DFT study of electron absorption and emission spectra of pyramidal LnPc(OAc) complexes of some lanthanide ions in the solid state.

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Kolekcja

Naukowa

Streszczenie

The electron absorption and emission spectra were measured for the pyramidal LnPc(OAc) complexes in the solid state and co-doped in silica glass, where Ln=Er, Eu and Ho. The theoretical electron spectra were determined from the quantum chemical DFT calculation using four approximations CAM-B3LYP/LANL2DZ, CAM-B3LYP/CC-PVDZ, B3LYP/LANL2DZ and B3LYP/CC-PVDZ. It was shown that the best agreement between the calculated and experimental structural parameters and spectroscopic data was reached for the CAM-B3LYP/LANL2DZ model. The emission spectra were measured using the excitations both in the ligand and lanthanide absorption ranges. The possibility of energy transfer between the phthalocyanine ligand and excited states of lanthanide ions was discussed. It was shown that the back energy transfer from metal states to phthalocyanine state is responsible for the observed emission of the studied complexes both in the polycrystalline state and silica glass.

Słowa kluczowe

pyramidal complexes, emission spectra, solid state, quantum calculations, phthalocyanine ligand

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