A Theoretical Approach to Unexpected Chemistry: Tunneling, Orbital Theory and Halogen Bonds.

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Lunes 6 de Julio de 2015, 13 hs
Aula de seminarios del 3er Piso - Departamento de Qca. Inorg., Analítica y Qca. Física

Abstract
Frontier chemistry is built from the unexpected. In this talk, three topics will be discussed at the light of different theoretical tools: (a) heavy atom tunneling, (b) a tetrahedral penta-coordinated $(SiO)_4$ system, and (c) halogen bonding.

(a) Quantum mechanical tunneling is a non-classical process where small mass particles can cross through potential energy barriers instead of over it. However, in specific circumstances “heavy” elements (period 2) can tunnel. We will review the factors that enable this effect, comparing the theoretical predictions with experimental observations.

(b) Square planar $(CO)_4$ in its ground state is a triplet, an unexpected outcome for a seemingly ordinary organic molecule. The analogous planar $(SiO)_4$ has an even more stable triplet state. Yet, once again unexpectedly, it spontaneously rearranges to a tetrahedral hyper-coordinated system. We will try to comprehend this outcome by the analysis of their molecular orbitals.

(c) Halogen bonds, in spite of having been observed for a long time, are the latest accepted member of the family of “non-covalent interactions”. Their nature is still a matter of dispute, sharing several characteristics with the also controversial hydrogen bond. A brief overview of some theoretical tools for the analysis of halogen bonds will be presented.