Structure and optical properties of 3-bromo-4-methylthio-2,6-lutidine N-oxide and its eight-coordinate europium(III) and terbium(III) aqua complexes.

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Streszczenie

New europium and terbium $[LnCl_3L_3(H_2O)_2]$ polycrystalline complex were synthesized with the ligand L = 3-bromo-4-methylthio-2,6-lutidine N-oxide. IR, Raman, electron absorption UV-VIS and emission spectra measurements were carried out for these compounds. Re-crystallization of these materials led to formation of single crystals with another composition $[LnL(H_2O)_7]Cl_3{\cdot}L_3$, they were characterized by X-ray diffraction technique and spectroscopic measurements. Both types of the materials consist of eight coordinated $LnCl_3O_3O'_2$ or $LnOO'_7$ polyhedrons containing O - oxygen atoms of the N-oxide group, chlorine atoms or O' - oxygen atoms of the water units. The crystal structure was solved for two complexes of the formula $[Ln(L)(H_2O)_7]Cl_3{\cdot}(L)_3$ where Ln = Eu and Tb. X-ray diffraction analysis reveals that these complexes are isostructural with *P*21/*m* space group. The optimization of the molecular system and frequency calculations were carried out using density functional theory (DFT). The DFT quantum chemical calculations of the vibrational wavenumbers were performed for the ligands used for the Eu^{3+} and Tb^{3+} ions complexation. The emission measurements were carried out with the femtosecond excitation. The effective ligand-to-metal energy transfer was discovered in the $[LnCl_3L_3(H_2O)_2]$ complexes formed in the polycrystalline state.

Słowa kluczowe

Eu3+, Tb3+, Lutidine complex, Optical, Femtosecond, Energy transfer

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