Synthesis, X-ray studies, spectroscopic investigation, and DFT calculations of [$ReBr_3$(dppt)($OPPh_3$)].

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Streszczenie

The reaction of [ReOBr3(PPh3)2] with 5,6-diphenyl-3-(2-pyridyl)-1,2,4-trazine(dppt)hasbeenexamined and [ReBr3(dppt)(OPPh3)] has been obtained. Itwas characterised by IR, UV–Vis spectroscopy, magneticmeasurements, and X-ray crystallography. The electronicstructure of [ReBr3(dppt)(OPPh3)] has been studied byDFT/B3LYP level calculations, and TDDFT calculationswere employed for discussion of its electronic spectrum inmore detail. The magnetic behavior is characteristic ofmononuclear complexes with d4low-spin octahedralRe(III) complexes (3T1gground state) and arise because ofthe large spin–orbit coupling (f=2500 cm-1), whichgives diamagnetic ground state.

Słowa kluczowe

Rhenium complexes, 6-Diphenyl-3-(2-pyridyl)-1, molecule, 4-trazine, X-ray and electronic structure, DFT calculations, magnetic measurements

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