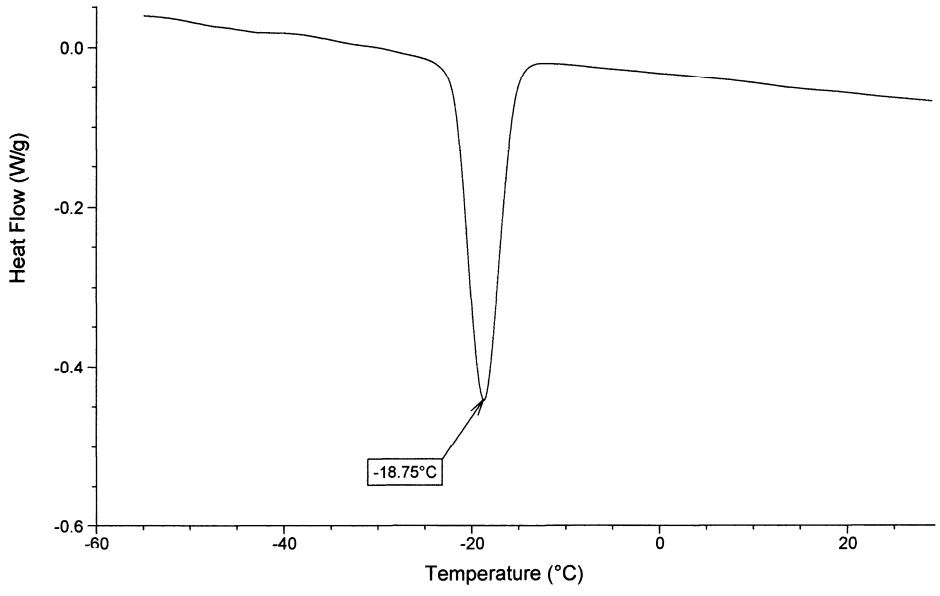



**Figure S4** Powder diffraction data for dried **3**, and simulated powder patterns from the two crystalline acetone solvates. The data show the powder is poorly crystalline, but suggest that most, or all, of the material is derived from the low-spin di-acetone solvate.




