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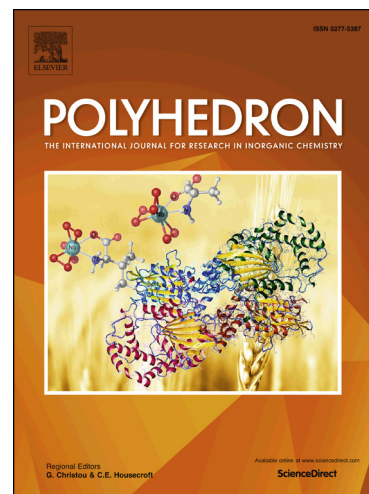
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High-spin Fe(III) Schiff based complexes with photoactive ligands. Synthesis, EPR study and magnetic properties.

M. S. Gruzdev,^[1] V. E. Vorobeva,^[2] E. M. Zueva,^[3,4] U. V. Chervonova,^[1] M. M. Petrova,^[5]
N. E. Domracheva^[2]*

^[1] G.A. Krestov Institute of Solution Chemistry, Russian Academy of Sciences, Akademicheskay str. 1, 153045 Ivanovo, Russia

^[2] Zavoisky Physical-Technical Institute of FRC Kazan Scientific Center of RAS, Sibirsky Tract 10/7, 420029 Kazan, Russia

^[3] A.E. Arbuzov Institute of Organic and Physical Chemistry of FRC Kazan Scientific Center of RAS, Arbuzov str. 8, 420088 Kazan, Russian Federation

^[4] Kazan Federal University, Kremlyovskaya str. 18, 420008 Kazan, Russian Federation

^[5] Kazan National Research Technological University, K. Marx str. 68, 420015 Kazan, Russian Federation

Corresponding Authors

Dr. Gruzdev Matvey Sergeevich

* E-mail: gms@isc-ras.ru

Phone: +7(4932)336265

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ABSTRACT

A series of three novel Fe(III) compounds of the formula $[\text{FeL}_2]\text{X}$ (where $\text{X} = \text{Cl}^-$ (**1**), PF_6^- (**2**), NO_3^- (**3**), and L is a photoactive ligand, (4)-4-(((2-(ethylamino)ethyl)imino)methyl)-3-hydroxyphenyl 4-bromobenzoate) was synthesized and studied by means of electron paramagnetic resonance (EPR) and pulsed laser irradiation. The Fe^{3+} ions in these compounds are in a high-spin state. A thorough analysis of the EPR data suggests that compounds **1** and **2** undergo an order-disorder ferroelectric phase transition, and below the phase transition temperature ($T_c = 100$ and 200 K for compounds **1** and **2**, respectively) a nonzero average electric dipole moment appears. To get an insight into molecular structure of Fe^{3+} ions and their supramolecular organization in low-temperature (LT) and high-temperature (HT) phases of compounds **1** and **2**, a series of density functional theory calculations was performed. On the basis of our

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