

SHORT TERM SCIENTIFIC MISSION (STSM) SCIENTIFIC REPORT

This report is submitted for approval by the STSM applicant to the STSM coordinator

Action number: CM1405

STSM title: Is Conformational Switching Through Vibrational Overtone Pumping Selective?

STSM start and end date: 04/03/2019 to 17/03/2019

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PURPOSE OF THE STSM:

(max.200 words)

The purpose of the STSM to the LaserLab at Coimbra University in Portugal was to perform NIR vibrational overtone excitation experiments, as well as to obtain knowledge of the necessary techniques and equipment to possibly create a similar setup In Copenhagen. The goal with these experiments was to investigate if conformational changes could be induced by NIR overtone pumping and/or UV irradiation for selected molecules.

DESCRIPTION OF WORK CARRIED OUT DURING THE STSMS

(max.500 words)

During the work performed, explanations of the required theory and experimental setup was provided by the host, as well as possible adjustments to the present setup.

We managed to study two of the molecules we brought with us from Copenhagen. The first week we spent on the first molecule (the dimethoxy-pyrimidine). We tested several possible wavenumbers as possibilities for NIR overtone excitations. Hereafter we also tested with UV excitation in an effort to induce conformational changes (not easily seen with NIR excitation). We also tested whether the dimethoxy-pyrimidine could change its conformation without the excitation laser present, to rule out switching induced by the spectrometer from photoinduced switching from a specific excitation. Furthermore, we used annealing to see the possible changes due to heating.

The second week we started with the second molecule (the mercapto-pyrimidine). Upon arrival we were made aware of the possibility of the lowest energy conformer would not be as expected (rather with an double bonded O and S). Therefore we started by investigating this molecule via UV light to see which conformers were visible before and after irradiation. NIR overtone pumping would require this knowledge to know which overtones to irradiate.

After having found the UV irradiation needed to induce conformational change, we tried it again and let it irradiate for approximately 30 minutes to produce a significant amount of the other conformation(s). Following this, we used the laser to irradiate the sample at 280nm for 5-10 minutes four different times. Again, tests were made to ensure that the observed switching events were caused by the UV irradiation and not the spectrometer itself.

In general the overall process was delayed due to complications with the laser.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

It was possible to induce conformational changes in both the molecules we studied here, 4-amino-2,6-dimethoxypyrimidine (dimethoxy-pyrimidine) and 4-amino-6-hydroxy-2-mercaptopyrimidine monohydrate (mercapto-pyrimidine), by using UV irradiation. We had some difficulties inducing changes via NIR overtone pumping, but nevertheless got a good idea of the technique, as well as the range in which to irradiate when further experiments are to be performed.

The mercapto-pyrimidine spectra will take a lot of time to analyze due to the many possible conformers in which it can be. It will definitely be an interesting process, especially when comparing to calculations and the spectra in which other conformers have appeared. In the dimethoxy-pyrimidine we believe to have seen signs of selectivity in the UV range.

FUTURE COLLABORATIONS (if applicable)

The group at Universidade de Coimbra have a vast amount of knowledge and experience within the field over NIR overtone pumping and like techniques to induce conformational changes. For further work it would be a great source for advice and guidance to keep contact. No additional visits have been planned so far, but further work on the compounds will most likely be done both in Coimbra and Copenhagen.