Dalton Transactions

Electronic Supplementary Information (ESI)

Synthesis and mononuclear complexes of the bis-bidentate ligand 2,5-di-(2-pyridyl)-1,3,4-thiadiazole (dptd): spin crossover in $[Fe^{II}(dptd)_2(NCSe)_2]$ and $[Fe^{II}(dptd)_2(NCBH_3)_2]\cdot H_2O$

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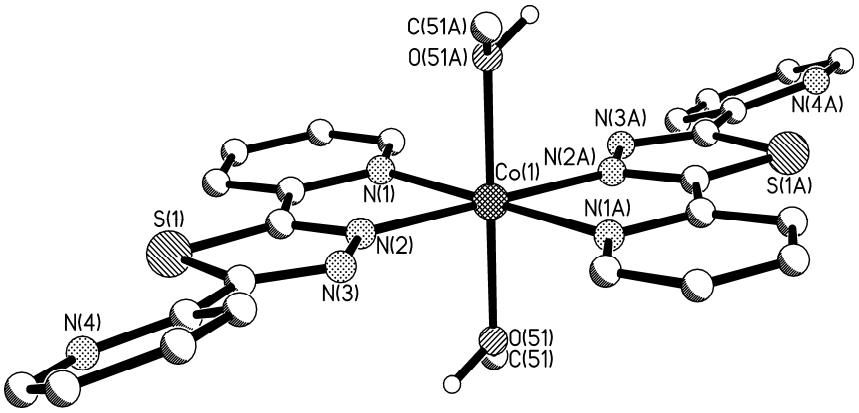

Fig. S1. View of the molecular structure of the complex cation of $[Co^{II}(\mathbf{dptd})_2(MeOH)_2](ClO_4)_2$ (**7**). Hydrogen atoms, except those of the MeOH co-ligands, have been omitted for clarity. Symmetry operation to used to generate equivalent atoms: (A) –x, –y, –z.

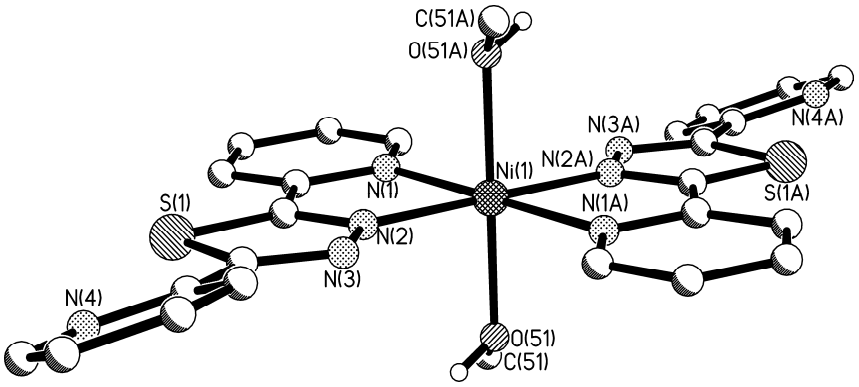

Fig. S2. View of the molecular structure of the complex cation of $[Ni^{II}(\mathbf{dptd})_2(MeOH)_2](ClO_4)_2$ (**8**). Hydrogen atoms, except those of the MeOH co-ligands have been omitted for clarity. Symmetry operation to used to generate equivalent atoms: (A) –x+1, –y+1, –z+1.

