

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

### Autorzy

Barbara Machura

Jerzy Mroziński

Rafał Kruszyński

Joachim Kusz

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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<sub>3</sub>(dpk-N,O)(PPh<sub>3</sub>)] (**1**), [ReCl<sub>3</sub>(dpk-N,N')(OPPh<sub>3</sub>)] (**2**) and [ReOBr<sub>3</sub>(dpk-OH)]·2(dpkH<sup>+</sup>Br<sup>-</sup>) (**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<sup>4</sup> low-spin (<sup>3</sup>T<sub>1g</sub> ground state) and arise because of the large spin-orbit coupling ( $\zeta = 2500 \text{ cm}^{-1}$ ), which gives diamagnetic ground state. DFT and time-dependent (TD)DFT calculations have been carried out for [ReCl<sub>3</sub>(dpk-N,N')(OPPh<sub>3</sub>)] and [ReOBr<sub>3</sub>(dpk-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

### Adres publiczny

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