

## Synthesis, characterization and molecular structure of Re(III) complexes containing 2-benzoylpyridine.

### Autorzy

Barbara Machura

Jerzy Mroziński

Joachim Kusz

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### Streszczenie

The paper presents a combined experimental and computational study of Re(III) complexes containing 2-benzoylpyridine (bopy). Two novel complexes  $[\text{ReX}_3(\text{bopy})(\text{PPh}_3)]$  ( $X = \text{Cl}, \text{Br}$ ) have been obtained in the reactions of  $[\text{ReX}_3(\text{MeCN})(\text{PPh}_3)_2]$  with 2-benzoylpyridine in dichloromethane and have been studied by IR, UV–Vis spectroscopy and X-ray crystallography. The electronic structure of  $[\text{ReCl}_3(\text{bopy})(\text{PPh}_3)]$  has been calculated with the density functional theory (DFT) method. The spin-allowed electronic transitions of  $[\text{ReCl}_3(\text{bopy})(\text{PPh}_3)]$  have been calculated with the time-dependent DFT method and the UV–Vis spectrum has been discussed on this basis.

### Słowa kluczowe

Rhenium(III) complexes, 2-Benzoylpyridine, X-ray structure, electronic structure, DFT calculations

### Adres publiczny

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