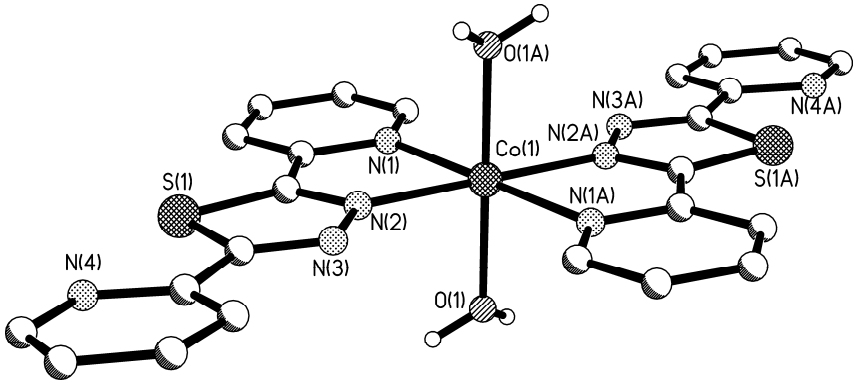

Fig. S3. View of the molecular structure of the complex cation of $[Co^{II}(\mathbf{dptd})_2(H_2O)_2](ClO_4)_2 \cdot 0.5H_2O \cdot \mathbf{dptd}$ (**10**$\cdot 0.5H_2O \cdot$**dptd**). Hydrogen atoms, except those of the H_2O co-ligands, have been omitted for clarity. Symmetry operation to used to generate equivalent atoms: (A) –x, –y, –z.

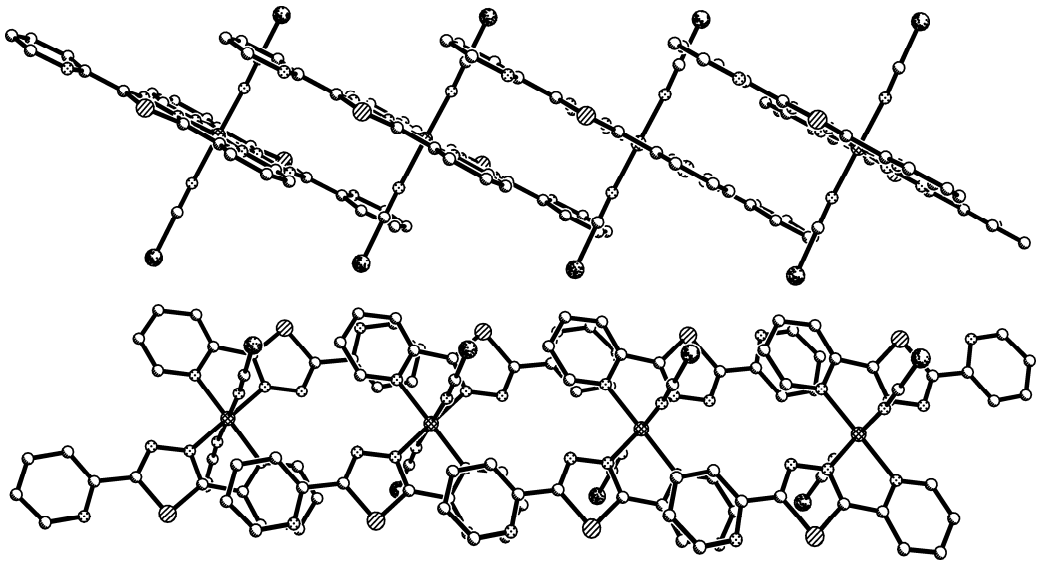

Fig. S4. Side and top views of the crystal structure of **2**·1.5DCM·1.5H_2O, emphasizing the chain motif running along the *a* axis. Hydrogen atoms and solvent molecules have been omitted for clarity.

