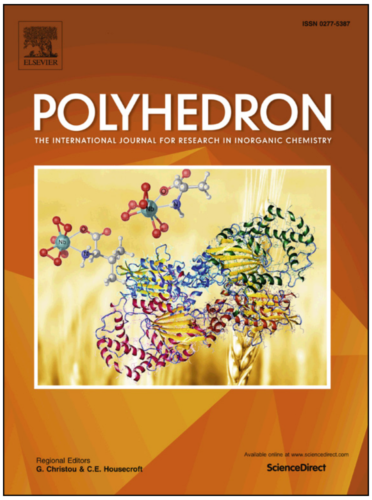

Synthesis, characterization and interactions with 9-methylguanine of ruthenium(II) η ^{6}-arene complexes with aromatic diimines

Theodoros Tsolis, Konstantinos Ypsilantis, Andreas Kourtellaris, Achilleas Garoufis

PII: S0277-5387(18)30202-X
DOI: https://doi.org/10.1016/j.poly.2018.04.025
Reference: POLY 13127

To appear in: *Polyhedron*

Received Date: 16 March 2018
Accepted Date: 20 April 2018

Please cite this article as: T. Tsolis, K. Ypsilantis, A. Kourtellaris, A. Garoufis, Synthesis, characterization and interactions with 9-methylguanine of ruthenium(II) η ^{6}-arene complexes with aromatic diimines, *Polyhedron* (2018), doi: https://doi.org/10.1016/j.poly.2018.04.025

Synthesis, characterization and interactions with 9-methylguanine of ruthenium(II) η^6-arene complexes with aromatic diimines.

Theodoros Tsolis [a], *Konstantinos Ypsilantis* [a], *Andreas Kourtellaris* [b] *and Achilleas Garoufis* [a] *

[a] Department of Chemistry, University of Ioannina, GR-45110 Ioannina, Greece.

[b] Department of Chemistry, University of Cyprus, P.O. Box 20537, CY-1678 Nicosia, Cyprus

ABSTRACT

The complexes of the formula [(η^6-arene)Ru(L)Cl]PF_6, where arene is benzene (bz) or p-cymene (cym) and L is 2,(2′-pyridyl)quinoline (pqn), were synthesized and characterized by means of NMR spectroscopic techniques, HR-ESI mass spectrometry and, in the case of [(η^6-cym)Ru(pqn)Cl]PF_6, by X-ray single crystal diffraction. Their resistance in hydrolysis was also studied. A comparative NMR study of their 9-methylguanine (9-MeG) complexes, [(η^6-arene)Ru(pqn)(9-MeG)]$(PF_6)_2$, with similar diimine complexes revealed that the unimpeded rotation of 9-MeG is hindered by interactions between the 9-MeGO6 and the p-cymene aromatic proton H2 and, by the bulky shape of the pqn. This conformation forces the 9-MeGH8 to be in close proximity to the aromatic ring system of pqn. NMR spectroscopic techniques lead to the conclusion that the strong shielding effect on 9-MeGH8 depends on the extension of the aromatic system of the ligand. Also, we conclude that the strong deshielding on the 9-MeGNH1 is influenced by both the N7 ruthenation of 9-MeG and the addendum electron density in the 9-MeG ring system, due to the proximity to the aromatic ring system of pqn.

Keywords: *η^6-arene ruthenium; 9-methylguanine; cancer chemotherapy; NMR; mass spectrometry*

* Corresponding author: AG, agaroufi@cc.uoi.gr