COMPARATIVE CRYSTAL FIELD ANALYSIS OF THE Ni^{2+} ENERGY LEVEL SCHEME IN $CdCl_2$, $CdBr_2$, CdI_2 CRYSTALS

Mikhail G. BRIK[1], Nicolae M. AVRAM[2], Calin N. AVRAM[3]

Abstract. *The exchange charge model of crystal field was used to calculate the crystal field splitting of all Ni^{2+} energy levels ($3d^8$ electron configuration) in three structurally similar crystals of $CdCl_2$, $CdBr_2$, and CdI_2. The influence of the nature of the ligands and interionic distances on the values of the crystal field parameters and location of the split energy levels and relative intervals between them was identified. Comparison of the calculated energy levels with the experimental results available in the literature yielded good agreement.*

Keywords: Crystal field theory; Transition metal ions; Crystal field strength; Racah parameters.

1. Introduction

The transition metal ions with the unfilled 3d electron shell are widely used in various applications, such as lasing [1,2], lighting [3], optical thermometry [4,5] etc. Their absorption and emission spectra are essentially dependent on the host matrix, since the electronic states arising from the open 3d electron shell strongly interact with the nearest crystalline environment.

The theory of crystal field is a powerful tool that has been successfully applied to analyze the optical spectra of the transition metal and rare earth ions in crystals [6]. Different models of crystal field that have been developed so far allow to establish firm and deep connections between the crystal structure (the nearest surrounding of an impurity ion) and chemical nature of the surrounding ions on the one hand and the overall splitting of the impurity ion's energy levels on the other hand.

In this connection, comparative studies of the crystal field effects and impurity ions energy levels splitting for a number of similar or different systems are of special importance. For example, calculations of energy level schemes of the same impurity ion in several isostructural crystals highlight the role of the host material in the formation of the impurity ion's spectra [7, 8]. Alternatively, calculations of spectra

[1]Prof., Dr. hab., College of Sciences & CQUPT-BUL Innovation Institute, Chongqing University of Posts and Telecommunications, Chongqing, 400065, People's Republic of China; Institute of Physics, University of Tartu, W. Ostwaldi Str. 1, Tartu, 50411, Estonia; Institute of Physics, Jan Dlugosz University, PL-42200, Czestochowa, Poland, (e-mail: mikhail.brik@ut.ee).
[2]Prof., PhD, Department of Physics, West University of Timisoara, Bd. V. Parvan, No. 4, 300223, Timisoara, Romania and Academy of Romanian Scientist, Independentei 54, 050094, Bucharest, Romania (e-mail: n1m2marva@yahoo.com).
[3] Assistant Prof., PhD, Department of Physics, West University of Timisoara, Bd. V. Parvan, No. 4, 300223, Timisoara, Romania (e-mail: calin.avram@e-uvt.ro).