

A novel rhenium(III) complex with bis(pyrazol-1-yl)methane: X-ray structure and DFT calculations for [ReCl₃(bpzm)(PPh₃)].

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Streszczenie

The [ReCl₃(MeCN)(PPh₃)₂] complex reacts with bis(pyrazol-1-yl)methane (bpzm) to give [ReCl₃(bpzm)(PPh₃)]. This compound has been studied by IR, UV–Vis spectroscopy, magnetic measurement and X-ray crystallography. The molecular orbital diagram of [ReCl₃(bpzm)(PPh₃)] has been calculated with the density functional theory (DFT) method. The spin-allowed triplet–triplet electronic transitions of [ReCl₃(bpzm)(PPh₃)] have been calculated with the time-dependent DFT method, and the UV–Vis spectrum of the title compound has been discussed on this basis. The magnetic behavior is characteristic of a mononuclear d⁴ low-spin octahedral Re(III) complex (³T_{1g} ground state) and arises because of the large spin–orbit coupling ($\zeta = 2500\text{ cm}^{-1}$), which gives a diamagnetic ground state.

Słowa kluczowe

Rhenium(III) complexes, Bis(pyrazol-1-yl)methane ligand, X-ray structure, DFT calculations, Magnetic measurement

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