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Modeling of the Valence Tautomeric Transformation in Heterometallic [Cr-dhbq-Co] Molecules

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In the present communication we report a model that describes the valence tautomeric transformation in a crystal consisting of heterometallic [Cr-dhbq-Co] molecules. The model takes into account the states arising from two different configurations of the molecule, namely, Cr^{3+}-$dhsq^{3-}$ -Co^{3+} and Cr^{3+}-$dhsq^{2-}$- Co^{2+}, the Heisenberg exchange interaction between the $dhsq^{3-}$ ligand and the Cr^{3+} ion as well as the cooperative electron-deformational and dipole-dipole interactions. The problem is solved in the mean field approximation. The main peculiarities of the valence tautomeric transformation are elucidated. It is demonstrated that the electron transfer ligand-Co is accompanied not only by the significant increase of the effective magnetic moment but also by the appreciable change in the microscopic polarization. The model provides quite a good description of the experimental data on the temperature dependence of the effective magnetic moment in the $[(Cr(SS\text{-cth}))(Co(RR\text{-cth}))(\mu\text{-dhbq})](PF_6)_3$ compound.