

Plasmon mediated isomerization dynamics in proton-PAH collisions at intermediate velocities

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Synopsis Smaller PAH, naphthalene and its isomer azulene is allowed to interact with energetic proton (50-150keV). Various fragment and parent ion is analysed in electron emission and electron capture mode. The rather similarity in energy loss mechanisms is quantitatively demonstrated for two isomeric targets. The fast decay of azulene⁺ is explained on the basis of isomerization dynamics. A model based on the multiplasmon resonance explains the observed proton velocity dependence of double ionization cross sections.

Collective excitation plays a very important role in the electronic energy-loss mechanism when a charged particle interacts with molecules like polycyclic aromatic hydrocarbons (PAHs) at intermediate velocities (≈ 1 a.u) [1]. Single ionization is observed to be the most prominent channel followed by double ionization in these collective excitations. PAHs and their cations have been investigated much for astrophysical purposes during the past few decades [2]. The resilience of PAHs against harsh interstellar radiations can be attributed to its collective response as well as structural features. Collective excitation is shown to be coupled with inner valence electrons and the outgoing electron carry minimal kinetic energy [3]. Average energy loss due to single plasmon excitation is 17eV. The first ionization potential of PAH is about 7-9eV. The remainder of excitation energy is stastically redistributed over all vibrational modes of ground electronic surface. Hence the statistical processes of PAHs is used as a tool to investigate the details of complex ion-PAH collisional mechanism.

Simplest PAH, naphthalene and its isomer molecule azulene is used as target in energetic proton (50-150keV) collision. Various intact and fragment ion is analysed in coincidence with ejected electron and neutralized projectile. The two targets being isomers, the rather obvious similarity in the fundamental ion-molecule collision energetics is quantitatively verified. The striking feature of the mass spectra is the

quasisimilarity in the mass spectra of the two isomers. But there was a clear difference in the C₂H₂ loss peak in the two spectra. These very primitive observations directed us to look for the possible role of isomerization provided one can explain the origin of specific points like excess acetylene loss of az⁺ in comparison to nph⁺. The fast decay of singly charged azulene is successfully explained by its isomerization energetics for the relevant internal energy regime. A first ever attempt is reported here wherein single plasmon excitation in conjunction with isomerization dynamics.

The next dominant peak in the mass spectrum was double ionization. The same plasmon model is used to explain dication formation and its dissociation dynamics in microsecond time scales. Using double plasmon excitation model we could successfully predict the double ionization cross section at all proton energies. Moreover an attempt is made to reinforce the proposition of double plasmon excitation by explaining the observed suppression of neutral H loss from dications as opposed to monocations.

References

- [1] P. M. Mishra *et al* 2013 *Phys. Rev. A* **88**, 052707
- [2] A.G.G.M. Tielens 2008 *Annu.Rev. Astron.astrophys.* **46** 289
- [3] P. M. Mishra *et al* 2014 *J. Phys. Chem. A* **118**, 3128

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