

On the interpretation of the optical spectra of iron-group ions

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Abstract

The positions of the energy levels of free ions of the iron group V²⁺, Cr³⁺, Mn⁴⁺, Fe⁵⁺, and Co⁶⁺, whose ground configuration is 3d³, and Co²⁺, Ni³⁺, Cu⁴⁺, and Zn⁵⁺, whose configuration is 3d⁷, are interpreted theoretically within the framework of the single-configuration approximation with a Hamiltonian that takes into account real electrostatic, spin-orbit, and spin-spin interactions, as well as electrostatic and spin-orbit interactions correlated by configuration mixing. It is shown that the correct positions of all the energy levels are determined when the Hamiltonian includes the operators of the theory of the nonlinear configuration interaction. The most correct theoretical description of the experimental spectra is obtained by taking into account relativistic interactions and correlation effects of spin-orbit interactions. Semiempirical parameters of the interactions included into the Hamiltonian are found for all the ions. © Nauka/Interperiodica 2006.

<http://dx.doi.org/10.1134/S0030400X06030039>
