A newly built setup for small bio-molecule fragmentation study in Lanzhou

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Abstract. A new setup for studying ion induced small bio-molecule fragmentation processes has been built in Lanzhou, China. A preliminary collision experiment between a 30 keV He2+ ion beam and gas phase adenine molecules was performed. Partial TOF spectra associated to well-defined scattered projectile final charge states, He+ or He0 were recorded. Coincidence spectra between fragments were also obtained.

1. Introduction

In radiation therapy, the damage of DNA molecules is not only induced by direct impact of the primary high-energy particles, but also by low energy secondary species such as radicals, cations, anions, and secondary electrons, etc., generated in the track of the primary ionizing radiation. Studies involving low energy electron impact on DNA films and gas-phase bio-molecules showed that strand breaks in DNA or dissociation of the bio-molecules can occur at energies well below the ionization energy thresholds, and it was found that the formation of transient anions played an important role in the fragmentation processes [1, 2]. Fragmentation of bio-molecules induced by ion beams at low energy has also attracted much attention during the last years. Using multi-coincidence techniques, detailed information concerning fragmentation dynamics of molecule dissociation under ion impact has been revealed [3-8].

In this work, we report a setup built in Lanzhou aiming at performing collision experiments between ion and small bio-molecules. The specificity of this setup is to be able to detect scattered projectiles at all final charge states, including neutrals and negative ions, in coincidence with the detection of charged fragments. The first running experimental results using 30 keV He2+ beam and Adenine (C5H5N5) molecules are presented in this paper.

2. Experimental setup

A schematic view of the experimental setup is shown in Fig. 1. He2+ projectiles at 30 keV were delivered by the ECR ion source of the Institute of Modern Physics in Lanzhou. The ion beam was guided into the experimental line after a 45° magnet. It was collimated by two sets of adjustable slits separated by a distance of 800 mm (not shown in the sketch) and then cleaned by a 30° coaxial electrostatic deflector (Beam cleaner). In the collision chamber, the beam crossed a gas-phase adenine jet evaporated from an oven heated at 135°C. A liquid nitrogen cooled trap was mounted above the
collision region to collect the molecular jet. Two sets of electrostatic plates in horizontal and vertical planes were set before the interaction region in order to optimize the crossing between the projectile beam and the molecular jet. After the collision region, the outgoing projectiles were deflected according to the charge states by a parallel-plate analyzer. The intense primary beam was collected into a Faraday Cup (FC) beside the detector. Scattered particles that have undergone charge exchange were detected by a two-dimensional position sensitive detector (PSD). The charge of a scattered particle was mapped by the positions on the PSD. The hitting time of a scattered projectile on the PSD provided the time reference for each collision event. Charged recoil products were extracted by a homogeneous electrostatic field of 85V/cm perpendicular to both the ion beam and the target jet. After acceleration and passing through a field free drift Time Of Flight (TOF) tube, the recoil products were detected by a MCP detector (MCPs). The recoil signals were sent to a LeCroy 4208 TDC, which was operated at single channel multi-hit (8) mode, for analyzing the arrival times with respect to the reference signal provided by the PSD. The length of the acceleration region and that of the TOF tube were designed to fulfill the first-order focusing condition of Wiley-McLaren.

![Diagram of Experimental Setup](image)

**Figure 1.** Schematic view of the experimental setup.

With the equipped Analyzer and PSD, the final charge states of the outgoing projectiles can be determined, and all projectiles undergoing charge exchange can be measured under the same experimental conditions. Partial TOF spectrum corresponding to a given scattered projectile charge state can be extracted from the total TOF spectrum by adding a filter on the charge of the scattered projectiles.

### 3. Results and discussion

In collisions between He$^{2+}$ ion beam and adenine molecules, one or two electrons can be kept by the projectile. These two channels were differentiated by the detection of two spots mapped on the PSD assigned respectively to mono-charged and neutral scattered projectiles, He$^+$ and He$^0$. By selecting the main spot associated to the scattered He$^+$ ions, partial TOF spectrum corresponding to single electron capture process was extracted, as shown in Fig. 2 a). In this spectrum, mono-charged stable parent ion C$_6$H$_5$N$_5^+$ is observed with high intensity. The small peak located next to the parent ion is assigned unambiguously to the heavy fragment C$_6$H$_5$N$_4^+$ resulted from the loss of a HCN fragment. Smaller fragments, such as C$_2$H$_m$N$_2^+$, C$_2$H$_m$N$^+$, CH$_m$N$^+$, H$^+$, etc (Here $m$ stands for the number of hydrogen atom), are also present in the spectrum with lower intensities. Unfortunately, this part of the spectrum is dominated by O$_2^-$, N$_2^-$, and H$_2$O$^+$ peaks due to a leakage of our vacuum chamber.
Fig. 2 b) presents the partial TOF spectrum obtained by selecting the spot associated to the neutral scattered projectiles He\(^0\). It corresponds to processes where two electrons are kept by the scattered projectile. In this spectrum, only light fragments resulted from multi-fragmentation of the molecules are observed. This is in consistence with the formation mechanism of neutrals. Let’s consider first two electrons primarily captured at large distance via two-electron-transfer process. Due to the very different potential energy wells on the two doubly charged centers (79 eV for He\(^{++}\) and 22 eV for adenine\(^{+++}\)), these electrons occupy a doubly excited state on the projectile that decays mainly by autoionisation. Such events are classified in the partial TOF spectrum extracted in coincidence with the detection of He\(^+\) (Fig.2.a). Therefore, in collisions between a highly charged ion and a target with limited dimension, the neutral formation channel is attributed to direct multi-electron-capture at short distance in frontal collisions [9]. In such cases, the energy deposited in the target during the collision leads to complete breakup of the target after the collision.

![Figure 2. Partial TOF spectra for a) one electron stabilized on scattered the projectile; b) two electrons stabilized on scattered the projectile.](image)

Fig. 3. TOF-TOF correlation spectrum of fragments in a single collision.

![Figure 3. TOF-TOF correlation spectrum of fragments in a single collision.](image)
When multifragmentation occurs, two or more charged particles are produced in one collision event. Fig. 3 is a correlation spectrum between TOF of the first two fragments in a single collision. Horizontal axis corresponds to the TOF of the faster/lighter one, and vertical axis to the TOF of the slower/heavier one. This spectrum was built without differentiation of the projectile final charge state. It shows that most of the coincidences occur between small fragments for both He$^+$ and He$^0$ channels. To get a better fragment ion collection efficiency, a stronger extraction field of 254V/cm was applied in this case.

4. Summary
With the experimental setup developed in Lanzhou, we are able to provide partial TOF spectra according to the final charge state of the scattered projectiles. The TOF spectrum obtained in coincidence with the detection of neutrals is a typical multifragmentation mass spectrum. It is attributed to short distance frontal collisions. TOF-TOF coincidence spectrum between fragments emerged in a single collision provides detailed information on the molecule dissociation dynamics. With this setup, we have also performed collision experiments using F$^{2+}$ projectiles. Partial TOF spectra have been obtained not only for neutral but also for negative scattered projectiles. These results will be published in a forthcoming paper. Based on the experiences from these preliminary experiments, an improved experimental setup is under development in Lanzhou.

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