CHEMISTRY JOURNAL OF MOLDOVA. General, Industrial and Ecological Chemistry. 2023, 18(2), 78-86
ISSN (p) 1857-1727 ISSN (e) 2345-1688
http://cjm.ichem.md
http://doi.org/10.19261/cjm.2023.1146

ON THE CALCULATION OF LANTHANIDE SYSTEMS. THE SPECTRAL PARAMETERS OF PRASEODYMIUM TRIVALENT ION

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Abstract. In this work, taking the Pr(III) ion as a suitable case study, the authors test the capacity of a series of Gaussian Type Orbitals (GTOs) basis sets to account for the atomic spectra of lanthanide ions. An extended relevance of this assessment can be found in modeling the luminescence of lanthanide-based materials. It was selected the Pr(III) case because it shows a rather rich collection of experimental data, emerging from the f^2 and *fd* configurations. The energy barycenters of spectral multiplets can be equated analytically in terms of the so-called Slater-Condon parameters. By multi-configurational *ab initio* procedures, with basis sets from existing GTO repositories, the calculated $f \rightarrow f$ transitions are moderately higher than the experimental values, while the relative energies of $f \rightarrow d$ states undergo both under- and over-estimation. The GTO shortcomings, that are impacting the accuracy, were debated, the critical perspective spreading the seeds of future development.

Keywords: lanthanide ion, luminescence, spectral term, Slater-Condon parameter, a*b initio* calculation.

Received: 26 November 2023/ Revised final: 14 December 2023/ Accepted: 15 December 2023