SYNTHESIS OF TRIPODAL AZOLE-BASED LIGANDS FOR REDOX ACTIVE TETRANUCLEAR IRON CLUSTER

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Poly-substituted boron compounds featuring three coordination sites have been recognized for intriguing spin crossover (SCO) behaviour in iron(II) complexes. In our approach, we introduced a central carbon [1] linker capable of subsequent post-functionalization, leading to a hydroxy-functionalized tripodal ligand. To investigate the steric influences within the ligand architecture, we varied the heterocyclic moiety in addition to the substitution at the N1-position [2].

By employing diverse synthetic conditions and varying ligand-metal ratios, we successfully synthesized iron(II) complexes displaying distinct coordination arrangements. The kinetic product, an octahedral complex, exhibited SCO activity upon heating due to the removal of a coordinating imidazole ligand [3]. Upon further heating, a Fe₄O₄-cluster emerged as the thermodynamic product. Cyclic voltammetry profiles revealed the redox capacity of the M₄O₄-cubane core, enabling facile cycling through multiple oxidation states and indicating an antiferromagnetic nature. This underscores the intricate interplay between ligand design and the resultant properties, offering valuable insights into the design of multifunctional molecular materials with tailored redox attributes for catalytic or electron-shuttling applications.

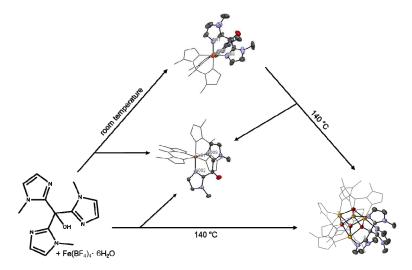


Figure 1. Reaction scheme for the complexation of the three different complexes, with hydrogens, anions, and solvates omitted.

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^[2] Seifried, M. et. al. . *Magnetochemistry*. 2022, 8(9), 95.

^[3] Bruijnincx PCA. ; et. al. Inorg. Chem. 2011, 50(19); 9243-9255