

# Stepwise Magnetic Behavior of the Liquid Crystal Iron(III) Complex

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## Abstract

EPR and Mossbauer spectroscopy is used to study a new liquid crystal complex of iron(III) with a Schiff base: 4,4'-dodecyloxybenzoyloxybenzoyl-4-oxosalicylidene-2-aminopyridine with a PF<sub>6</sub><sup>-</sup> counterion. It is shown that Fe(III) ions exist only in the high-spin (HS,  $S = 5/2$ ) state. It is found that under the influence of temperature the system demonstrates the stepwise behavior of the product of the integrated intensity of EPR lines ( $I$ ) and temperature (proportional to "where" is the magnetic susceptibility) with an inflection point at 80 K. Above 80 K a new EPR spectrum is detected due to the excited  $S = 2$  state and the formation of dimeric molecules (through oxygen bridges) with a strong intramolecular antiferromagnetic exchange interaction  $J_1 = 162.1$  cm<sup>-1</sup>. Below 80 K iron(III) complexes are organized in 1D chains where the exchange value  $J_2 = 2.1$  cm<sup>-1</sup>. At 80 K there is a structural phase transition in the system: the transition from a 1D chain organization of HS Fe(III) centers to dimeric molecules. Based on quantum chemical calculations a model of the binuclear iron(III) complex is proposed. Copyright © 2013 by N. E. Domracheva, V. E. Vorob'eva, A. V. Pyataev, R. A. Manapov, E. M. Zueva, M. S. Gruzdev, U. V. Chervonova.

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## Keywords

DFT., Electron paramagnetic resonance (EPR), Fe(III) complexes, Liquid crystals, Mossbauer spectroscopy, Magnetic properties, Quantum chemical calculations, Schiff bases, Spin-crossover