Uniwersytet Wrocławski

Repozytorium

Plik pochodzi z repozytorium Wydziału Chemii Uniwersytetu Wrocławskiego

Novel rhenium(III) complexes with the picolinate ligand: synthesis, spectroscopic investigations, X-ray structures and DFT calculations for $[ReX_2(pic)(PPh_3)_2]$ complexes.

Autorzy

Barbara Machura

M. Wolff

Rafał Kruszyński

Jerzy Mroziński

Joachim Kusz

Rok wydania

2009

Czasopismo

Polyhedron

Numer woluminu

28

Strony

2377-2384

DOI

10.1016/j.poly.2009.05.032

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The paper presents a combined experimental and computational study of novel rhenium(III) complexes with the picolinate ligand – $[ReCl_2(pic)(PPh_3)_2]$ (**1**) and $[ReBr_2(pic)(PPh_3)_2]$ (**2**). Both complexes **1** and **2** have been characterised spectroscopically and structurally (by single-crystal X-ray diffraction). Complex **1** has been additionally studied by magnetic measurement. The magnetic behavior is characteristic of a mononuclear d^4 low-spin octahedral Re(III) complex ($^3T_{1g}$ ground state) and arises because of the large spin–orbit coupling (ζ = 2500 cm^{-1}), which gives a diamagnetic ground state. DFT and time-dependent (TD)DFT calculations have been carried out for complex **1**, and UV–vis spectra of the $[ReX_2(pic)(PPh_3)_2]$ compounds have been discussed on this basis.

Słowa kluczowe

Rhenium complexes, Picolinate ligand, X-ray, Electronic structure, DFT calculationsmagnetic measurement

Adres publiczny

https://doi.org/10.1016/j.poly.2009.05.032

Strona internetowa wydawcy

http://www.elsevier.com

Plik został wygenerowany dnia 2026-11-11 02:10:33

Adres w repozytorium https://old.chem.uni.wroc.pl/pl/repozytorium/f5YBnYm.