

Report of the STSM of Miss Alina Wildenberg at the LISA in UPEC

Action number (CM1405)

Start and end dates:

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Name of the host institution:

Laboratoire LISA

CNRS UMR 7583, Univ. Paris Est-Créteil

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FRANCE

TITLE OF THE STSM

“Large amplitude motion in 2,3-Dimethylanisol – Spectroscopic, crystallographic, and theoretical characterization”

During my visit within the MOLIM action, I carried out state-of-the-art quantum chemical calculations at the B3LYP and MP2 levels of theory to calculate 2D potential energy surfaces of the 2,3-dimethylanisol. The investigated angles are shown in figure 1. These calculations are important to understand the intramolecular coupling effect of the molecule and to determine all barriers to internal rotation of the molecule to be able to assign the microwave spectra. Parts of the calculations at the MP2 level are still in progress.

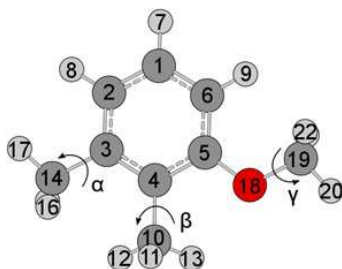


Figure 1. Structure of 2,3-Dimethylanisol. For the 2D potential energy surfaces, the angles alpha and beta, as well as the angles beta and gamma, were rotated against each other in steps of 10 degrees.

In addition to the calculations, I was able to perform some high resolution measurements on the small molecule 2-methylthiazol using the MB-FTMW spectrometer at LISA. The high resolution measurements are used to obtain highly accurate rotational constants and quadrupole coupling constants of this molecule. Figure 2 shows the structure of 2-methylthiazol and a high resolution measurement I performed on the microwave spectrometer in LISA. After finishing the fit, we will be able to publish the results in form of a manuscript in a peer-reviewed journal such as Molecular Structure of the Journal of Molecular Spectroscopy.

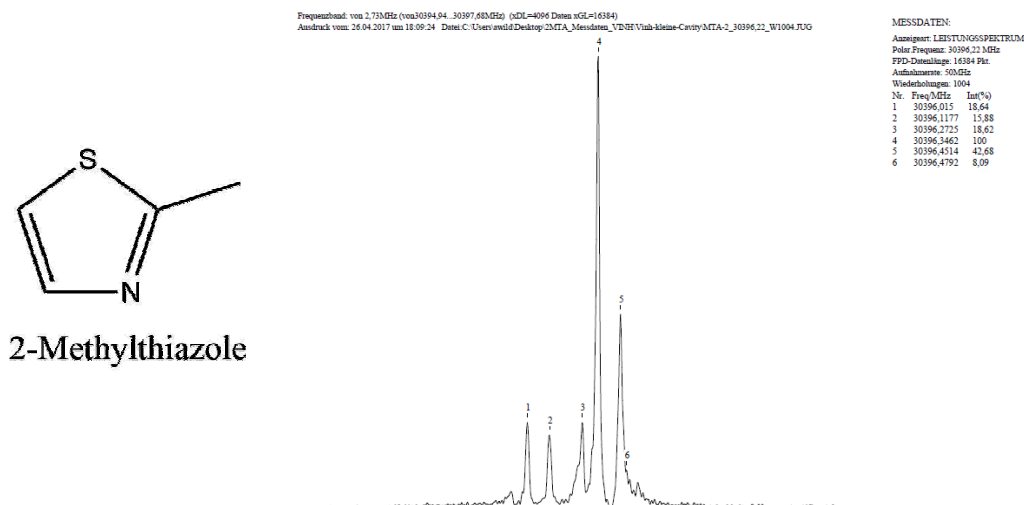


Figure 2. Left hand-side: Structure of 2-methylthiazole. **Right hand-side:** High resolution measurement of 2-methylthiazole recorded at a frequency of 30396.22 MHz.

In summary, I very much enjoyed working on a project within a research group and did highly benefit from my visit at the LISA laboratory. The STSM motivated me to plan future projects after my M.Sc. degree and to pursue a career in science which might include applying for a PhD position in Germany or another European country. I am definitely interested in the field of molecular physics and chemistry and was able to meet several experts in these fields.