Synthesis, crystal, molecular and electronic structure of $[ReOCl_3(phen)]$ and $[ReCl_2(phen)(PPh_3)_2](ReO_4)$ complexes.

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Streszczenie

The reactions of $[ReOCl_3(OAsPh_3)(AsPh_3)]$ and $[ReOCl_3(PPh_3)_2]$ with 1,10-phenanthroline (phen) have been examined and the complexes $[ReOCl_3(phen)]$ (**1**) and $[ReCl_2(phen)(PPh_3)_2](ReO_4)$ (**2**) have been obtained. The crystal and molecular structures of **1** and have been determined. The geometric parameters of **1** and **2** have been examined with the density functional theory (DFT) method. The spin-allowed electronic transitions have been calculated with the time-dependent DFT method for $[ReOCl_3(phen)]$, $[ReCl_2(phen)(PPh_3)_2]^+$ cation and anion, and the UV–Vis spectra of the title compounds have been discussed on this basis.

Słowa kluczowe

Rhenium oxo complexes, Phenanthroline, X-ray structure, DFT calculations

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