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

Action number: CA21126

Grantee name: Pavol Jusko

Details of the STSM

Title:Growth of small polycyclic aromatic hydrocarbons from 5 membered rings - $C_5H_5^+$, $C_9H_7^+$

Start and end date: 27/05/2024 to 08/06/2024

Description of the work carried out during the STSM

The STSM started right after the superconducting magnet of the cryogenic FTICR setup PIRENEA was restarted after 2 years of break due to difficulty in supplying liquid helium. The team at IRAP (group of C. Joblin) had checked that the different components were functioning properly before the STSM so everything was ready at arrival and the scientific program could proceed. PIRENEA was operated at room temperature. The "building block" of interest, $C_9H_7^+$ ion, was produced from 2-methylnaphtalene vapor pressure pulsed into the trap (ICR cell) in the presence of intense 266 nm radiation (>5 mJ/pulse). The multiphoton process leads to ionisation and subsequent fragmentation. The $C_9H_7^+$ ion (115 *m/z*) was then mass selected inside the trap to react with 2-methylnaphtalene and produce a cluster of mass 257 *m/z*. The clusters were then fragmented using either photons from a tunable OPO laser in the visible or from activation by collisions with helium. For this STM, our focus was to characterize the structure of the 179 and 178 *m/z* fragments, by using action spectroscopy in the visible range. The species at 178 *m/z* were identified as anthracene cations. It was more difficult to assign 179 *m/z.* Protonated anthracene and phenanthrene are obvious candidates but they both have several isomers and the resulting electronic spectrum can be quite complex as shown in the literature. We however noticed that 179 *m/z* fragments into 178 *m/z*, which suggests that 179 *m/z* is protonated anthracene. Interpretation of the spectral analysis will continue over the coming weeks.

In addition of the grantee (P. Jusko), the experimental campaign involved the PIRENEA team at host institution (C. Joblin, technical staff in particular A. Bonnany and O. Coeur-Joly, as well as a junior post-doctoral fellow who took the opportunity to familiarize herself with the technique).

During my stay, I also gave a talk about my current work on the weekly Institute Seminar of the LCAR/ FERMi institute at the Université Paul Sabatier – Toulouse 3.

[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.

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

The main achievement of the STSM was to demonstrate that the photo-reactivity of 2-ring aromatic species can lead to efficient formation of 3-ring aromatic species. This provides a possible additional route for PAH growth in astrophysical environments. The obtained results combined with theoretical calculations performed at the DFT level will be used to finalise a publication on the growth of PAHs induced by reactivity of the 5-membered rings ions $C_5H_5^+$ and $C_9H_7^+$. We plan to submit this publication to A&A within 2-3 months. A virtual meeting with the colleague involved on the theoretical side is planned for the end of June.

This STSM also re-started a longer term collaboration between the STSM host and the grantee's home institutes beyond the current publication in preparation and was the opportunity to train a junior post-doc on using PIRENEA to progress on her scientific program dedicated to the isomers of the -H fragment of methylated PAH cations.