**α-1**




**2**

**Figure S5** Differential scanning calorimetry (DSC) data for α-**1** and **2**.

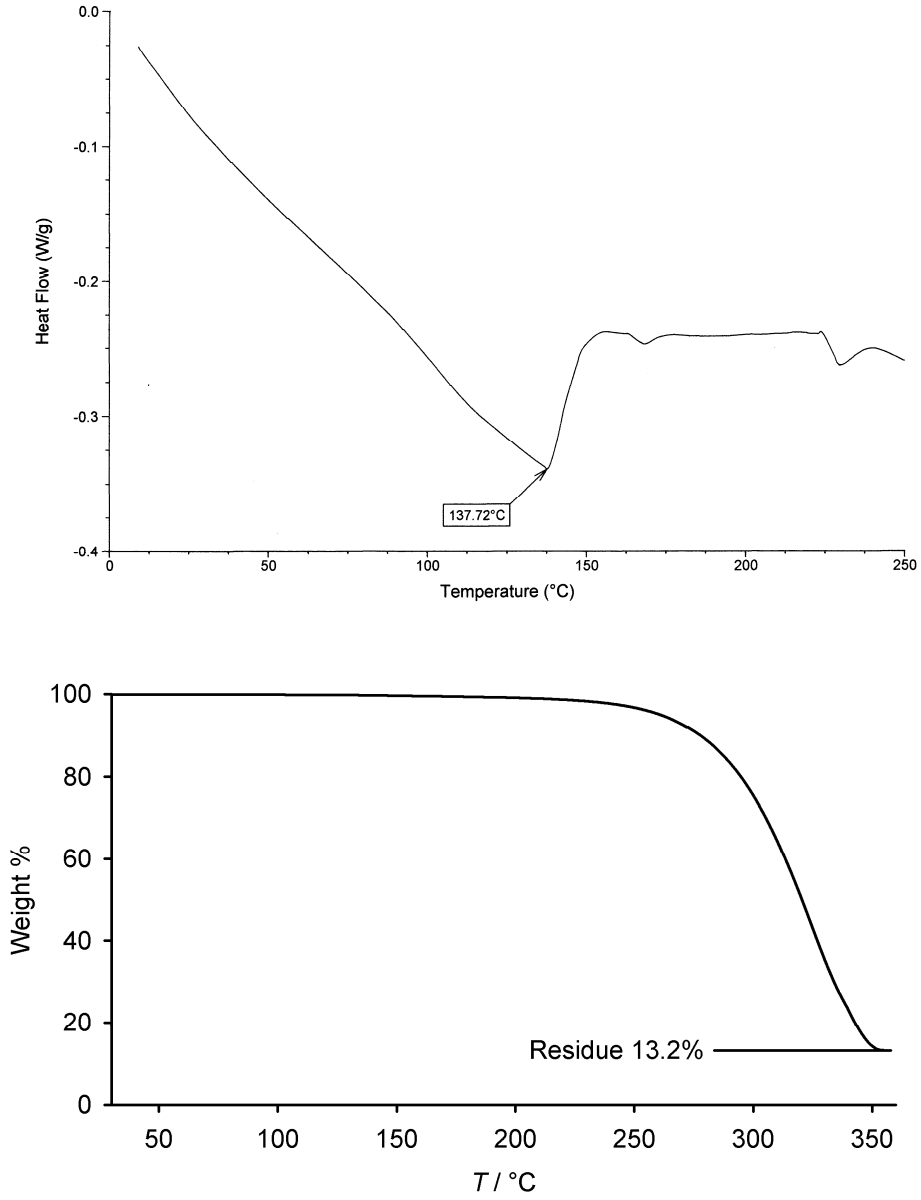



**Figure S6** Differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) data for β-**1**.

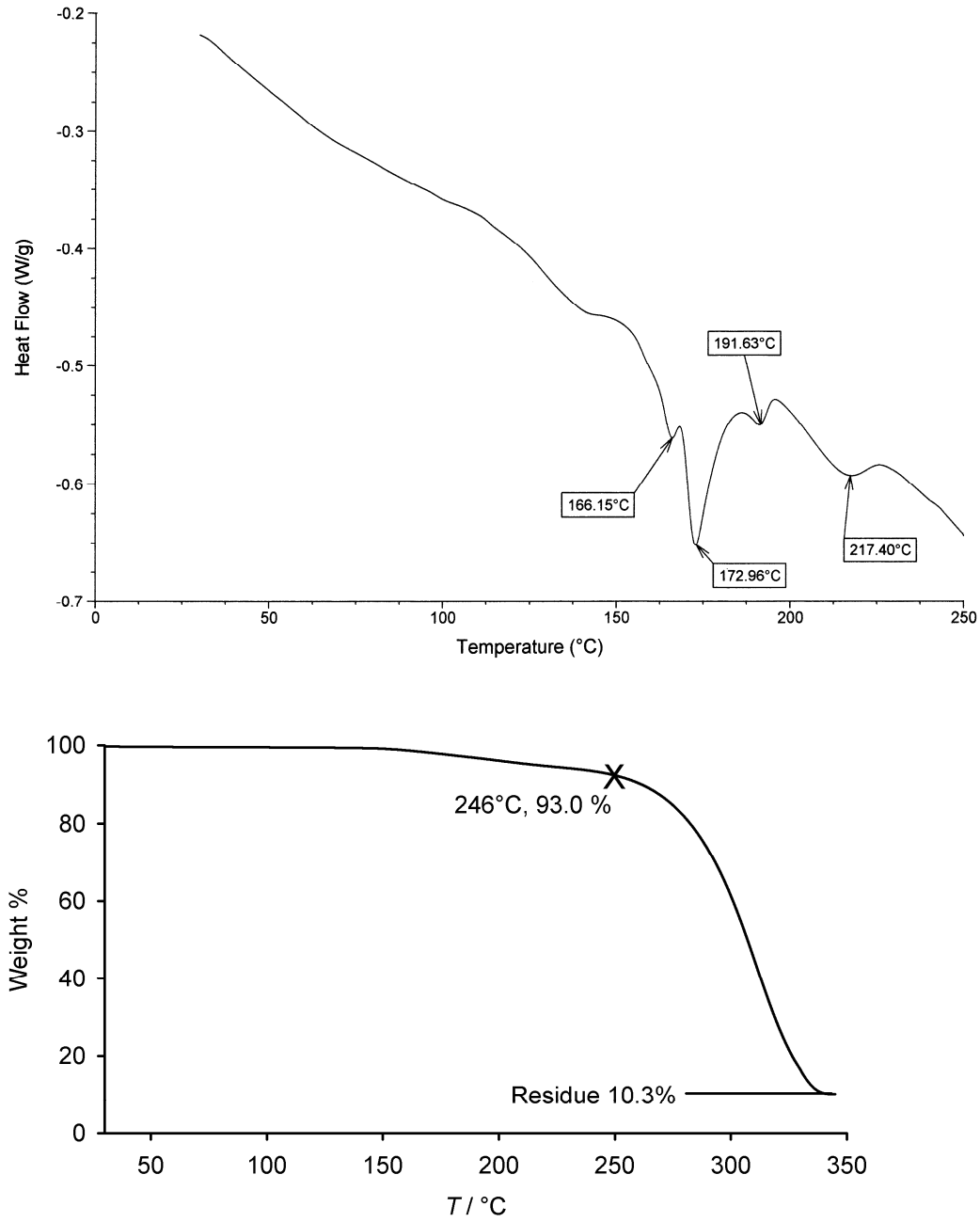



