

S3-1.5

Spin Crossover in Trinuclear and Protonated Tetranuclear Iron(II) Complexes: DFT Modelling

S.I.Klokishner and O.S.Reu

Institute of Applied Physics, Academy str. 5, MD 2028, Chisinau, Republic of Moldova

In the present study the course of spin transformation in the linear trinuclear $[\text{Fe}_3(\text{bntrz})_6(\text{tcnset})_6]$ complex, exhibiting a complete one step transition at $T=318\text{K}$, and in the tetranuclear protonated $[\text{Fe}_4(\text{H}_6\text{L}_4)]^{6+}$ and $[\text{Fe}_4(\text{H}_8\text{L})]^{8+}$ complexes is examined with the aid of DFT single point energy calculations. The suggested approach allowed to explain the peculiarities of spin crossover observed in the $[\text{Fe}_3(\text{bntrz})_6(\text{tcnset})_6]$ compound. The DFT study of the energy pattern of the tetranuclear $[\text{Fe}_4(\text{H}_8\text{L})]^{8+}$ complex at low and high temperatures revealed, that upon deprotonation of the complex the number of the Fe^{II} ions participating in the spin crossover transformation is reduced from two Fe^{II} ions to one.