Regium Bonding and its relevance in the context of inorganic and bioinorganic chemistry from a theoretical viewpoint

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Regium bonding is the term that has been proposed to identify noncovalent interactions that involve atoms from group XI of the periodic table. These interactions of weak nature have been found in a series of biological systems[1][2] and their relevance and applications have been studied theoretically in further depth using state of the art computational chemistry tools such as the combined *Atoms in Molecules/Non Covalent Interaction Plot (AIM/NCIplot)*, *Molecular Electrostatic Potential (MEP)* and *Energy Decomposition Analyses (EDA)*.

To better understand the potential of the regium bond and its possible applications and implications in the fields of crystal engineering, bioinorganic chemistry and inorganic chemistry, we have studied models that can illustrate the regium interaction by taking directly structures from crystallographic databases such as the Protein Data Bank; or by designing simpler arbitrary models to further expand the concept of the regium bond. In the recent years, we've made contributions to expand our knowledge of this interaction involving nucleobases[3], we have explored the strength of the noncovalent interaction depending on the size of model constructed nanoparticles[4] and we have proposed some equations to identify the energy of the interaction between silver atoms and gold atoms, providing new insights into the argentophilic and aurophilic interactions[5].

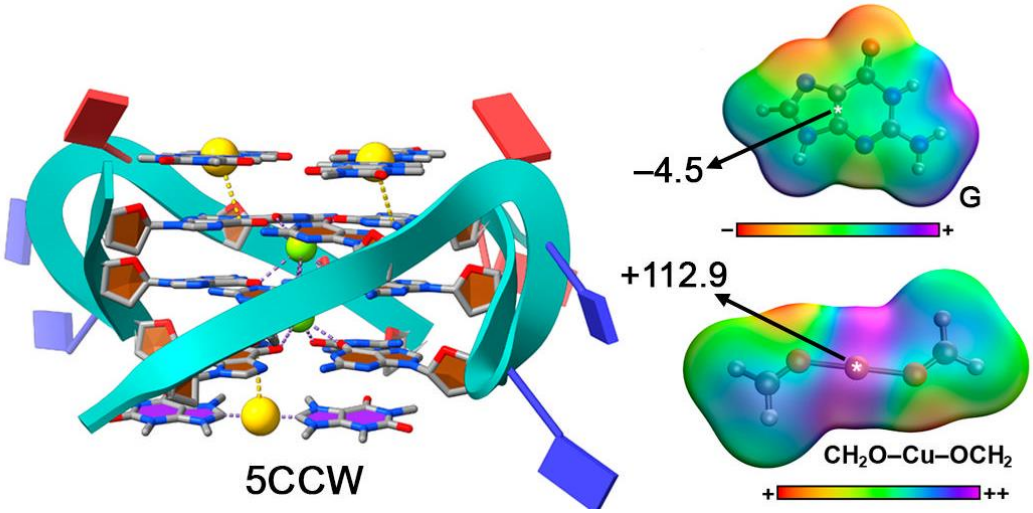

Figure 1. Regium-π bonds in a Protein Data Bank structure where gold atoms interact with the π surface of nucleic acids, left, the MEP of Guanine and a simple model of a constructed Cu system are presented on the right.

[1] Piña, M. N.; Frontera, A.; Bauzá, A. *J. Phys. Chem. Lett.* **2020**, *11*, 8259– 8263

[2] Piña, M.N.; Mooibroek, T. J.; Frontera, A.; Bauzá, A. *Phys. Chem. Chem. Phys.* **2022**, *24*, 24983– 24991

[3] Burguera, S.; Frontera, A.; Bauzá, A. *Inorg. Chem.* **2023**, *62*, 6740– 6750

[4] Burguera, S.; Piña, M. N.; Bauzá, A. *Phys. Chem. Chem. Phys.*, 2024,**26**, 20522-20529

[5] Burguera, S.; Bauzá, A.; Frontera, A. *Phys. Chem. Chem. Phys.*, 2024,**26**, 16550-16560