Two novel rhenium complexes derived from [ReO(OMe)Cl_2(dpphen)]- synthesis, crystal structure, spectroscopic and magnetic properties.

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Rok wydania

2011

Czasopismo

Polyhedron

Numer woluminu

30

Strony

354-363

DOI

10.1016/j.poly.2010.10.025

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The reaction of [ReO(OMe)Cl_2(dpphen)] (dpphen = 4,7-diphenyl-1,10-phenanthroline) with triphenylphosphine has been examined and two novel rhenium complexes – [$Re^{III}Cl_3$(dpphen)(PPh_3)]·Me_2CO (**1**) and [$Re^{IV}Cl_4$(dpphen)]·$CHCl_3$ (**2**) – have been obtained. The compounds have been characterised by elemental analysis, IR, UV–Vis spectroscopy, magnetic measurements and X-ray crystallography. The electronic structures of [$ReCl_3$(dpphen)(PPh_3)] and [$ReCl_4$(dpphen)] have been studied by DFT/B3LYP level calculations, and TD-DFT calculations have been employed for discussion of the electronic spectra in more detail. The magnetic behaviour of **1** is characteristic of mononuclear complexes with d^4 low-spin octahedral Re(III) complexes ($^3T_{1g}$ ground state) and arise because of the large spin–orbit coupling (ζ = 2500 cm^{-1}), which gives diamagnetic ground state. For complex **2** the results of calculations revealed value of zero-field splitting parameter D = 10.8 cm^{-1}, $g_{||}$ = 2.49 and $g_{\perp}$ = 1.51

Słowa kluczowe

Re(III) and Re(IV) complexes, lanthanides, 7-diphenyl-1, 10-phenanthroline, X-ray structure, Electronic structure, DFT calculation

Adres publiczny

https://doi.org/10.1016/j.poly.2010.10.025

Strona internetowa wydawcy

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