Report on the outcomes of a Short-Term Scientific Mission[1]

Action number: CA21126

Grantee name: Maëva Louis

Details of the STSM

Title: **Electronic spectroscopy of space-relevant oxygenated or sulfurated interstellar complex organic molecules.**

Start and end date: 04/05/2026 to 24/05/2026

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)

The STSM was carried out as part of Petrignani's group (UvA) in collaboration with Jennifer Noble and Jordan Dezalay in the PIIM laboratory at Aix-Marseille Université (AMU), using the cryogenic ion trap and electrospray ionisation (ESI) for 3 weeks. The initial working plan was to record the electronic action spectra of three species: protonated anthrone, protonated oxanthrene and protonated thianthrene under cold, high-vacuum conditions. Anthrone got replaced by fluorenone (our initial backup molecule) in this STSM.

The first week was dedicated to getting familiar with the ESI setup, optimization and recording spectra and mass spectra (MS). We prepared solutions of the compounds of interest in different MeOH:H2O solvent ratios, in which we added a few drops of acetic acid for protonation. Optimization of the ESI (temperatures, voltages, flow rates, pressures, solutions etc...) and of the ion path for both protonated thianthrene and fluorenone were attempted. For the fluorenone, we successfully recorded the action spectra of the protonated parents and the photofragments in the range [210 - 430] nm, as well as mass spectra with and without laser at a resonant wavelength. We faced two limitations: the signals were quite weak (parent and fragments) and some fragments created independently of the laser were detected, limiting the quality of the recorded data. For the protonated thianthrene, the instability, the broadening and the intensity of the signal did not allow us to perform any reliable measurements.

Because both the signal to noise ratio and the stability of the signal for thianthrene and fluorenone was not satisfying enough, we decided to adjust the plan for the second week: we switched from protonated

[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.

species to radical ions (still for thianthrene, fluorenone and oxanthrene) using a discharge, unsuccessfully. We decided then to switch back to the original plan, the protonated species, and renew our effort with the ESI for the third week.

The third and last week of the visit was focused on the protonated thianthrene and oxanthrene. The signal of both the thianthrene and the oxanthrene were still very unstable, very weak and disappeared over time. We suggested then that the optimization of the ion paths was hindered and decided to check using protonated aza-indole. 7-Aza-indole has been previously successfully recorded by the hosts (Noble+2020 PCCP 10.1039/d0cp03608k). Its signal was also not as intense as expected, confirming our suspicions. As the stability of the signal using this benchmark protonated molecule was stable enough, we continued our effort with the protonated oxanthrene and thianthrene. Some preliminary data were obtained for the thianthrene, mostly MS, including the observation of S-loss. Despite many attempts, we have not been successful in recording any data related to the protonated oxanthrene

Overall, the main challenges we faced during these three weeks of experiments were due to the weak intensities of the protonated species, their instabilities and the separation of the fragments created by the photofragmentation from the fragments created by collision in the trap. This limited the acquisition of experimental data but these three weeks led to the measurements of a good set of base data on the molecules, that will be refined by the host group in the coming months.

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)

Main achievements:

During these three weeks, we successfully measured the MS and action spectrum protonated fluorenone. We also were able to record the MS of protonated thianthrene and preliminary results of the thianthrene action spectrum, in which S-loss was observed. Regarding the challenges faced during this STSM, we identified (some) experimental problems hindering the experiments. Those three weeks were dedicated to this explorative work described above and we were able to get preliminary data regarding the action spectra, enabling the follow-ups described below.

Follow up action plans:

The follow-ups of this collaborative project between Petrignani's group, Jennifer Noble and Jordan Dezalay includes new measurement attempts by the host team in July. In parallel, TDDFT calculations will be performed by the grantee to have a better insight on the preferred protonation sites of these molecules. The observation S-loss of the thianthrene was also one of the unexpected highlights of this STSM, and its understanding needs further experimental and theoretical work to study its dissociation pathways and energy.

The results obtained during this STSM is a good basis and, with further experiments and calculations, we expect to be able to write an article about the photochemical behaviour of protonated fluorenone and protonated thianthrene, contributing to the understanding of their potential role in the interstellar medium. This article as well as contributions related to this STSM at international conferences will be prepared, highlighting the COST Action NanoSpace network. As mentioned in the application form, this study is directly related to the broader goals of the Action MoU, with the enhancement of our knowledge of interstellar matter, providing data for computational models, and allowing interdisciplinary and international collaboration between PIIM and UvA. These outcomes are directly relevant to the Action MoU objectives and deliverables, contributing to the advancement of our understanding of astrochemistry and organic material in space.