Coordination chemistry of di-2-pyridylketone. Synthesis, spectroscopic investigations, X-ray studies and DFT calculations of Re(III) and Re(V) complexes.

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Streszczenie

The paper presents a combined experimental and computational study of Re(III) and Re(V) complexes containing di-2-pyridylketone and its gem-diol form – $[ReCl_3(dpk\text{-}N,O)(PPh_3)]$ (**1**), $[ReCl_3(dpk\text{-}N,N')(OPPh_3)]$ (**2**) and $[ReOBr_3(dpk\text{-}OH)]\cdot 2(dpkH^+Br^-)$ (**3**). All the complexes have been characterized spectroscopically and structurally (by single-crystal X-ray diffraction). The complex **2** has been additionally studied by magnetic measurement. The magnetic behavior of **2** is characteristic of mononuclear octahedral Re(III) complex with d^4 low-spin ($^3T_{1g}$ ground state) and arise because of the large spin–orbit coupling (ζ = 2500 cm^{-1}), which gives diamagnetic ground state. DFT and time-dependent (TD)DFT calculations have been carried out for $[ReCl_3(dpk\text{-}N,N')(OPPh_3)]$ and $[ReOBr_3(dpk\text{-}OH)$, and their UV–vis spectra have been discussed on this basis.

Słowa kluczowe

Rhenium complexes, Di-2-pyridylketone, X-ray, Electronic structure, DFT and TDDFT calculations, Magnetic measurement

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