First-Principles Analysis of the Rb_2CrF_6 Absorption Spectrum

Mikhail G. Brik

Department of Chemistry, School of Science and Technology, Kwansei Gakuin University,
2-1 Gakuen, Sanda, Hyogo 669-1337, Japan

Reprint requests to Dr. M.G. B.; E-mail: brik@fukui.kyoto-u.ac.jp and brik@ksc.kwansei.ac.jp

Z. Naturforsch. **61a,** 293 – 298 (2006); received February 27, 2006

A systematic first-principles analysis of the energy level scheme and absorption spectrum of Cr^{4+} in Rb_2CrF_6 crystal is presented. The recently developed first-principles approach to the analysis of the absorption spectra of ions in crystals based on the discrete variational multi-electron (DV-ME) method was used in the calculations. The method is based on the numerical solution of the Dirac equation and has a wide area of applicability. As a result, the complete energy level scheme of Cr^{4+} and its absorption spectrum were calculated, assigned and compared with available experimental literature data on the ground state absorption. Numerical contributions of all possible electron configurations to the wave functions of the calculated states were determined. By analysing the molecular orbitals population, numerical contributions of the fluorine 2p- and 2s-orbitals to the 3d-molecular orbitals were determined. The significant contribution of the ligand's wave functions shows the high degree of covalency in the considered crystal. – PACS numbers: 71.70.Ch, 71.70.Ej

Key words: First-Principles Calculations; Crystal Field Theory; 3d-Ions; Ground State Absorption.