

Complexes of Yb³⁺ with EDTA and CDTA - molecular and electronic structure.

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Two Yb³⁺ compounds, [C(NH₂)₃]₂[Yb(EDTA)(H₂O)₂]ClO₄·6H₂O and [C(NH₂)₃][Yb(CDTA)(H₂O)₂]·4H₂O, where EDTA is the ethylenediaminetetraacetate anion and CDTA is the *trans*-1,2-diaminecyclohexane-*N,N,N',N'*-tetraacetate anion, were obtained and their crystal structures and spectroscopic properties were determined. In both compounds, the coordination geometries of the eight-coordinate Yb³⁺ ion are very similar. In each case, the inner sphere of the metal ion consists of four carboxyl oxygen atoms, two nitrogen atoms and two water molecules. The complexes were characterized by UV/Vis/NIR absorption at different temperatures and IR spectroscopy. The spectroscopic results revealed high sensitivity of the electronic 4f¹³ configuration upon minor changes in the coordination geometry around the Yb³⁺ ion. These data also demonstrate that species present in solutions of Yb³⁺–EDTA are similar to those found in the crystal, whereas in solutions of Yb³⁺–CDTA an equilibrium between at least two different forms exists. For the Yb³⁺–EDTA complex in solution and in the crystalline state, a charge-transfer transition was detected. Theoretical calculations revealed its complicated (Yb → ligand and ligand → Yb) character.

Słowa kluczowe

X-ray diffraction, Absorption, Density functional calculations, N, O ligands, Ytterbium

Adres publiczny

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