A New User-Friendly Software for Effective Analysis of Rare Earth Spectroscopy

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Abstract

Based on Racah's [1] famous angular momentum tensor operator techniques, the complex spectra of *f*-shell electrons (including lanthanide and actinide ions) have been successfully parametrized with both free-ion and crystal field interactions. The free-ion interactions consist of not only the major electrostatic and spin-orbit interactions but also many minor correctional terms such as configuration interactions (in the form of odd rank two-particle operators and three-electron effective operators) and several kinds of intra-atomic magnetic interactions (i.e. spin-spin, spin-other-orbit and electrostatically-correlated spin-orbit interactions) for *f*-shell electrons. The crystal field interactions are sometimes extended from a one-particle Hamiltonian to a two-particle one for incorporating correlation crystal field effects. However, there are several gaps recently found in the literature on the proper use (or the corresponding computer programme) of this model Hamiltonian to fit the atomic spectra of *f* electrons. Examples include the errors in the reduced matrix elements for some magnetic interactions [2], omission of the spin-spin interaction [3], truncation of the Hamiltonian matrix for f^4 to f^{10} configurations, high correlation between some parameters in incomplete set of observed energy levels, improper use of parameters or reduced matrix elements for conjugate configurations as well as negligence and/or incorrect identification of the irreducible representations of the observed states [4]. Therefore, a new user-friendly Windows-based computer package has been independently developed (i.e. not based on or modified from any other researchers' package) to address the aforementioned issues in the analysis of the lanthanide spectroscopy. In particular, it allows the researcher to interactively carry out the fitting of various parameters to the observed energy levels with different tentative assignment of irreducible representations for any one of the 32 crystallographic point groups.

References:

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