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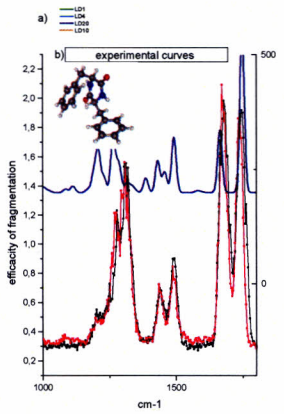
STSM REPORT OF Feriel Ben Nasr

My mission was conducted at the Institut des Sciences Moléculaires d'Orsay (ISMO) of CNRS and of Paris Sud University, from 15 October 2015 to 15 January 2016. The work performed during this intership is a part of my thesis which consists in a theoretical and experimental study of stereochemistry effects on the structure and the photoreactivity of biomolecules. This mission was realized under the supervision of Dr. Anne Zehnacker-Rentien Research director at CNRS.

During this mission, I did a theoretical and experimental study, in the gas phase, of vibrational spectroscopy of protonated molecular complexes having of biological relevance.

1- **Theoretical study of the structure of $Cd_2H_2^+HSO_4^-$ complex :**
This complex consists of a protonated dimer of cinchonidine (Cd), a cinchona alkaloid, interacting with sulfuric acid. Its study is an extension of that of the $CdH_2^+HSO_4^-$ complex I previously did in my thesis. Due to the complexity of the system, this work requires a careful exploration of the potential energy surface. Then la structure and the vibrational spectra of these systems are determined within the frame of the density functional theory (DFT). The aim is to simulate the vibrational spectra obtained at rhe Free Electrons Laser CLIO in Orsay. Two methods were used. First, ri-b97-d/TZVPP for saving calculation time thanks to the ri method (resolution of identity) and secondly b3lyp/6-31++g (d,p) known for giving acceptable harmonic frequencies.



2- **Experimental and theoretical study of the structure of protonated cyclic diphenylalanine peptides.**
I participated in experiments coupling mass spectrometry and IR laser spectroscopy in collaboration with D.Scuderi in the Laboratoire de Chimie Physique/CLIO in Orsay. The aim is to see the influence of chirality on the structure of a cyclic dipeptide by comparing cyclic diphenylalanines LL (LPheLPhe) and LD (LPheDPhe). The comparison between experimental spectra and calculated spectra shows that the system is protonated on oxygen. This figure shows the comparison between the calculated spectrum and the obtained spectrum for LPheDPhe in the region 1000-2000 cm^{-1}, in which a slight difference is seen between LPheLPhe and LPheDPhe. Calculation for Les LPheLPhe are in progress.

3- **Conclusion :**
During this mission I became familiar with the softwares and the methods which are used in quantum chemical calculations. I modelled many conformers of $Cd_2H_2^+HSO_4^-$ complex and selected the one observed experimentally by comparing their IR calculated spectra to experimental IR spectra. An article is in preparation, which includes these calculations and those I did earlier in my thesis. I participated in experiments coupling mass spectrometry and IR spectroscopy, other experiments are planned in 2016 to complete the results. I will continue the calculations on the dipeptides and an article will be published based on these results. So this mission allowed me to progress efficiently in the preparation of my thesis.

This report is consistent with the work of F. Ben Nasr

Anne Zehnacker

Bernard Bourguignon, director of ISMO

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