# Ten-coordinate neodymium(III)complexes with triethylenetetraaminehexaacetic acid.

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The crystal structures and spectroscopic (IR, Raman, UV/Vis) data for the complexes $[C(NH_2)_3]_2[Nd(HTTHA)]\cdot 3H_2O$ (**I**) and $[C(NH_2)_3]_3[Nd(TTHA)]\cdot 6H_2O$ (**II**) are presented. Crystals of **I** are triclinic, $P$, $a$ = 9.998(2), $b$ = 10.730(2), $c$ = 15.557(3) Å, $\alpha$ = 106.89(3)°, $\beta$ = 90.27(3)°, $\gamma$ = 93.24(3)°, $V$ = 1594.0(5) Å$^3$, $Z$ = 2, while the chiral crystals of **II** are monoclinic, $P2_1$, $a$ = 10.157(2), $b$ = 15.958(3), $c$ = 12.788(3) Å, $\beta$ = 112.68(3)°, $V$ = 1912.5(7) Å$^3$, $Z$ = 2. Both structures consist of the complex monomeric anions, guanidinium cations and water of hydration. The $Nd^{III}$ ions are ten-coordinate. The TTHA ligand coordinates to the $Nd^{III}$ ions with six of its carboxyl oxygen atoms and four nitrogen atoms. Although the coordination environments of both $Nd^{III}$ cations are essentially the same, the spectral results of both crystals reveal the influence of the degree of protonation of the ligand on the $Nd^{III}$ ion. The IR and Raman spectra allowed us to assign some important frequencies. A comparison of the electronic absorption spectra of $Nd^{III}$–TTHA complexes in solution and in single crystals of **I** and **II** allows the detection of a small elongation of the Nd–O and Nd–N bonds in these complexes as compared to the $[Nd(TTHA)]^{3-}$ moiety in the previously reported complex $Na_3[Nd(TTHA)]\cdot 2.5NaClO_4\cdot 7.617H_2O$ and indicates that the coordination geometry of the ten-coordinate neodymium complex in solution is the same as in the chiral crystal **II**. The intensities of the f–f transitions in $Nd^{III}$–TTHA solutions and of crystals **I** and **II** were analysed on the basis of the Judd–Ofelt theory.

Adres publiczny

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