A Density Functional Study of Ruthenium(II) and Ruthenium(III) interaction with Nucleobases

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It has been well established for several years that Ru(II) and Ru(III) complexes display interesting anticancer, antimetastatic properties, and some of these compounds are under intensive preclinical and clinical investigation.[1,2] Following these studies, there has been considerable interest in the interaction of simple Ruthenium complexes, such as $[Ru(NH_3)_5]^{2+}$ and $[Ru(NH_3)_5]^{3+}$ with DNA and it's purine and pyrimidine constituents.[3] In this work, density functional calculations have been performed on $[Ru(NH_3)_5B]^{z+\ (z=2,\ 3)}$ complexes, where B is an adenine, guanine or citosine nucleobase. Calculations were based on a Becke and Perdew exchange-correlation potential using triple-ζ plus polarization basis sets and include scalar relativistic corrections. Geometry optimizations have been performed for all possible coordination modes between the $[Ru(NH_3)_5]^{z+}$ fragment and the nucleobases. Bond energies have been calculated for all considered metal binding sites. Our results allow to built a binding order for the nitrogen atoms of the considered nucleobases and indicate that the N7 atom of guanine is the thermodinamically preferred coordination site.

1) Michael J. Clarke, Fuchun Zu, Dominic R. Frasca, Chem. Rev. 99, 2511-2533 (1999).
2) R. Cini, G. Tommasi, S. Defazio, M. Corsini, P. Zanello, L. Messori, G. Marcon, F. Piccioli, P. Orioli, Inorg. Chem. 42, 8038-8052 (2003)
3) Michael J. Clarke, Coordination Chem. Rev. 232, 69-93 (2002).