S3-1.9

Temperature Induced Spin Transition in Co(II) Complex

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A crystal containing a Co(II) ion in the octahedral cubic surrounding as a structural element is examined. The total Hamiltonian of the crystal includes the crystal field acting on the Co(II) ion, the spin-orbital interaction within the high spin $^4T_1$ –state of this ion, the interaction of the Co ions with spontaneous lattice strains arising on the $^2E \rightarrow {}^4T_1$ transition, the electron-vibrational interaction and free molecular vibrations. The mechanism responsible for the observed spin conversion is assumed to be the interaction of the Co ions with two spontaneous lattice strains, namely, with the fully symmetric (A_1) and tetragonal E one. The interaction with E symmetry strain is strong only for the low spin ^2E –state arising from the d^7 electronic configuration with a single d-electron in the e-orbital, while for the high spin state $^4T_1$ it can be neglected. Basing on the experimental X-ray data, in the model only the u-component of the E type deformation is accounted for. In fact in the model there are examined two types of A_1 and E vibrations, namely, the molecular ones and those of the intermolecular type. The molecular vibrations directly coupled to the electronic shells of the spin crossover ions form the energy spectra of these ions, while the intermolecular vibrations transmit the local strains throughout the crystal and are responsible for cooperativity. The problem of interacting Co ions is solved in the mean-field approximation. The main characteristic parameters of the model are calculated microscopically. An explanation of the experimental magnetic behavior of the $[Co(pyterpy)_2](PF_6)_2$ compound is given. The different role of the cooperative interactions, namely, the electron-deformational one and that arising from the Jahn-Teller interaction in the spin transformation is demonstrated.

The support of the National Agency for Research and Development of Moldova (project 20.80009.5007.19) is highly appreciated.