Report on the outcomes of a Short-Term Scientific Mission[[1]](#footnote-1)

Action number: CA18212

Grantee name: Dominik Jank

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| **Details of the STSM**  Title: Experimental and Theoretical Investigation of wavelength-dependent photochemistry on atmospheric important molecules.  Start and end date: 09/07/2023 to 22/07/2023 |
| **Description of the work carried out during the STSM**  Description of the activities carried out during the STSM. Any deviations from the initial working plan shall also be described in this section. |
| *(max. 500 words)*  After arrival and some general discussions for the plans of the upcoming two weeks, an introduction to the lab and especially the cluster beam (CLUB) apparatus together with the necessary safety instructions was given. The experimental work started with the setting up of the apparatus for the molecule of interest.  For the first week, we worked with acetyl chloride (H3C2ClO) which is one of the *X*3C2ClO molecules (*X* = F, Cl, H…), study of them and their clusters is the goal of this STSM. As the apparatus was used for other experiments, we had to clean it and change source and nozzle (*d* = 90 mum) for the use of a gaseous sample. The waiting time for the evacuation of the vacuum chamber allowed further instruction on the used laser and the velocity map imaging (VMI) which we used for the first experiments. The goal of the first measurement was to carry on with the last measurement which was done two months earlier on the same molecule, by reproducing the VMI image of photodissociation with co-expansion of the molecule together with argon clusters. The photoionization and dissociation are done via a resonant enhanced multiple photon ionization (REMPI) at a wavelength of 235 nm. Here, we found some discrepancies in the kinetic energy distribution when looking at the intensity part of the VIM. However, in the ion counting mode, the results were comparable. Thus, we tried to find the cause of this error, and after some other modifications, we could reason that the most probable cause for this was the too short time of acquisition of the multichannel plate which we could not change in this frame, but as the ion counting delivered correct results, we continued with this mode for the rest of the measurement. The next step was the switching from co-expansion to pick-up experiments, which means the pick-up of the molecule after the forming of the argon clusters. For this also VMI and mass spectrum measurements were performed.  In the second week, we started with the measurement of trichloroacetic acid (CCl3COOH). As this was a solid sample, we had to change from the rare gas source to the solid source. We started with tuning the parameters for heating of the source and nozzle, and adjusting the argon backing pressure for most intense electron ionization (EI) gains for larger cluster sizes. With the obtained settings, EI mass spectra at 70 eV and also electron attachment (EA) measurements with electron energies between 0 and 15 eV could be taken. Repetition of the measurement showed a strong dependence of the drying time of the solid sample in the apparatus. So, we repeated the measurements with even higher reservoir and nozzle temperatures together with a longer time of the sample inside the apparatus for drying it to get rid of water. Lastly, we switched from argon to helium as a buffer gas and performed also EI and EA measurements. However, this measurement will be continued in the next weeks. |
| **Description of the STSM main achievements and planned follow-up activities**  Description and assessment of whether the STSM achieved its planned goals and expected outcomes, including specific contribution to Action objective and deliverables, or publications resulting from the STSM. Agreed plans for future follow-up collaborations shall also be described in this section.  *(max. 500 words)*  Employing the STSM, we could obtain VMI images for acetyl chloride (H3C2ClO) in the ion counting mode, both for co-expansion of the molecule in argon and helium buffer gas and for pickup of the molecule on argon clusters. Further, mass spectra for the different processes were taken. For trichloroacetic acid (CCl3COOH), we recorded mass spectra for EI as well as for EA on the molecule and molecular clusters which were created with the solid source and the use of argon and helium as buffer gases with different amounts of water attached to the clusters.  Overall, the measurements went as well as expected, and delivered a considerable amount of output for the short period of two weeks. Also, a better understanding and connection between theory and experiment was obtained by lively discussions about results, experimental procedure, and observations, which yielded a benefit for both sides.  For the follow-up of the STSM, the obtained data of the experiments still needs to be evaluated fully. This, and the interpretation of the results will still be done in cooperation of both sides. Moreover, we will start the theoretical investigation of the molecules with the help of quantum chemical calculations. We will model different possible isomers of the observed clusters and fragments to get a picture of the structural changes during the processes. Further, we will try to follow the energetics of both photodissociation, which was recorded via AIM, and EI and EA obtained by mass spectroscopy.  The experimental outcome should fit well to the objective of working group 2 of the COST action - survival and destruction of molecules following energetic processing, where we could contribute to the task – Develop models to accurately describe how energetic processing affect the competition between structural changes and emission of photons, electrons and heavy particles on ultraslow timescales.  In the end, it is expected that the experimental part as well as the theoretical contribution are published in a cooperative research paper.  The STSM was a good possibility for strengthening the collaboration between the theoretical group of Dr. Milan Ončák and the experimental group of Dr. Michal Fárník and paved the way for further collaborations and student exchanges.  Personally, the chance to work on the CLUB apparatus allowed me to get in touch with a new experimental setup and to work with spectroscopic components like VMI which beforehand I only knew from different lectures. Further, I really enjoyed the opportunity to contribute to the experiment with my own thoughts, ideas, and decisions always well supported by the group. And I already look forward to the theoretical investigations as some results of the experiment still need a better theoretical background for a full understanding of the underlying processes. |



1. This report is submitted by the grantee to the Action MC for approval and for claiming payment of the awarded grant. The Grant Awarding Coordinator coordinates the evaluation of this report on behalf of the Action MC and instructs the GH for payment of the Grant. [↑](#footnote-ref-1)