

Crystal structure and absorption spectroscopy of neodymium(III) complex with triethylenetetraaminehexaacetic acid, $\text{Na}_3[\text{Nd}(\text{TTHA})] \cdot 2.5\text{NaClO}_4 \cdot 7.617\text{H}_2\text{O}$.

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The crystal structure and absorption spectroscopy results of the $\text{Na}_3[\text{Nd}(\text{TTHA})] \cdot 2.5\text{NaClO}_4 \cdot 7.617\text{H}_2\text{O}$ compound are presented. The crystal structure of the complex was determined by X-ray analysis. Crystals are monoclinic, space group $C2/c$, with $a = 38.446(8) \text{ \AA}$, $b = 10.552(2) \text{ \AA}$, $c = 25.796(5) \text{ \AA}$, $\beta = 130.51(3)^\circ$, and $Z = 4$. The structure consists of monomeric (triethylenetetraaminehexaacetato)neodymate anions, perchlorate anions, sodium cations, and water molecules. The Nd(III) ion adopts a 10-coordinate geometry with six oxygen atoms and four nitrogen atoms from a ligand molecule, which is best described as a bicapped square antiprism. Absorption spectra of a single crystal were measured at room and liquid helium temperatures. Intensities of the f-f transitions were analyzed on the basis of Judd-Ofelt theory. The good correspondence between the spectra of $[\text{Nd}(\text{TTHA})]^{3-}$ in solution and in the single crystal suggests close similarity of both coordination polyhedra.

Adres publiczny

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<https://www.acs.org/content/acs/en.html>