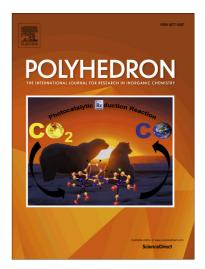
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Synthesis, characterization, X-ray crystallography and stability in aqueous medium of *trans*- $[Ru(CO)(NH_3)_4P(OH)_3]^{2+}$

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ACCEPTED MANUSCRIPT

Synthesis, characterization, X-ray crystallography and stability in aqueous medium of trans-[Ru(CO)(NH₃)₄P(OH)₃]²⁺

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Abstract

Here, we report the synthesis, characterization, crystal data and DFT calculation of a new water-soluble ruthenium(II) carbonyl complex. The *trans*-[Ru(CO)(NH₃)₄P(O)(OH)₂]Cl is a robust complex in aqueous media. The pK_a of 3.3 for the phosphorous acid ligand in this complex was measured by infrared spectroscopy. The *trans*-[Ru(CO)(NH₃)₄P(O)(OH)₂]⁺ exhibits just two slow reactions at pH 7.5: CO-Ru-P(O)(OH)₂ to CO-Ru-(O)P(OH)₂ isomerization (k = $1.1 \times 10^{-5} \text{ s}^{-1}$ at 25°C) and subsequent P(O)(OH)₂ dissociation (k = $1.7 \times 10^{-7} \text{ s}^{-1}$ at 25°C). The formation of O-bonded *trans*-[Ru(CO)(NH₃)₄(O)P(OH)₂]⁺ was supported by IR, UV-vis and ³¹P NMR spectroscopies and DFT calculations.

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