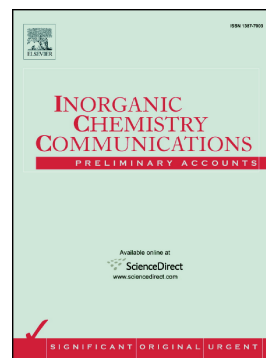


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(Pyrazolyl)pyridine ruthenium(III) complexes: Synthesis, kinetics of substitution reactions with thiourea and biological studies

Reinner O. Omondi,¹ Stephen O. Ojwach,*¹ Deogratius Jaganyi,¹ Amos A. Fatokun²

¹School of Chemistry and Physics, University of KwaZulu-Natal, Private Bag X01, Scottsville, Pietermaritzburg, 3209, South Africa

²School of Pharmacy and Biomolecular Sciences, Faculty of Science, Liverpool John Moores University, Liverpool L3 3AF, England, UK

Abstract

Reactions of 2-bromo-6-(3,5-dimethyl-1H-pyrazol-1-yl)pyridine (**L1**), 2,6-di (1H-pyrazol-1-yl) pyridine (**L2**) and 2,6-bis(3,5-dimethyl-1H-pyrazol-1-yl)pyridine (**L3**) with RuCl₃·3H₂O led to the formation of their respective metal complexes [RuCl₃(**L1**)] (**1**), [RuCl₃(**L2**)] (**2**) and [RuCl₃(**L3**)] (**3**). Solid state structure of complex **3** established the formation of a six-coordinate mononuclear compound in which **L3** is tridentately bound. The order of reactivity of the studied complexes with thiourea (**TU**) nucleophile is in the form **1** > **2** > **3**, in line with density functional theory (DFT) studies. The complexes displayed minimal cytotoxic activity against the HeLa cell line, consistent with molecular docking experiments which showed weaker DNA binding affinities.

Keywords: ruthenium complexes; ligand substitution; cytotoxicity, anti-cancer activities; DFT; molecular docking

*Corresponding author: Tel.: +27 (33) 260 5239; Fax: +27 (33) 260 5009

E-mail: ojwach@ukzn.ac.za (S. O. Ojwach)

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