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

Action number: CA20129 MULTICHEM

Grantee name: Antonella Cartoni

Details of the STSM

Title: Study of mutual neutralization reactions in low energy collisions between organic cations and atomic oxygen anions

Start and end date: 17/03/2024 to 23/03/2024

Description of the work carried out during the STSM

During the STSM in Stockholm we performed experiments of mutual neutralisation (MN) between organic pyrimidine cation ($C_4H_4N_2^{\cdot+}$, Pyr^+) and oxygen anion (O^-), and a preliminary measurement using the accessible chlorine anion (Cl^-).The Pyr^+ beam was produced on the high energy platform using the ECR source, accelerated to 32kV and injected into 'symmetric ring' of DESIREE. The O^- beam was produced on the low energy platform using a cesium-sputtering SNICS source, accelerated at 7kV and injected in the 'asymmetric ring' of DESIREE, see Figure 1.

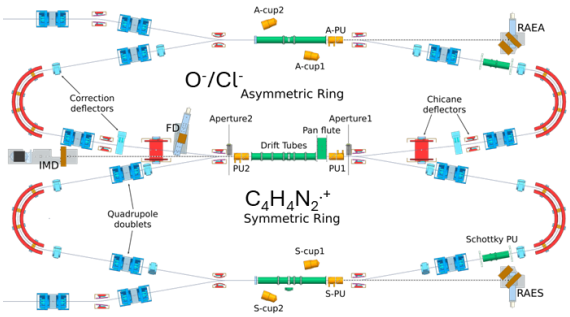

Figure 1.
The DESIREE storage rings. In the merging section, where the two beams overlap, tube electrodes can be biased to control the collision energy down to about 100 meV. Scheme is taken form the DESIREE web page, https://www.desiree-infrastructure.com/desiree

The first day was spent in optimizing the working conditions in the two rings using Ar^+ and O^- ion beams, and finding the best overlap between the two with apertures, to have the best possible starting conditions for the mutual neutralisation (MN) experiments.
Then the Ar^+ beam was replaced by Pry^+ in the symmetric ring, and the MN experiments between Pyr^+ and O^- (and in the last days with Cl^-) with a collision energy of the centre of mass of about 0.1 eV were performed. This condition is achieved by tuning the velocity of the two beams along a relatively short region in the 'drift tube', i.e. the merging section between the two rings. When the complex is formed by

[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.

the MN, then two or more correlated neutral products are ejected sharing a certain amount of energy that can be 'stored' as internal energy of the fragments or spent in their kinetic energy. Therefore, the neutral particles depart of each other with a well-defined relative kinetic energy distribution and direction of motion. The neutral fragments hit the neutral detector located straight ahead along the drift tube direction. Recording and correlating the (*x,y,t*) coordinates of each hit on this position sensitive detector allows to reconstruct a simple picture of the collision and interaction between cation and anion.
The coincidence data are sorted by events that involve two or three (or more) particles. Two particle events are most likely due to neutralised Pyr and O (or Cl) molecule/atom and provide information on the excited states of the Pyr molecule where the electron has been captured. The preliminary step of the analysis is reported in Figure 2 where the kinetic energy release E_K distribution can be reconstructed by the measurements of the *x,y* position and timing, *t*, of hit of each particle on the detector. The choice of the two anions (O^- and Cl^-) is driven by their very different electron affinity value, 1.439157 ± 0.000004 and 3.613577 ± 0.000044 eV respectively. This in turn is expected to lead to different MN and collisional dynamics with Pyr (IE=9.33 ± 0.07 eV), with a closer interaction in the case of Cl^-. At a closer interaction, not only different electronic states of Pyr are expected to be populated, but also the probability of a direct head-on collision could increase.

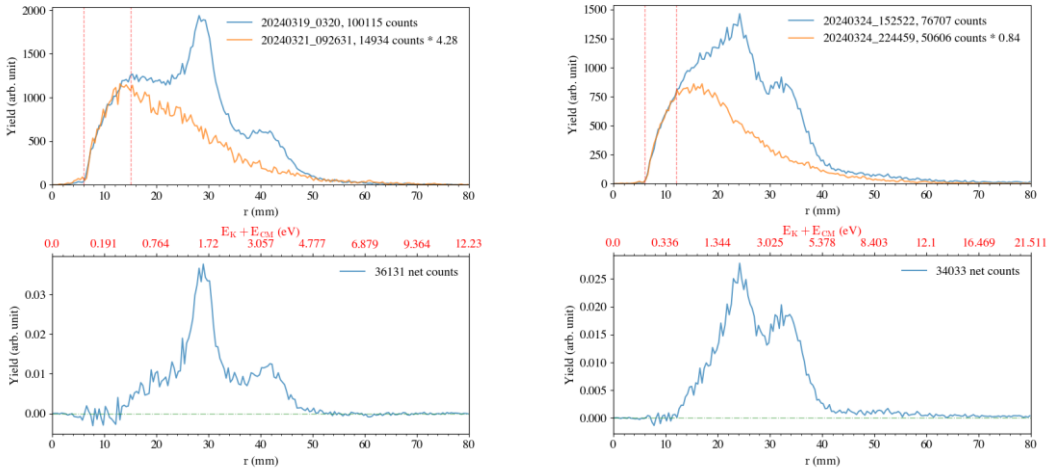

***Figure 2**. Preliminary results of MN experiments between Pyr^+ and O^- (on the left) and Cl^- (on the right). In the top panels, the background, due to high energy collisional processes are also displayed (orange line). The bottom panels report the background subtracted data. The kinetic energy released scale is also reported in red.*

Indeed, the preliminary analysis reported in Figure 2 shows clear differences between the two anions. Moreover, three-particle events were observed and provide access to the interesting break-up dynamics. In our case, the main fragmentation channels have been identified in the HCN and 2HCN loss. A detail data analysis is in progress and theoretical simulation will be undertaken to understand and explain these results.

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

The STSM has allowed the first joint experiment between University of Rome La Sapienza/CNR and SU at DESIREE, and it has been very successful, on many respects. From the scientific point of view, the experiments fulfilled the experimental plan, and even added and explorative measurement using the accessible Cl^- anion, further than O^-. Preliminary analysis has shown data of good quality, and that pyrimidine is an excellent target, with a good compromise of complexity (typical of biomolecular systems) and feasibility in the theoretical calculation/simulation of the results. This international collaboration, with different expertise, has the aim to achieve the best results in data analysis and theoretical support to better understand the dynamics in cation-anion collision when biomolecular systems are involved. From the practical point of view, this STSM has been the invaluable opportunity to work, hands one, at DESIREE. The training received will facilitate the ability to propose follow up of the present experiments, as well as new class of experiments. These have already been discussed during the visit in Stockholm. New visits and on-line discussion will be the essential tools to continue collaboration and produce a publishable articles.