

Relationships between structure and spectroscopic properties of Nd³⁺ ethylenediaminetetramethylene-phosphonates and ethylenediaminetetraacetates.

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The structural and spectroscopic properties of the Nd³⁺ compounds [C(NH₂)₃]₇[Nd(EDTMP)(CO₃)]·10H₂O, K₁₇H₃[Nd₄(EDTMP)₄]·36H₂O, [C(NH₂)₃][Nd(EDTA)(H₂O)₃] and Na[Nd(EDTA)(H₂O)₃]·5H₂O are presented (H₄EDTA = ethylenediaminetetraacetic acid, H₈EDTMP is a phosphonic acid analogue of H₄EDTA). The obtained monomeric [Nd(EDTMP)(CO₃)]⁷⁻ and tetrameric [Nd₄(EDTMP)₄]²⁰⁻ structures, in which bidentate carbonate and tridentate bridged phosphonate coordination patterns appear, are exceptional. The use of different countercations has allowed us to assess their role in crystal formation and their influence on the spectroscopic properties of the investigated crystals. The countercations slightly change the geometry of [Nd(EDTA)(H₂O)₃]⁻ and some subtle modifications of the geometry of the carboxylic groups is observed. These changes are discussed in the context of hypersensitive transition intensities. The intensities of the f–f transitions in all studied crystals were determined and analyzed basing on the Judd–Ofelt theory. Luminescence of the Nd³⁺ ions in the NIR region could be observed solely in the phosphonate complexes. The luminescence quantum yields were calculated from the luminescence lifetimes and the Judd–Ofelt parameters. The Φ value for the rigid tetramer [Nd₄(EDTMP)₄]²⁰⁻ is twice as large (7 %) as that for the monomer [Nd(EDTMP)(CO₃)]⁷⁻ (3.5 %).

Słowa kluczowe

lanthanides, structure elucidation, luminescence,
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