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Spin Crossover in Iron(II) Complexes with Mixed Nitrogen-Sulfur Coordination: DFT Modeling

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The majority of known Fe^{II} spin crossover (SCO) complexes are based on a homogeneous octahedral nitrogen coordination of the metal ion. Currently a new type of compounds with mixed nitrogen-sulfur ligand surroundings of the iron(II) ions demonstrating spin transitions has attracted much attention. Despite the comprehensive experimental characterization the origin of SCO phenomena in these complexes has not been elucidated. In the present paper on the basis of DFT calculations we describe the course of the spin transformation in the γ-polymorph of the $[Fe(bpte)(NCSe)_2]$ compound containing in the unit cell two different types of iron(II) ions which differ in the geometry of the $\{N_4S_2\}$ ligand surroundings. To prove the adequacy of the suggested approach in the present paper the well known picture of SCO in the thoroughly characterized classic $[Fe(ptz)_6](BF_4)_2$ compound is also reproduced.