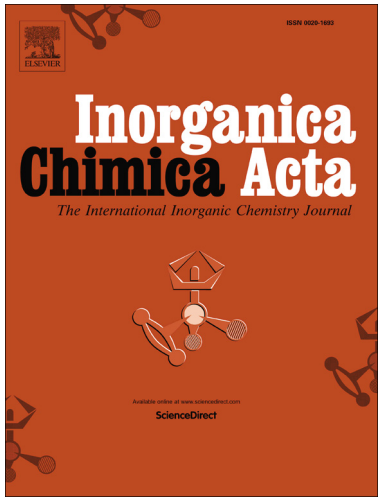

Research paper

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A theoretical and experimental study of six novel new complexes of alkyl substituted isothiosemicarbazone

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Abstract

Six closely related [UO_2L'(solvent)] complexes, where L' is the *N*-2-hydroxy-3-methoxybenzaldehyde-*N*'-2'-hydroxyacetophenone-*S*(*R*)isothiosemicarbazone ligand (*R* = methyl, ethyl, allyl, butyl, pentyl and benzyl), are synthesized. Characterization of the complexes is accomplished using elemental analysis, FT-IR, ^{13}C and ^{1}H NMR and UV-Vis spectroscopic techniques. Fluorescence emission of the complex with *R* = benzyl gives the maximum quantum yield while in the other complexes the quantum yield decreases markedly with increasing length of the linear *R* groups. TGA/DSC showes that the thermal stability decreases to the lenght of the *R* group. Crystal structures of the complexes determined by X-ray crystallography indicate that the tetradentate isothiosemicarbazone ligands in addition to solvent molecule are coordinated to the uranyl center in distorted pentagonal bipyramid geometries. All of the six uranyl complexes form dimers through some pairwise hydrogen bonds mainly between OH of solvent molecules and phenoxy oxygen atoms. Molecular geometries and vibrational frequencies are compared using the density functional method (B3LYP) with the SDD basis set for uranium and 6-311G++(d,p) basis set for the other atoms. Electronic absorption spectra of compounds are predicted with TD-DFT studies and HOMO-LUMO orbitals as well as charge delocalization are determined using natural bond orbital analysis.

Keywords

Isothiosemicarbazone, Uranyl complex, Tetradentate ligand, DFT calculations, Fluorescence, X-ray analysis.

1. Introduction