Physical and Computational Organic Chemistry

Spring 2015 (C. Corminboeuf)

Presentation of an article linked to computational organic chemistry

A. Literature of your choice (to be approved first).

or

B. Article from the following list

Reaction/Rearrangement Mechanisms

- *Nonamethylcyclopentyl Cation Rearrangement Mysteries Solved.* Tantillo and Schleyer *Organic Letters* **2013**, *15*, 1725.
- *The Inherent Competition Between Addition and Substitution Reactions of Br_2 with Benzene and Arenes* Schleyer et al. *Angew. Chem. Int. Ed.* **2011**, *50*, 6809-6813.

Physical Organic Chemistry

- *Do Special Noncovalent π -π stacking Interactions Really Exist?* Grimme *Angew. Chem. Int. Ed.* **2008**, *47*, 3430-3434.
- *The "Bond-Stretched Invertomer" of Hexafluorocycloprpoane-a New Type of Reactive Intermediate.* Borden et al. *Angew. Chem. Int. Ed.* **2007**, *46*, 2666-2668.
- *Squeezing C-C Bonds.* Huntley and Hoffmann *Angew. Chem. Int. Ed.* **2005**, *44*, 7549-7553.

Transition State Theory

- *Dynamics and the Failure of Transition State Theory in Alkene Hydroboration* Singleton et al. *J. Am. Chem. Soc.* **2009**, *131*, 3130-3131.

Properties of Organic Molecules (A good choice for the physical chemists)

- *Large First Hyperpolarizabilites in Push-Pull Polyenes by Tuning of the Bond Length Alternation and Aromaticity* Marder et al. *Science* **1994**, *263*, 511.

Quantification of Chemical Concepts:

A: The Anomeric Effect

Can we sense the anomeric effect? (the following two articles go together)

- *Sensing the Anomeric Effect in a Solvent-Free Environment.* Cocinero et al. *Nature* **2011**, *76*, 469.
- *Sensing or No Sensing: Can the Anomeric Effect Be Probed by a Sensing Molecule?* Mo et al. *J. Am. Chem. Soc.* **2011**, *133*, 13731.

B: Atomic Charges (A good choice for those interested in quantum chemistry)

How do we quantify the charge of an atom in a molecule?

- Quantification of "Fuzzy" Chemical Concepts: A Computational Perspective" Corminboeuf et al. *Chemical Society Reviews* **2012**, *41*, 4671. **Part 2**