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

Action number: CA18212

Grantee name: João Ameixa

|  |
| --- |
| **Details of the STSM**  Title: Survival of fragments of cyano-containing polycyclic aromatic hydrocarbons  Start and end date: 12/12/2022 to 16/12/2022 |
| **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. |
| We have successfully carried out the planned measurements of survival times of fragment ions produced upon the collision of fast benzonitrile (BN) and 1-cyanonaphtalene (1-CNN) cations with He during the STSM. Such studies involving 2-cyanonapthalene will be the focus of a future proposal for beamtime at the DESIREE infrastructure. For both systems, BN and 1-CNN, we have measured, in a first step, the collision-induced dissociation mass spectrum (CID MS) of the intact parent cation at an energy of about 100 eV (lab-of-frame energy), where He served as a collision partner. For a mass-selected ion, we have subsequently measured the ion yield as function of the storage time in DESIREE for the intact parent cations, as well as that for the most abundant fragment ions using two different experimental schemes: (i) measurement of spontaneous emission of neutrals and (ii) ion-beam dump onto a detector after progressively longer storage times.  Figure 1 shows the CID MS of BN+ (C6H5CN+) where the most abundant fragments are ascribed as C6Hx+ due to -HxCN loss, as well as C6Hx+ and C3Hx+ due to -HxC2N and -HxC3N losses, respectively. In the absence of He in the collision cell, it is observed a contribution from a metastable decay process leading to -HxCN loss to yield the ion C6Hx+. For each observed fragment of BN+ formed upon a collision with He, we measured subsequently the spontaneous emission decay yielding neutral fragment yield as a function of the storage time in DESIREE. In a further experiment, we measured the remaining ionic yield by directly dumping the ion beam onto a detector at different storage times in DESIREE ranging from 270 μs up to 1 s. The data acquired from the latter experiment is currently under analysis.   |  | | --- | |  | | *Figure 1. Mass spectra from (i) the metastable decay of BN+ (black line), and (ii) the collision-induced dissociation mass spectrum of BN+ upon collisions with He at a center-of-mass energy of about 100 eV(blue line).* |   The CID of 1-CNN+ produces a rich fragmentation pattern as shown in Figure 2. The most abundant fragments are C10Hx+ due to a loss of –HxCN along with a series of six lighter fragments with molecular structure C10-*n*Hx+ with *n* ≤ 6 (–HxC*n*N loss), in which the dominant ion is ascribed as C6Hx+. As observed in fragmentation pattern of BN, the parent ion 1-CNN+ undergoes a metastable decay, by which the neutral fragment HxCN gets dissociated to yield the counterpart ion C10Hx+.   |  | | --- | |  | | *Figure 2. Mass spectra from (i) the metastable decay of 1-CNN+ (black line), and (ii) the collision-induced dissociation mass spectrum of 1-CNN+ upon collisions with He at a center-of-mass energy of about 100 eV(blue line).* | |
| **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.  Through the present STSM, the survival of fragments of benzonitrile and 1-cyanonaphtalene were successfully studied using the unique storage conditions of the DESIREE cryogenic ion storage ring. The next activity is to analyse the data related with the spontaneous decay of (i) parent cation BN+, (ii) fragments produced by CID as well as (iii) the 1-CNN+ fragments produced by CID. Classical molecular dynamics simulations will be also conducted by the Stockholm groupto help to interpret the experimental data, namely by simulating the mass spectra measured experimentally, the energy distribution of the fragmentation products as well as fragmentation routes. In this spirit, we intend to prepare a publication to be submitted in a high-impact journal in the field of astrochemistry or physical chemistry, where we plan to provide key insights to understand the chemistry of cyano polycyclic aromatic hydrocarbons in conditions close to those of the interstellar medium. Therefore, the expected outcomes of this STSM are in line with the MD-GAS COST Action objectives. To extend the knowledge acquired herein, a further application for a STSM to the DESIREE infrastructure may be submitted, through which a similar set of experiments could be performed on the isomer 2-cyanonaphtalene. |
|  |



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)