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

Action number: CA20129 - MultiChem

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Details of the STSM

Title: Mutual neutralization reactions in collisions between biological relevant cations and 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 pyrimidine cations ($C_4H_4N_2^+$, Pyr+) and oxygen anions (O-), and with chlorine anions (Cl-).
The Pyr+ beam was produced on the high energy platform using the ECR source, accelerated to 32kV and injected into the '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.

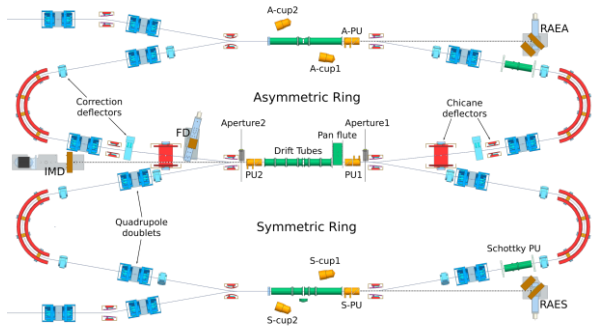

Figure 1.
The DESIREE storage rings. In the merging section, where the two beams overlap, tube electrodes can be biased to control the collision energy down to about 100 meV.
Scheme is taken form the DESIREE web page, https://www.desiree-infrastructure.com/desiree

The first day was spent optimizing the ion-beam storage conditions in the two rings with 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 Pyr+ in the symmetric ring, and the MN experiments between Pyr+ and O- (and then Cl-) with a centre of mass collision energy of about 0.1 eV was 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 of the two rings. When the complex formed by the MN undergoes fragmentation, 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

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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 determine the kinetic energy of the reaction products.
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 after electron transfer from the atomic anion. 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 motivated by their very different electron affinity values, 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 increases, as observed in the case of pilot DESIREE studies of MN interactions involving PAH cations and atomic anions.

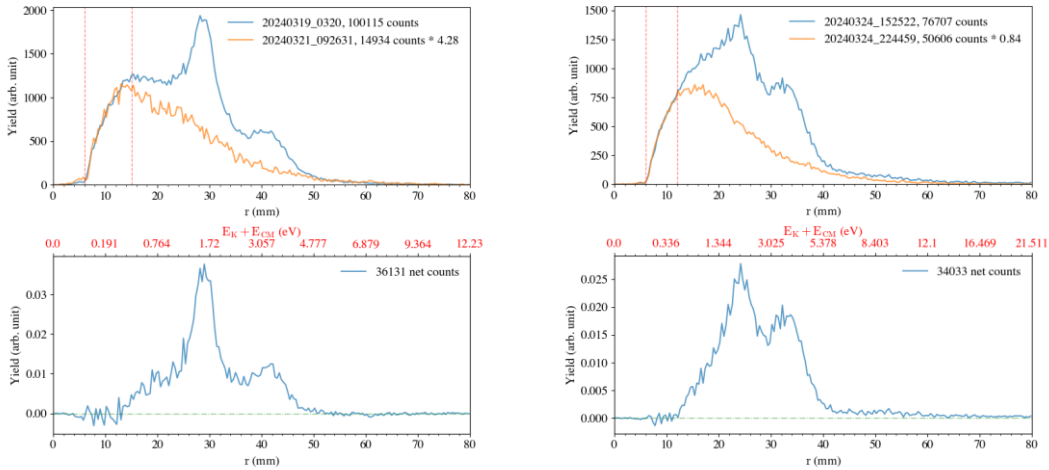

***Figure 2**. Preliminary results of MN experiments between Pyr+ and O- (on the left) and Cl- (on the right). In the top panels, the back ground, due to high energy collisional processes are also displayed (orange line). The bottom panels report the background subtracted data. The kinetic energy released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

The preliminary analysis reported in Figure 1 shows clear differences between the two anions. Theoretical simulation will be undertaken to understand and explain these results.
Three particles event provide access to the 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.

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

The STSM has allowed the first joint experiment between the team from CNR and SU at DESIREE, and it has been very successful, in many respects.
From the scientific point of view, the experiments fulfilled the experimental plan, and even had time to perform additional experiments with Cl^- as the anionic collision partner. 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. The two teams will continue to work closely together to achieve the best results in data analysis and theoretical support, relaying on the long standing expertise of the SU team in these experiments.
From the practical point of view, this STSM has been the invaluable opportunity for the CNR team 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

article.

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