Accepted Manuscript

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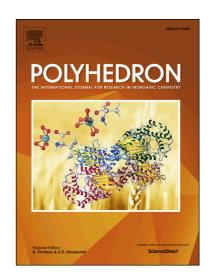
PII: S0277-5387(18)30202-X

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

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ACCEPTED MANUSCRIPT

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

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ABSTRACT

The complexes of the formula $[(\eta^6\text{-arene})Ru(L)Cl]PF_6$, 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 $[(\eta^6\text{-cym})Ru(pqn)Cl]PF_6$, by X-ray single crystal diffraction. Their resistance in hydrolysis was also studied. A comparative NMR study of their 9-methylguanine (9-MeG) complexes, $[(\eta^6\text{-arene})Ru(pqn)(9\text{-MeG})](PF_6)_2$, 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

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