SPECTROSCOPIC STUDIES OF CHIRAL RECOGNITION AT THE MOLECULAR LEVEL

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Chirality and stereochemistry effects play a key role in life chemistry. Our group is conducting gas-phase experiments for isolating and studying these effects in isolated molecules and weakly bound complexes without the perturbation brought to the solvent. Size- and conformer-selective laser-based experiments combining either supersonic expansion or ion traps are employed to characterize chirality and stereochemistry effects in spectroscopy, stability and photofragmentation of molecular complexes[1,2]. Very recent experiment aiming at determining the structure of photoproducts combine an ion trap with both UV laser and IR free-electron laser, in collaboration with Debora Scuderi (Laboratoire de Chimie Physique Orsay).[3] In parallel, we also apply chiroptical methods in solution and in the solid phase like Vibrational Circular Dichroism (VCD) to gain complementary information on the role of the environment in shaping the structure of chiral molecules[4].

Ab initio calculations are performed as an aid to the interpretation of the experimental results.

Depending on his/her skills and taste, the hired student will focus either on the gas-phase experiments, on the condensed-phase experiments, or on the *ab initio* calculations

References

(1) Zehnacker, A.; Suhm, M. A. *Angewandte Chemie-International Edition* **2008**, *47*, 6970.

(2) Scuderi, D.; Le Barbu-Debus, K.; Zehnacker, A. *Physical Chemistry Chemical Physics* **2011**, *13*, 17916.

(3) Scuderi, D.; Lepere, V.; Piani, G.; Bouchet, A.; Zehnacker-Rentien, A. *Journal of Physical Chemistry Letters* **2014**, *5*, 56.

(4) Sen, A.; Bouchet, A.; Lepere, V.; Le Barbu-Debus, K.; Scuderi, D.; Piuzzi, F.; Zehnacker-Rentien, A. *The Journal of Physical Chemistry. A* **2012**, *116*, 8334.