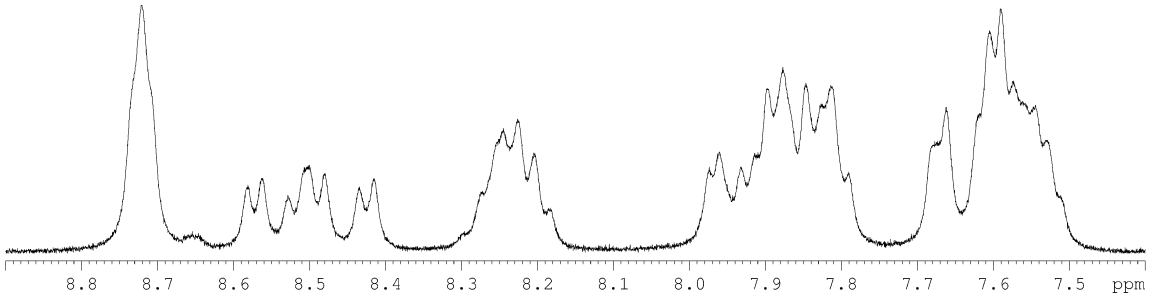

Fig. S5. Aromatic region of the ^{1}H NMR spectrum of [Fe^{II}(**dptd**)$_3$](OTf)$_2$·1.25DCM·0.5H_2O (**5**·1.25DCM·0.5H_2O) in MeCN-d_3 at 243 K.

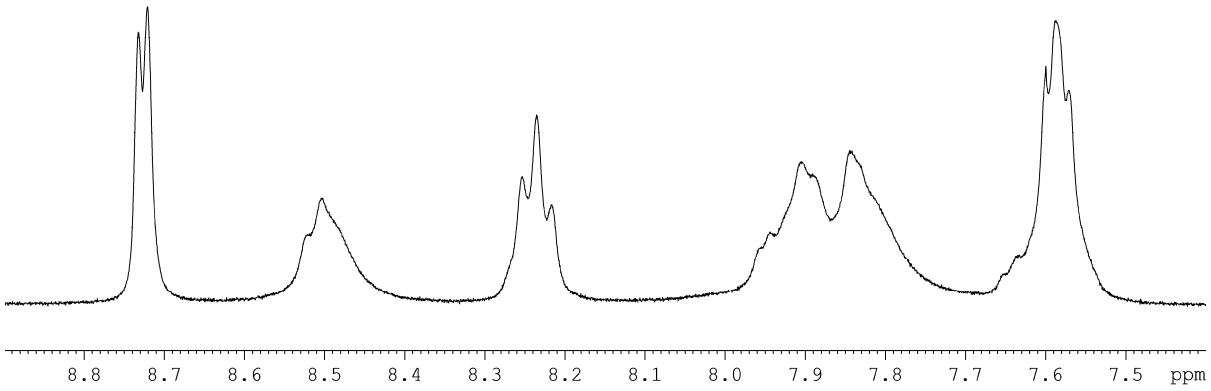

Fig. S6. Aromatic region of the ^{1}H NMR spectrum of [Fe^{II}(**dptd**)$_3$](ClO_4)$_2$·H_2O (**6**·H_2O) in MeCN-d_3 at 298 K.

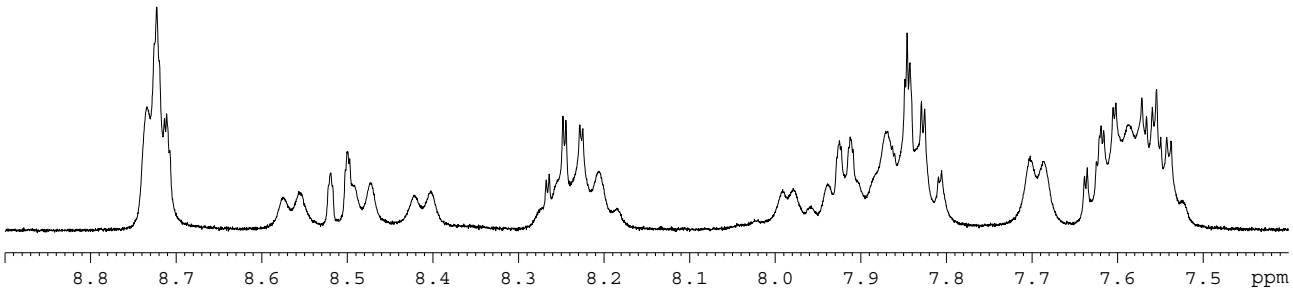

Fig. S7. Aromatic region of the ^{1}H NMR spectrum of $[Fe^{II}(\mathbf{dptd})_3](ClO_4)_2 \cdot H_2O$ (**6**·H_2O) in MeCN-d_3 at 273 K.