Optical spectroscopy and structure of neodymium complexes with 2,6-pyridine-dicarboxylic acid in solution and single crystal at room and low temperatures.

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Streszczenie

X-ray characterization of a compound reported as $Na_3[Nd(dpa)_3].15H_2O$ by Albertsson was repeated and it was found to be a 14-hydrate. Absorption spectra of the crystal were measured along the a axis at room temperature and at 5 K. The results for the crystal were compared with those for Nd(III) aquoion and Nd(III)-dipicolinate solutions. Intensities of the f-f transitions were analyzed according to the Judd-Ofelt theory. The good correspondence between the values of oscillator strength of the hypersensitive transition for $[Nd(dpa)_3]^{3-}$ complex in solution and in the crystal suggests an analogy between the coordination polyhedra; however, the crystal field splitting is different, best seen for the $I^4_{9/2} \rightarrow {}^2P$ transition. The contribution of polarization and electrostatic field mechanisms to the oscillator strengths is discussed.

Słowa kluczowe

X-Ray structure, Absorption, Intensity analysis, Nepheloauxetic effect

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