**Figure S7** Differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) data for **3**.

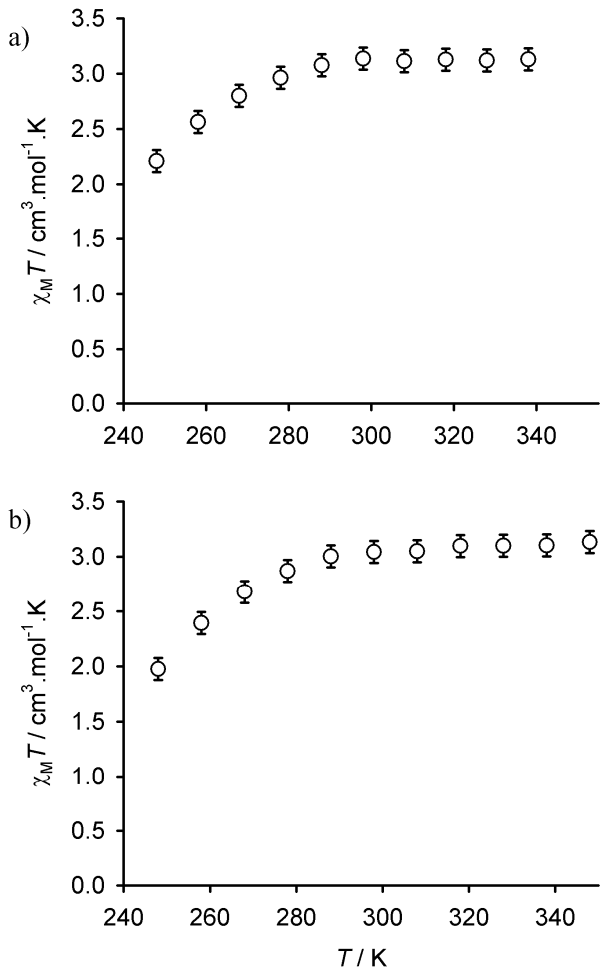



**Figure S8** Solution-phase magnetic data in $CD_3NO_2$ for: a) **1** and b) **2**.