Synthesis, characterization, structural studies and Hirshfeld surface analysis of Re(III) and Re(V) complexes with picolinohydrazone ligands

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Rok wydania

2025

Czasopismo

Journal of Molecular Structure

Numer woluminu

1341

Strony

142614/1-142614/9

DOI

10.1016/j.molstruc.2025.142614

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Two mononuclear rhenium coordination compounds with hydrazone ligand, $[ReOBr_2(PPh_3)(HL)]\cdot(CH_3CN)$ (**1**) and $[ReCl_2(PPh_3)_2(HL)]\cdot(CH_3CN)$ (**2**), were synthesized by the reaction of $ReOBr_3(PPh_3)_2$ or $ReOCl_3(PPh_3)_2$ with H_2L in acetonitrile (H_2L = (*E*)-*N*'-(1-(4-hydroxy-6-methyl-2-oxo-2H-pyran-3-yl)ethylidene)picolinohydrazide).

Compounds **1** and **2** were characterized by spectroscopic methods and their structures were determined by single crystal X-ray analysis. Structural studies indicated that despite the similarity of the reactions and structures, the oxidation state of rhenium ion in **1** is mainly Re(V) but, in compound **2** it is reduced to Re(III) during the synthesis procedure. The hydrazone ligand in these compounds has similar coordination mode and it is coordinated as a bidentate N- and O-donor mononegative ligand, HL^{-1}. TGA analysis showed that these compounds are stable up to 200 °C and they decompose in two steps in the range of 200–700 °C. The intermolecular interactions in these compounds were investigated by Hirshfeld surface analysis which revealed there are several intermolecular C−H···N, C−H···X (X = Br and Cl) and C−H···π interactions which contribute in the stabilization of the crystal structures.

Słowa kluczowe

Rhenium coordination compound, Crystal structure, Hydrazone ligands, Hirshfeld surface analysis, Spectroscopic studies

Adres publiczny

http://dx.doi.org/10.1016/j.molstruc.2025.142614

Strona internetowa wydawcy

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