

Switching of Magnetic and Polarizability Characteristics of Dinuclear [CrCo] Complexes via Intramolecular Electron Transfer

S.I. Klokishner, O.S. Reu and M.A. Roman

Institute of Applied Physics, Academy str. 5, MD 2028, Chisinau, Republic of Moldova

A model has been developed to describe the valence tautomeric transformation in a crystal containing as a structural element trinuclear complexes with electronic configurations $\text{Cr}^{3+} - dhsq^{3-} - \text{low-spin Co}^{3+}$ and $\text{Cr}^{3+} - dhbq^{2-} - \text{high-spin Co}^{2+}$ at low and high temperatures, respectively. The model takes into account the antiferromagnetic exchange coupling between the $dhsq^{3-}$ -ligand with the itinerant electron and the Cr^{3+} - ion, the ferromagnetic exchange coupling $\text{Cr}^{3+} - \text{high-spin Co}^{2+}$ as well as the interaction of the Co-ion with the full symmetric breathing mode of the nearest crystal surrounding producing a strong localizing effect. In the model there are also accounted for the cooperative dipole-dipole and electron-deformational interactions. The parameters of the main interactions governing the observed phenomena are evaluated through DFT calculations. The interplay between the intracluster exchange coupling and the cooperative interactions has been demonstrated to lead to gradual and abrupt spin transitions as well as to those accompanied by a hysteresis loop. Within the framework of the suggested model a qualitative and quantitative explanation is given of the magnetic susceptibility of the $[(\text{Cr}(\text{SS-cth})(\text{Co}(\text{RR-cth})(\mu - dhbq)))(\text{PF}_6)_2\text{Cl}]$ compound.