Novel rhenium(III) complexes with the picolinate ligand: synthesis, spectroscopic investigations, X-ray structures and DFT calculations for $[ReX_2(pic)(PPh_3)_2]$ complexes.

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Streszczenie

The paper presents a combined experimental and computational study of novel rhenium(III) complexes with the picolinate ligand – $[ReCl_2(pic)(PPh_3)_2]$ (**1**) and $[ReBr_2(pic)(PPh_3)_2]$ (**2**). Both complexes **1** and **2** have been characterised spectroscopically and structurally (by single-crystal X-ray diffraction). Complex **1** has been additionally studied by magnetic measurement. The magnetic behavior is characteristic of a mononuclear d^4 low-spin octahedral Re(III) complex ($^3T_{1g}$ ground state) and arises because of the large spin–orbit coupling (ζ = 2500 cm^{-1}), which gives a diamagnetic ground state. DFT and time-dependent (TD)DFT calculations have been carried out for complex **1**, and UV–vis spectra of the $[ReX_2(pic)(PPh_3)_2]$ compounds have been discussed on this basis.

Słowa kluczowe

Rhenium complexes, Picolinate ligand, X-ray, Electronic structure, DFT calculationsmagnetic measurement

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