Optical absorption spectra of divalent neodymium (Nd^{2+}) in bromide and iodide hosts.

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Streszczenie

Optical Absorption Spectra of Divalent Neodymium (Nd2+) in Bromide and Iodide Hosts The electronic spectra for Nd2+ions in bromide andiodide hosts are reported for the first time. These spectra, to-gether with the recently obtained spectra for the chloride ma-trix, constitute a substantial series of Nd2+spectra in crystals.Importantly, these crystals differ in the factors important for thephysical properties of the divalent lanthanide Ln2+ions; that is,the ligand's chemical character and the symmetry of the crystalfield. The available experimental data allow systematic investi-gations of the impact of these factors on the electronic spectra,and thus, spectroscopic properties of Nd2+ions. These investi-gations are the main aim of this study. The results indicate that Optical Absorption Spectra of Divalent Neodymium (Nd2+) in Bromide and Iodide Hosts due to the increasing covalence of the Nd2+environment in theCl–Br–I series, the energy of the first f–d transition shifts intothe infrared region, from 6121 cm–1for SrCl2/Nd2+to ca.5260 cm–1for SrI2/Nd2+, whereas the strength of the crystalfield decreases along this series. Calculations using the para-metric Hamiltonian and superposition model are carried outto quantitatively interpret the measured spectra. The simulatedspectra exhibit good agreement with the experimental spectra.Using the proposed approach, a meaningful interpretation andassignment of the bands observed in the spectra has beenachieved.

Słowa kluczowe

neodymium, structure elucidation, ligand effects, lanthanides, divalent neodymium