Report of the STSM of Miss Rihab Hakiri at the RWTH Aachen University entitled

Structure and dynamics of Flavors in different states of aggregation

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Name of the host institution:

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During my visit within the MOLIM action, I was be able to finish up the experiments on ethyl 2-ethyl butyrate completing my previous data set with a large number of high resolution measurements. The fit of the most abundant conformer using ethyl 2-ethyl butyrate which I made using the XIAM code consists of 87 transitions and yielded a set of highly accurate rotational and centrifugal distortion constants. Part of the recorded and predicted spectrum of ethyl 2-ethyl butyrate using the experimental spectroscopic constants I obtained from the fit are shown in Figure 1. We will soon submit a manuscript with my results in a peer-reviewed international journal (such as JPCA or CHEMPHYSCHEM). The manuscript is currently in progress.

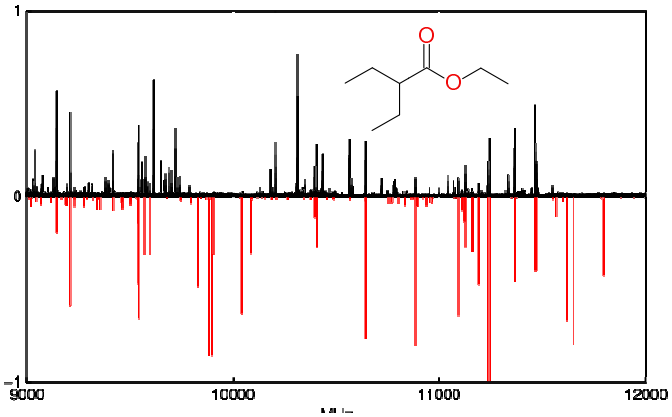

Figure 1.
Recorded spectrum of ethyl 2-ethyl butyrate in the frequency range from 9 to 12 GHz (upper trace) using the low resolution mode of the spectrometer and the theoretical spectrum (lower trace) of the assigned conformer predicted using the XIAM code at a rotational temperature of 1 K.

After completing the work on ethyl 2-ethyl butyrate and I started the attribution of the microwave spectrum of a much more complex system, the **3-(5-Methyl-2-furyl)-butanal** which is currently ongoing and will finish up at my home institute. I was able to study the conformational landscape of these molecules in detail using quantum chemical calculations. This was crucial to analyze and assign the first microwave data which I already recorded during my last stay at the RWTH University of Aachen. The results obtained during my stay with the MOLIM STSM are crucial to know which conformations are be most relevant for the activation of ligand-protein-complexes in biological media.
In addition, I was able to highly benefit from my visit to plan future projects within the scope of my PhD thesis in the field of quantum chemical calculations and high resolution spectroscopy. I started an active collaboration with the group of Prof. Englert at the RWTH Aachen who is currently analyzing the structure of my molecular systems using x-ray crystallography.