Non-uniform coupling model of the Cr_8Ni ring

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We analysed the magnetic properties of a ring of eight chromium ions doped with one nickel ion, denoted in short Cr_8Ni. By making calculations for smaller rings we have demonstrated that the chromium and nickel anisotropies can be neglected for modeling the susceptibility in the considered temperature range due to their relatively low values. Omission of anisotropy allowed us to make simulations for three models with different degrees of diversification of the exchange integrals between chromium ions, using a genetic algorithm. The models revealed better agreement with experiment than those previously known from literature. We also calculated the magnetization in a magnetic field and compared the results with experimental data, which so far have not been taken into account for modelling. We calculated the energy structure as a function of the ratio of the exchange integral between chromium and nickel ions to the remaining integrals, and have determined the energy differences for the selected transitions, which may be expected to be observed in the INS experiment.

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