

Structure and optical spectroscopy of holmium(III) triethylenetetraaminehexaacetate in single crystal and in solution.

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The crystal structure of $[\text{C}(\text{NH}_2)_3]_3[\text{Ho}(\text{ttha})]\cdot 3\text{H}_2\text{O}$ (H_6ttha =triethylenetetraaminehexaacetic acid) has been determined. The coordination environment of the Ho^{III} ion is composed of five carboxylate oxygen atoms and four nitrogen atoms. Electronic absorption spectra of a $[\text{C}(\text{NH}_2)_3]_3[\text{Ho}(\text{ttha})]\cdot 3\text{H}_2\text{O}$ single crystal were measured at room and liquid helium temperatures and compared with those of the $\text{Ho}^{\text{III}}\text{--ttha}$ (1:1) complex in solution. The results suggest that a species of coordination geometry similar to that of the $[\text{Ho}(\text{N}_4\text{O}_5)]^{3-}$ type found in the crystal exists predominantly in solution at $\text{pH} > 5$. At lower pH values, as for other $\text{Ln}^{\text{III}}\text{--ttha}$ complexes, coordination equilibria are observed. This paper is a part of our investigation of lanthanide compounds with triethylenetetraaminehexaacetic acid (H_6ttha), a ligand with four nitrogen and six oxygen donor atoms (N_4O_6). Our previous results based on the electronic absorption spectra of $\text{Nd}^{\text{III}}\text{--ttha}$ crystals and solutions of the complex revealed the existence of two different species at equilibrium in solution.^{1,2} In those species, the inner sphere of the Nd^{III} ion comprises only donor atoms of the ttha ligand, forming $[\text{Nd}(\text{N}_4\text{O}_6)]^{3-}$ and $[\text{Nd}_2(\text{N}_3\text{O}_6)_2]^{6-}/[\text{Nd}(\text{N}_3\text{O}_6)]^{3-}$ entities with coordination numbers of ten and nine, respectively. In order to check how coordination arrangements around the Ln^{III} ion will change across the rare earth series in the ttha complexes, we have performed spectroscopic investigations of the $\text{Ho}^{\text{III}}\text{--ttha}$ complex in solution and in the form of a single crystal. Such studies seem to be essential since previously obtained results on complexes of heavy lanthanide ions with ttha in solution proved the absence of water molecules in the inner sphere of the Ln^{III} ion,^{3–5} formation of oligomeric species⁶ as well as a presence of multiple 1:1 species.^{3,7} So far two types of crystal structure of nine-coordinate ttha complexes with heavy lanthanide ions have been determined, namely: $[\text{Ln}(\text{N}_4\text{O}_5)]^{3-}$ (where $\text{Ln}^{\text{III}} = \text{Gd},^8 \text{Dy},^9 \text{Yb}^{10}$) and $[\text{Gd}_2(\text{N}_3\text{O}_6)_2]^{6-},^{11}$ the latter being similar to that found for the $\text{Nd}^{\text{III}}\text{--ttha}$ complex.² The aim of this paper is to recognize the solution structure of the $\text{Ho}^{\text{III}}\text{--ttha}$ (1:1) complex based on a comparison between the spectral properties of this complex in the $[\text{C}(\text{NH}_2)_3]_3[\text{Ho}(\text{ttha})]\cdot 3\text{H}_2\text{O}$ single crystal and in solution.

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