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Coupling of collective excitation in proton and photon interaction with PAHs

P M Mishra^{*}¹, L Avaldi[†], P Bolognesi[†], K C Prince^δ, J Rajput^Σ, R Richter^δ, C P Safvan^δ,
S Vig^λ, and U R Kadhane^φ

^{*} Max-Planck Institut für Kernphysik, Heidelberg 69117, Germany

[†] CNR-Instituto di Metodologie Inorganiche e dei Plasmi, CP10-00016, Monterotondo, Italy

^δ Elettra-Sincrotrone Trieste, Strada Statale 14, km 163.5, Area Science Park, I-34149 Basovizza, Italy

^Σ Department of Physics and Astrophysics, University of Delhi, Delhi 110007, India

^λ Inter-University Accelerator Centre, Aruna Asaf Ali Marg, New Delhi 110067, India

^λ Department of Earth and Space Science, Indian Institute of Space Science and Technology, Trivandrum 695547, India

^φ Department of Physics, Indian Institute of Space Science and Technology, Trivandrum 695547, India

Synopsis Collective excitation in polycyclic aromatic hydrocarbon molecule is studied in collision experiments with intermediate velocity (50-180 keV) proton and FUV (15-40 eV) photon energy. In proton impact experiments a clear comparison between pure ionization and capture ionization (or pure capture) process is done on the basis of ionization, evaporation, fragmentation process as a function of impact energy. Two mechanisms: large impact parameter collective excitation mode and closer encounters with higher amount of electronic energy loss leading to fragmentation were observed in proton collision process. The photon impact results were used to understand the origin of evaporation processes.

The structural and dynamical study for polycyclic aromatic hydrocarbons (PAHs) is important in astrophysics and in medical science. A typical photoabsorption spectra of PAH molecules is dominated by two main features, the $\pi-\pi^*$ resonance at about 6 eV and a very broad, strong $\sigma-\sigma^*$ at approximately 20 eV leading to collective excitation with large oscillator strength. This excitation is difficult to isolate from other physical processes due to broader energy deposition in ion-molecule collision. We have studied the contribution of collective excitation in various post collisional processes like fragmentation, ionization, and collision dynamics of PAHs in two independent ways such as pure ionization process and capture process (pure as well as capture ionization). The collision experiments of proton (ranging 50 to 180 keV) with a PAH molecule naphthalene (D_{2h} symmetry) was performed using electro cyclotron resonance source. It is observed that the coupling of this excitation is to pure ionization as well as evaporation processes like loss of neutral H, C_2H_2 (see Figure 1) [1]. The photoelectron spectroscopy experiments using synchrotron source with pyrene (D_{2h}) and fluorene (C_{2v}) showed that collective excitation is coupled to inner valence shell [2] and hence a good amount of excitation energy goes in heating which leads to above evaporation process. In addition to this the energetic of H, 2H and C_2H_2 loss, proton emission is also studied. The frag-

mentation dynamics is studied in both the process as a function of projectile impact energy.

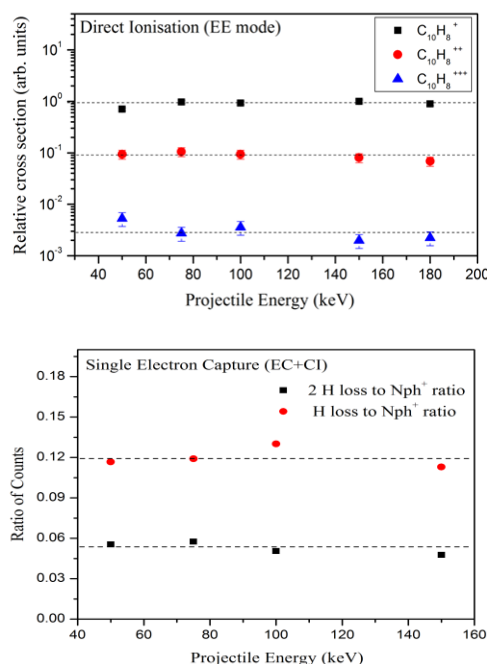


Figure 1. Ionization (top) and evaporation (bottom) behavior with proton impact energy.

References

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- [2] P. M. Mishra *et al* 2014 *J. Phys. Chem. A* **118** 3128

¹ E-mail: pmishra@mpi-hd.mpg.de