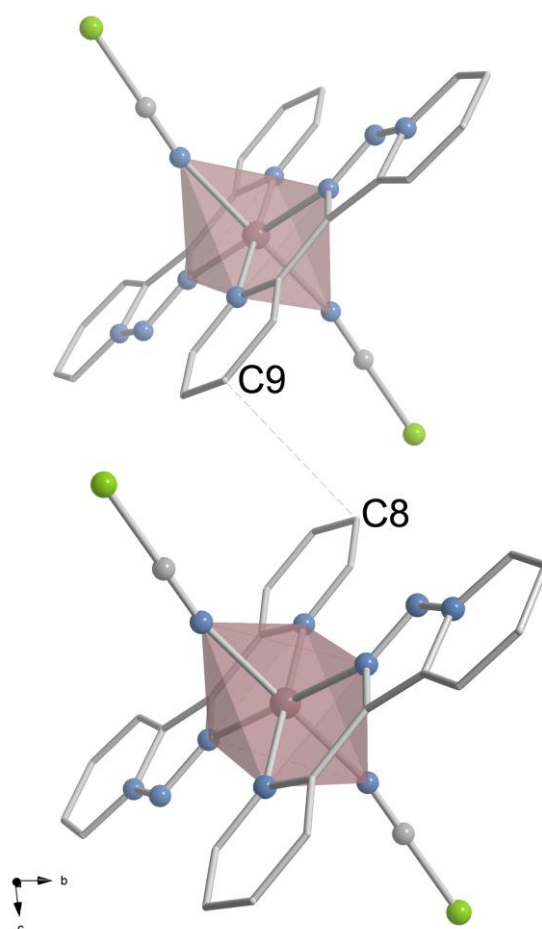


Supporting Information

Structural, magnetic and calorimetric studies of a crystalline phase of the spin crossover compound $[\text{Fe}(\text{tzpy})_2(\text{NCSe})_2]$

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Figure S1. Intermolecular interactions of complex molecules generated by symmetry operation $iii = -x, -y, -z+2$.



Synthesis of precipitated samples of $[\text{Fe}(\text{tzpy})_2(\text{NCSe})_2]$ (**4**)

To a solution of $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$ (69.5 mg, 0.25 mmol) in methanol (5 mL) was added an aqueous solution of KNCSe (51.5 mg, 0.5 mmol) and tzpy (98 mg, 0.5 mmol). The red-orange solution was stirred for two hours under an argon atmosphere. The solvent was removed at reduced pressure and the solid was washed with water to remove traces of K_2SO_4 giving an ocher precipitated of **4** (122 mg, 75%). Figure S2 displays the experimental X-ray powder diffraction pattern (XRPD) of a precipitated sample of **4** (left, red color) together with the XRPD calculated from single crystal data of **4** (left, black) and magnetic behavior (right) of precipitated samples.

Figure S2

