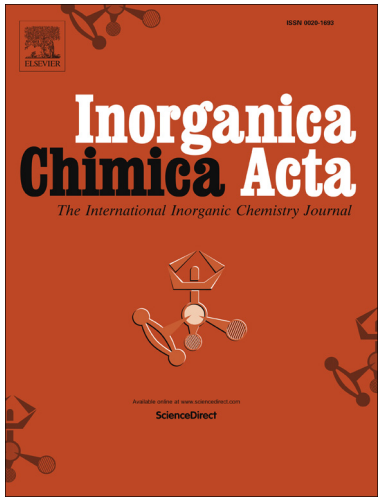

Research paper

Ruthenium Complexes of Pyridine Oxime and Azoimine Ligands: Syntheses, Crystallography, Electrochemical and Catalytic Properties

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Ruthenium Complexes of Pyridine Oxime and Azoimine Ligands: Syntheses, Crystallography, Electrochemical and Catalytic Properties

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Abstract

Five mononuclear ruthenium complexes of the type *trans*-[$RuCl_2$(Azo)(Py-C(R)N=OH)] (**C1-C5**) {Azo = C_6H_5N=NC($COCH_3$)=NC_6H_4X, R=CH_3, X = H (**C1**), Br (**C2**), CH_3 (**C3**), F (**C4**); R=H, X=CH_3 (**C5**)} have been synthesised and characterized by spectroscopic (IR, UV–Vis, and NMR) and electrochemical (cyclic voltammetry) techniques. In addition, **C2** complex has been further characterized by single crystal X-ray diffraction. The complexes (**C1-C3**) were also tested with respect to their catalytic activity in the liquid-phase hydrogenation of acetophenone. The electronic absorption spectrum of **C2** in acetonitrile has been modelled by time-dependent density functional theory.

Keywords: Ru (II) complex, oxime, X-ray structure, electrochemistry, DFT calculations, Transfer hydrogenation.