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Spin Crossover [Fe(qsal)2]X (X = Cl, SCN, CF3SO3) Complexes: EPR and DFT Study

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Abstract

The compounds [Fe(qsal)2]X (X = Cl, SCN, CF3SO3) were synthesized and investigated by electron paramagnetic resonance (EPR). The dependence of the Fe(III) spin state on the type of counterion X and on the temperature was established. On the basis of the density functional calculations, the geometrical parameters of compounds in high- and low-spin states were optimized and the difference in their internal energies was calculated. A correlation between the experimental EPR data and the theoretically calculated energy difference between the high-spin and the low-spin states of the compounds with different anions was obtained. © 2010 Springer-Verlag.

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