Novel rhenium(III) complexes with 5.6-diphenyl-3-(2-pyridyl)-1,2,4-trazine: X-ray structures and DFT calculations for [$ReCl_3(OPPh_3)(dppt)$] and [$ReCl_3(PPh_3)(dppt)$] complexes.

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The reaction of [ReOCl3(PPh3)2] with 5,6-diphenyl-3-(2-pyridyl)-1,2,4-trazine (dppt) has been examined and [ReCl3(OPPh3)(dppt)]has been obtained. The triphenylphosphine oxide can be easily replaced by PPh3in the reaction of [ReCl3(OPPh3)(dppt)] with an excessof triphenylphosphine. The [ReCl3(OPPh3)(dppt)] and [ReCl3(PPh3)(dppt)] complexes have been structurally and spectroscopically char-acterized. Their molecular orbital diagrams have been calculated with the density functional theory (DFT) method, and their electronicspectra have been discussed on the basis of time-dependent DFT calculations. The compound [ReCl3(OPPh3)(dppt)] has been studiedadditionally by magnetic measurement. The magnetic behavior is characteristic of mononuclear complexes with d4low-spin octahedralRe(III) complexes (3T1gground state) and arise because of the large spin–orbit coupling (f= 2500 cm1), which gives diamagnetic ground state.

Słowa kluczowe

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

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