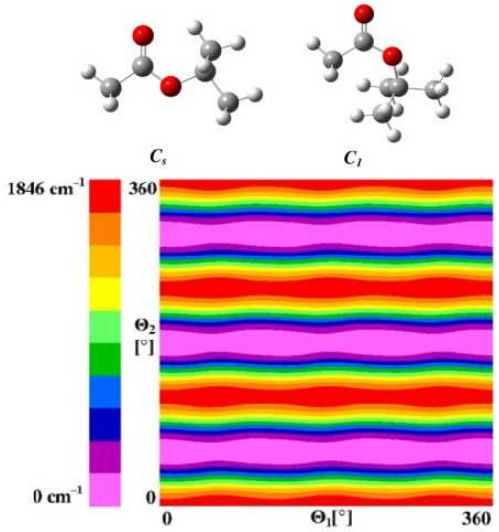
MOLIM STSM 2015: Understanding the structure and dynamic of odorant molecules in the gas phase using a combination of microwave spectroscopy and quantum chemical calculations

STSM Final Report of Dr. H. Mouhib in the laboratory of Dr. I. Kleiner, LISA, Paris

The main aim of the MOLIM STSM of Dr. Mouhib was to enforce the collaboration between the experimental group at the RWTH Aachen University in Germany (who are experts in high-resolution molecular beam Fourier transform microwave spectroscopy) and the LISA Créteil, in France (who are experts in the theoretical modeling of the rotational and vibration-rotational spectra of medium-sized molecular systems). The goal of the two months visit of Dr. Mouhib was to develop new competences in the theoretical modeling of large amplitude motions using the BELGI code, which was developed in LISA. This code uses an effective Hamiltonian to describe the effects present in molecules containing one or two internal rotors, as well as rotation and centrifugal distortion. Dr Mouhib accomplished this task successfully. The molecular targets studied during the STSM are ***tert*-butyl acetetate** (TBA)**, Melonal** (2,6-Dimethyl-5-heptenal), and the cyclic monoterpene **rose oxide** (Tetrahydro-4-methyl-2-(2-methylpropenyl)-2H-pyran)**.**

For TBA, a small blueberry like fruit ester, the C_s conformer was determined to be the most abundant structure in the molecular beam (see Figure on the left-hand side). The preliminary assignments were carried out using the high resolution microwave data recorded in Aachen previous to the STSM. Further assignments using the BELGI code were done at LISA. **The refinement of the fits pursued with BELGI allowed us to obtain highly accurate molecular parameters to describe the dynamics and the barrier high of the acetyl methyl group.** The results were compared to state-of-the-art *ab initio* calculations and are essential to evaluate future quantum chemical models that deal with the quantization of internal rotation. In contrast to the observation of *Oki et. al.* at room temperature in the infrared range, the *cis*-conformation (C_1 symmetry) of TBA could not be detected in the supersonic jet. In short, the suggested interaction between the methyl and the *tert*-butyl group that may result in an energetic stabilization of the *cis*-conformer does not apply for the isolated molecule under molecular beam conditions. **The results on this part of the work will be published at the beginning of 2016.**



In the case of the medium-sized odorants Melonal and rose oxide, highly accurate *ab initio* calculations were carried out to investigate the vast conformational landscape of the molecules. In addition to the *ab initio* calculations, the assignment of the barrier to internal rotation of rose oxide using the BELGI code is currently in progress and will be finished by Dr. Mouhib back at her home institute. The obtained results will serve as "benchmark" for large molecular system and be extended to more complex systems in future. The preliminary simulated and assigned microwave spectra with the corresponding observed conformer are shown in the figure on the right-hand side. **Altogether, the previously defined research goals for the STSM of Dr. Mouhib were successfully accomplished and will lead to further fruitful collaborations between the above mentioned groups in Aachen and Paris.** In addition to this, Dr. Mouhib and Dr. Kleiner contacted biologists from the IEES at the UPMC in Créteil to initiate scientific collaboration which combines molecular biophysics and molecular biology by joining theory and experiment. In the future, Dr. Mouhib will be able to expand this collaboration with the aim to deepen her expertise in computational biophysics and establish herself as a future female scientist on the European scientific labor market.