

Structural and spectroscopic studies of heavy lanthanide complexes with o-phenanthroline and isothiocyanate.

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Spectroscopic and structural properties of lanthanide (Tb, Dy, Ho) complexes with o-phenanthroline and isothiocyanate have been investigated as potential candidates for optical materials. The heavy lanthanide (Tb^{3+} , Dy^{3+} , Ho^{3+}) mixed complexes were synthesized in solution and as crystals. They were characterized by elemental analyses, IR absorption spectra and X-ray powder diffraction patterns. Spectroscopic investigations were performed using optical absorption spectra at room temperature and 4.2K. Luminescent spectra for Tb and Dy compounds as well luminescent decay curves at room temperature and 77K were measured. The crystal structures of isostructural complexes $[(\text{NCS})_3(\text{o-phen})_2(\text{H}_2\text{O})\text{Ln}]$ ($\text{Ln}=\text{Tb}$ (**1**), Dy (**2**), Ho (**3**)) obtained from ethanol solution were determined by X-ray diffraction analysis. All three complexes crystallized in the monoclinic system with space group $P2_1/c$, $Z=4$. In the inner-sphere coordination of the lanthanide ions there are 3 isothiocyanate N atoms, 4N atoms from o-phenanthroline molecules and a water molecule ($\text{C.N.}=8$). The optical spectra of the complexes indicate a single low symmetry Ln^{3+} ion site. Spectroscopic investigations of the crystals at room and low temperatures were performed in order to understand the nature of Ln^{3+} -ligand interactions. The variation of spectroscopic parameters of the title compounds (e.g. Sinha's parameter δ or "red shift") and their correlation with the nature of $\text{Ln}^{3+}-\text{N}$ or $\text{Ln}^{3+}-\text{O}$ bonds are discussed.

Słowa kluczowe

Heavy lanthanide complexes, o-Phenanthroline, crystal structure, UV/Vis spectroscopy, luminescence

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