Exploring Three Body Fragmentation of Acetylene Trication

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Synopsis Three body fragmentation of triply charged acetylene ($[C_2H_2]^{3+}$) into (H^+, C^+, CH^+) and (H^+, H^+, C_2^+) fragments is studied and different modes of breakup are identified and compared. Hydrogen migration in triply charged acetylene has been observed. Formation of $[C_2H]^{2+}$ intermediate molecular ion is observed in sequential breakup of $[C_2H_2]^{3+}$. *Ab- initio* calculations are performed for $[C_2H]^{2+}$ molecular ion and the experimental observations are discussed in light of these calculations.

We report on the three body fragmentation of $[C_2H_2]^{3+}$ into (H^+, C^+, CH^+) and (H^+, H^+, C_2^+) fragments formed in interaction of neutral acetylene with a slow highly charged ion (Xe^{9+} having a velocity of ≈ 0.5 a.u.). The experiment was performed at the Low Energy Ion Beam Facility (LEIBF) of Inter-University Accelerator Centre (IUAC), New Delhi, INDIA. The momenta of the set of three fragments were measured in coincidence using the technique of Recoil Ion Momentum Spectroscopy (RIMS).

The breakup of $[C_2H_2]^{3+}$ into (H^+, C^+, CH^+) is analysed using the method of "native frames" [1]. This method allowed us to conclude that breakup into this set of fragments proceed in three ways: concerted breakup in acetylene configuration, concerted breakup in vinylidene configuration and a sequential breakup via $[C_2H]^{2+}$ intermediate molecular ion. By collecting partial data which belongs primarily to concerted breakup events, a Newton diagram is plotted to study angular correlation between momentum vectors and is shown in figure 1.

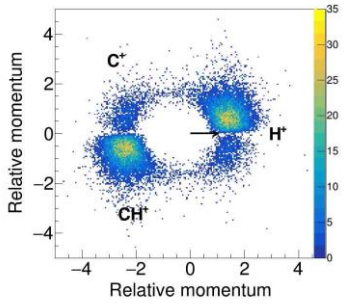

Figure 1. Newton diagram for breakup of $[C_2H_2]^{3+}$ into (H^+, C^+, CH^+).

From this diagram, concerted breakup from acetylene and vinylidene configuration can be clearly seen. The Newton diagram for the remaining data shows a semi-circular arc like feature and is a signature of the sequential breakup via $[C_2H]^{2+}$ intermediate molecular ion [2].

The *ab-initio* calculations of the potential energy surface (PES) for the lowest electronic state of $[C_2H]^{2+}$ are performed. This PES shows two dissociation pathways, one along the C–C stretch coordinate and another along the C–H stretch coordinate with potential barriers of ≈0.6 eV and ≈2.7 eV respectively. This indicates that it is easier for this electronic state to dissociate via the C–C stretch by tunnelling. The measured KER for the unimolecular breakup of $[C_2H]^{2+}$ along the C–C stretch is in good agreement with the *ab-initio* calculations indicating that the lowest electronic state of $[C_2H]^{2+}$ is populated in our experiment.

For the breakup of $[C_2H_2]^{3+}$ into (H^+, H^+, C_2^+), only concerted mode of breakup is observed [3] through the asymmetric and symmetric stretch of the C-H coordinate of the $[C_2H_2]^{3+}$ molecular ion.

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References

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