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Nuclear resonance scattering and Mössbauer studies of a trinuclear iron ferrocene complex

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In order to study the cooperativity between the three irons of the trinuclear iron ferrocene complex $[\text{Fe}_4\text{N}_4(\text{CH}_2\text{Fc})_2(\text{Cl})_2]$ synchrotron based spectroscopy such as nuclear inelastic scattering (NIS) and nuclear forward scattering (NFS) have been performed. These techniques are well suited to investigate valence tautomerism which denotes an intramolecular redox reaction over an energy barrier between two metal ions or between one metal ion and a redox active ligand. The NFS data display a quantum beat structure reflecting a quadrupole splitting of $\Delta E_Q = 0.99 (\pm 0.02)$ mms⁻¹. This is indicative of a ferric high-spin state for the central iron of this complex.

The partial density of vibrational states (pDOS) determined experimentally by NIS measurements provides information about the vibronic properties of the complex. For a better understanding of these results, density functional theory (DFT) calculations have been performed on this complex.

Furthermore, we have also carried out conventional Mössbauer spectroscopy to observe a possible electron transfer from the iron of the ferrocene ligand to the central iron ion. In addition, the zero field splitting D and the rhombicity E/D have been determined by measurements at 4.2 K and different external magnetic fields.

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