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

Action number: CA21126

Grantee name: Fatima Baterdouk

Details of the STSM

Title: Structure of Ionized PAH – Water Complexes of Astrophysical Interest

Start and end date: 25/02/2025 to 13/03/2025

Description of the work carried out during the STSM

During this STSM at the FELIX laboratory (Nijmegen, the Netherlands), I actively participated in the beamtime proposed and led by Dr. C. Joblin, co-director of my PhD thesis. The project aimed to study the interaction of water with polycyclic aromatic hydrocarbons (PAHs) in an astrophysical context and to quantify the infrared (IR) signatures of the complexes formed. This project took place at the FELIX facility on the FELion cryogenic ion trap tandem mass-spectrometer. For this run, the focus was on cationic pyrene ($C_{16}H_{10}^+$, Pyr^+) and protonated pyrene ($C_{16}H_{11}^+$, $PyrH^+$). However, during the preparation phase we were unable to optimize the production of these ions complexed with one or two water molecules at cryogenic temperatures. We therefore used 1-hydroxypyrene ions ($C_{16}H_{10}O^+$, $PyrOH^+$) as an alternative precursor and were able to produce its hydrated form $PyrOH^+$:H_2O.

The preparation phase included the optimization of the preparation of the PAH cations of interest with the storage ion source. The sample of 1-hydroxypyrene was evaporated at around 120°C and the ions were generated by electron impact ionization at energies between 10 eV and 50 eV. Pure and mixed helium and hydrogen gases were injected into the source to optimise the signal and to investigate the formation conditions of cationic and protonated 1-hydroxypyrene. The produced ions were then extracted by a (100-200 ms) pulse from the source, and the desired mass was selected by a quadrupole mass filter and transferred to the cryogenic 22-pole ion trap. Mixtures of He:Ne and He:H_2O were injected inside the trap to produce $PyrOH^+$:Ne complexes at 6 K and $PyrOH^+$:H_2O at (208 – 230) K, respectively. The free electron laser FEL-2 in the 5.5–15 µm (1800-600 cm^{-1}) spectral range was used to perform action spectroscopy by Infrared Pre-Dissociation (IRPD), trapping the ions up to 1.6 s. In case of H_2O tagging, the action spectroscopy technique could be Infrared Multiple-Photon Dissociation (IRMPD). The irradiated ions were then extracted from the trap by mass-selecting the parent ($PyrOH^+$:Ne or $PyrOH^+$:H_2O) using a QMS and counted by a Daly detector.

[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.

Depletion scans (studied ion counts vs. irradiation time) at wavelengths centred on some specific bands were also acquired. They will be used to study the diversity of isomer populations and the dissociation mechanism for the investigated bands.

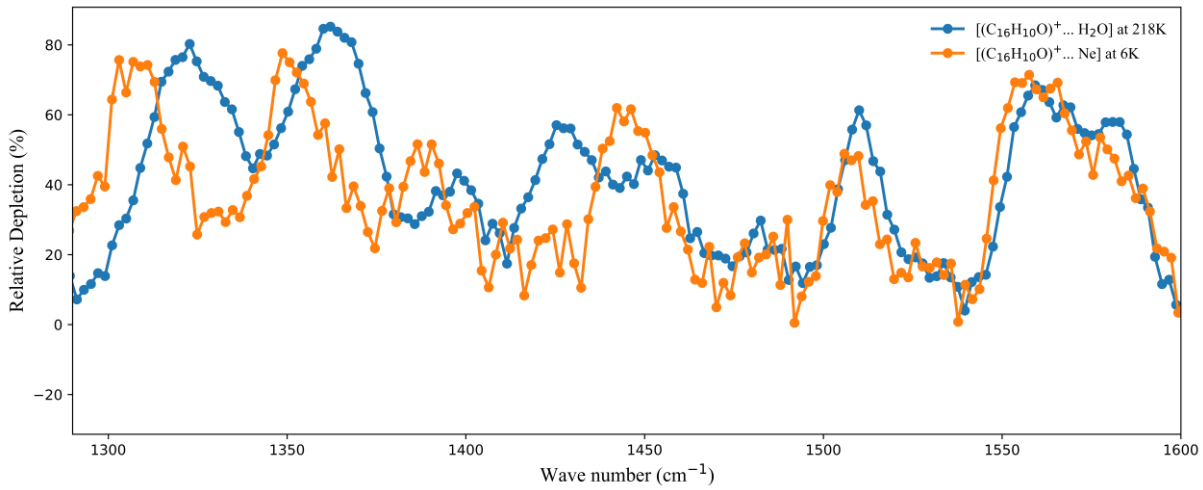


Figure 1 – IR spectra of $PyrOH^+$ tagged with Ne or H_2O (preliminary analysis) *highlighting the effects of water interaction on the $PyrOH^+$ spectrum in the 1290-1600 cm^{-1} (6.25-7.75 µm) range.*

Description of the STSM main achievements and planned follow-up activities

(max. 500 words)

This project at FELIX is part of a collaboration between several groups of experimentalists and theoreticians in Europe (France, Netherlands, Germany, Italy) to study the interaction of water with PAHs in an astrophysical context. The STSM gave me the opportunity to actively participate in the preparation and in the FELIX shifts using the FELion setup, and to improve my training on IR spectroscopy methodology, which is key in my PhD project led at LCAR/IRAP at Toulouse University. In addition, I am now strongly involved in the processing of the data. This is my first opportunity to work on a consistent scientific dataset since I have been more involved so far on the instrumental side. Although we were not able to reach the initial goal of the proposal, the obtained results are of high interest, highlighting the potential role of OH functional group in PAH-water interactions. Quantum chemistry calculations are ongoing by our collaborators in LCPQ (Toulouse) and OAC (INAF, Italy) to better characterize these interactions. This study will likely lead to a publication. Furthermore, the successful preparation of PAH-water complexes with FELion broadened our general scientific perspectives to further investigation of water tagging with different PAH molecules to better understand their intermolecular interactions.

Beyond the scientific achievements, this STSM provided an excellent opportunity to strengthen my scientific network. Collaborating with a new team, including PhD students from diverse backgrounds, enriched my research experience as an early-stage researcher and broadened my perspective. These activities were also featured in a NanoSpace outreach blog, highlighting the role of an early-stage researcher participating in an international collaboration during a beamtime mission at the FELIX facility.