The influence of different cations on the structure and spectral properties of Ln^{3+} tetrakis-complexes with the CAPh-type ligand dimethyl-*N*-trichloroacetylamidophosphate

Autorzy

Mariia B. Struhatska

Nataliia S. Kariaka

Viktoriya V. Dyakonenko

Svitlana V. Shishkina

Sergii S. Smola

Nataliia V. Rusakova

Paula Gawryszewska

Oscar L. Malta

Albano N. Carneiro Neto

Viktor O. Trush

Volodymyr M. Amirkhanov

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Streszczenie

Lanthanide coordination compounds $NMe_4[LnL_4]$, $NEt_4[LnL_4]$ and $PPh_4[LnL_4]$ (Ln^{3+} = Eu, Gd, Tb) with the carbacylamidophosphate (CAPh) ligand dimethyl-*N*-trichloroacetylamidophosphate (HL= $Cl_3CC(O)N(H)P(O)(OMe)_2$) were synthesized. These complexes are characterized using infrared, ultraviolet diffuse reflection, and luminescence spectroscopy as well as through elemental and X-ray analyses. The effect of changing the cation type on the structure and luminescence properties of the tetrakis-complex $[LnL_4]^-$ was analyzed. TD-DFT calculations reveal cation-specific contributions to the excited states in tetrakis complexes, with $[PPh_4]^+$ playing a central role in both singlet and triplet states. This leads to longer donor–acceptor distances compared to $NMe_4[LnL_4]$ and $NEt_4[LnL_4]$. Additionally, intramolecular energy transfer (IET) calculations for Eu^{3+} and Tb^{3+} tetrakis compounds reveal Tb^{3+} sensitization *via* S_1 and Eu^{3+}*via* the typical T_1 state.

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