

Photophysical and theoretical studies of structure and spectroscopic behaviour of axially substituted Yb(III) mono-phthalocyanines in different media.

Autorzy

Yuriy S. Gerasymchuk

L. A. Tomachynski

Małgorzata Guzik

Aleksander Koll

Jerzy Jański

Yannick Guyot

Wiesław Stręk

Georges Boulon

Janina Legendziewicz

Rok wydania

2015

Czasopismo

Journal of Photochemistry
and Photobiology A-
Chemistry

Numer woluminu

309

Strony

65-71

DOI

10.1016/j.jphotochem.2015.04.022

Kolekcja

Naukowa

Streszczenie

Lanthanide complexes with phthalocyanines (Pc) and porphyrins belong to the group of most investigated compounds because of their unique luminescence properties and variety of applications. The special interest is directed to medical applications, mainly in photodynamic therapy. This paper is devoted to photophysical studies of acetato- and chloro-ytterbium monophthalocyanine complexes in the solid state, solutions, silica matrices and PMMA polymer which can design their applicability. The structures, IR, and Raman spectra were calculated applying Hartree–Fock and density functional theory methods and further correlated with experimental findings. The theory reproduces reasonably spectroscopic frequencies of YbPcOAc₂DMSO chelate. Two molecules of DMSO with somewhat different spectroscopic behaviour were found to exist in this complex.

The mechanism of the effect of conformation changes, steric obstacles, extra-coordination of solvent molecules and molecule immobilization in polymer and inorganic matrices on lanthanide and phthalocyanine emission spectra was discussed. Attention was paid to the radiative and non-radiative processes, intramolecular energy transfer and the role of charge-transfer state in this process, electron–phonon coupling, multiion cooperative interactions, non-linear processes and dynamics in excited states. The role of solvent molecule exchange dynamic in possible interaction of Yb(III) complexes with biological systems was also analysed.

Słowa kluczowe

Ytterbium, Monophthalocyanine, DFT modelling method, Ab initio HF calculation, Spectroscopic properties, Sol–gel systems, Polymers co-doped by Yb-complexes

Język	Adres publiczny
Angielski	http://dx.doi.org/10.1016/j.jphotochem.2015.04.022
Typ publikacji	Strona internetowa wydawcy
Artykuł	http://www.elsevier.com

Plik został wygenerowany dnia 2026-08-26 16:09:32

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/BxWYkOZ>.