Crystal structure and absorption spectroscopy of a dimeric neodymium(III) complex with triethylenetetraaminehexaacetic acid. (H_6ttha), $Na_{0.5}H_{5.5}[Nd_2(ttha)_2]$.7.5 $NaClO_4$.16.83 H_2O.

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The crystal structure and absorption spectra (IR, UV/VIS) have been determined for $Na_{0.5}H_{5.5}[Nd_2(ttha)_2]\cdot 7.5NaClO_4\cdot 16.83H_2O$ (H_6ttha = triethylenetetraaminehexaacetic acid). The structure consists of the complex dimer, perchlorate anions, sodium cations and water of hydration. Both neodymium(III) ions are nine-co-ordinate. Each ttha ligand is bonded to one Nd^{III} through four of its carboxyl oxygen atoms and three of its nitrogen atoms. Two carboxyl oxygen atoms are bonded to the other Nd^{III}, and the fourth nitrogen atom remains unco-ordinated. The co-ordination spheres of both Nd^{III} are essentially the same and may be defined as distorted tricapped trigonal prisms. Absorption spectra of a single crystal were measured at room and liquid-helium temperatures. The intensities of the f–f transitions were analysed on the basis of Judd–Ofelt theory. Comparison of the absorption spectra of $[Nd(ttha)]^{3-}$ in solution to those of single crystals of $Na_3[Nd(ttha)]\cdot 2.5NaClO_4\cdot 7.617H_2O$ and $Na_{0.5}H_{5.5}[Nd_2(ttha)_2]\cdot 7.5NaClO_4\cdot 16.83H_2O$ compounds allowed us to estimate the ratio of mono- to di-meric species in solution.

Adres publiczny

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