Short Term Scientific Missions (STSM)

Action number (CM1405)

Title of the planned STSM

Structure and dynamics of Flavors in different states of aggregation

Start and end dates:
01. Mars-31.Mars2017

The Applicant is **Miss Rihab Hakiri**. She got her **M.Sc. degree at the beginning of 2016** and started her PhD right afterwards in the group of Prof. Nejm-Eddine Jaidane at the LSAMA Laboratory in Tunis. In June 2016 she received a scholarship to work in the group of Prof. Wolfgang Stahl at the RWTH Aachen University in Germany (for details see also attached CV).**Her scientific interests** are molecular spectroscopy and quantum chemical calculations of small flexible molecules in connection with their biological activity. **Her involvement in MOLIM will help on the promotion of WOMEN in science and motivate young people to envisage a scientific career in Europe.**

Name of the host institution:

Molecular Spectroscopy Unit
Institute of Physical Chemistry
RWTH Aachen University

Landoltweg 2, 52056 Aachen, Germany.

Financial data (amounts requested for travel and subsistence).

1) Travel expenses: Flight ticket from Tunis to Frankfurt and the train ticket Frankfurt to Aachen (and back): **600Euros**

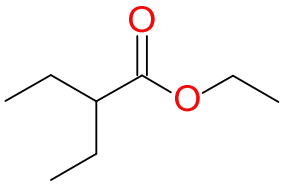
2) Subsistence expenses (including lodging, local transportation, meals):
For a stay of 30 days (1 month): **800 Euros**

TOTAL: 1400 Euros

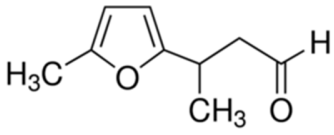
Work plan:
The work plan is to foster a collaboration between two groups, which are actively participating in the theme of the COST ACTION MOLIM. At the RWTH University in Aachen (Germany), they develop a state-to-the-art experimental microwave experiments using Fourier transform spectrometers combined with molecular jet with outstanding accuracy [1-3]. At LSAMA in Tunis (Tunisia), the group is specialized in theoretical modeling of the structure and dynamics of various medium-sized molecular systems in the gas phase, as well as in the solvated phase using implicit and explicit water models [4,5]. **Recently, the two groups have established a new collaboration which showed their complementarities to better understand the nuclear motions within these medium sized molecular species**. Within this collaboration, the applicant worked at the RWTH Aachen for three and analyzed two different molecular systems: **3-(5-Methyl-2-furyl)-butanal** and **ethyl 2-ethyl butyrate**. During her visit within the MOLIM action, the Applicant Rihab Hakiri will be able to finish up her

experiments on ethyl 2-ethyl butyrate and publish her results in peer-reviewed international journal such as JPCA or CHEMPHYSCHEM. Miss Hakiri **will also take advantage of her visit to increase her knowledge on microwave spectroscopy and design future project within the scope of her PhD thesis.** For this reason, Miss Hakiri previously contacted the group of Prof. Ulli Englert at the RWTH Aachen who will analyze the structure of her molecular system using X-ray crystallography. This will allow the applicant to immediately compare the structure of small flavors in different states of aggregation.

The molecular targets we are planning to study are: **First Miss Hakiri will complete her work on ethyl 2-ethyl butyrate** and then she will study the spectra of another organic molecule which is more complex, the **3-(5-Methyl-2-furyl)-butanal**(see Figure 1). The ethyl 2-ethyl butyratecompound is a small volatile ester with a fruity smell, often used for industrial purposes as flavor additive, while3-(5-Methyl-2-furyl)-butanal I a fresh flavor reminiscent of cucumber due to its fresh, green scent impression.



ethyl 2-ethyl butyrate



3-(5-Methyl-2-furyl)-butanal

Figure 1. Molecular Systems analyzed by the applicant.

The aim of Miss Hakiri is to study the conformational landscape of these molecules in detail using quantum chemical calculations. This is required to analyze and assign the microwave data which she already recorded during her last stay at the RWTH University of Aachen. This will help her to deepen her knowledge on these types of systems.
The analyzed structures in the gas-phase will subsequently be compared with results in the condensed phase and the solvated phase using different solvents, e.g., water and ethanol. The results are crucial to estimate which conformations will be most relevant for the activation of ligand-protein-complexes in biological media.

References

[1] J.-U. Grabow, W. Stahl, H. Dreizler, *Rev. Sci. Instrum.***1996**, *67*, 4072-4084.
[2] H. Mouhib, W. Stahl, M. Lüthy, M. Büchel, P. Kraft, *Angew. Chem. Int. Ed.***2011**, *50*, 5576-5580.
[3] H. Mouhib, D. Jelisavac, L. W. Sutikdja, E. Isaak, W.Stahl, *J. Phys. Chem. A***2011**, *115*, 118-122.
[4] N. Derbel, I. Clarot, M. Mourer, J.B. Regnouf-des-Vains and M.F. Ruiz-López, *J. Phys. Chem. A***2012**, *116*, *9404−9411*.
[5] O. Ouni, N. Derbel, N. Jaïdane and M.F. Ruiz-López, Computational and Theoretical Chemistry, **2012**, *990*, *209–213*.