Photophysical properties and ab initio HF and DFT calculations of the structure and spectroscopy of axially chloro substituted Yb(III) monophthalocyanines in different systems.

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Streszczenie

Lanthanide complexes with phthalocyanines (Pc) and porphyrins are of great interest because of unique luminescence behavior and many applications, mainly in medicine, optoelectronics, lasers and solar energy conversion. This paper is focused on photophysical studies of axially chloro substituted ytterbium mono-phthalocyanine chelate in the solid state, solutions, lattice of PMMA polymer. These latter systems are fundamental for applications. The structures, IR, and Raman spectra were calculated basing on Hartree-Fock (HF) and Density Functional Theory (DFT) methods. The theory reproduces correctly experimental results of spectroscopic frequencies of PcYbCl2 CH_3OH chelate. Recently we published the absorption spectra of metalophthalocyanine compound in PMMA polymer, however neither its structure nor emission properties were studied. Now we have made the effort to study the emission behavior of PcYbCl 2 CH_3OH chelate in different media. Immobilization of molecule in polymer and inorganic matrices on lanthanide ions and the phthalocyanine emission spectra were analysed. The radiative and non-radiative processes, energy transfer and multi-phonon relaxation were investigated. The non-linear processes and dynamics in excited states were discussed.

Słowa kluczowe

Ytterbium, Monophthalocyanine, DFT and ab initio HF calculations, Spectroscopic properties, Polymers co-doped by Yb-complex

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