



Fragmentation channels of naphthalene, azulene and related heterocyclic PAHs under fast proton collision

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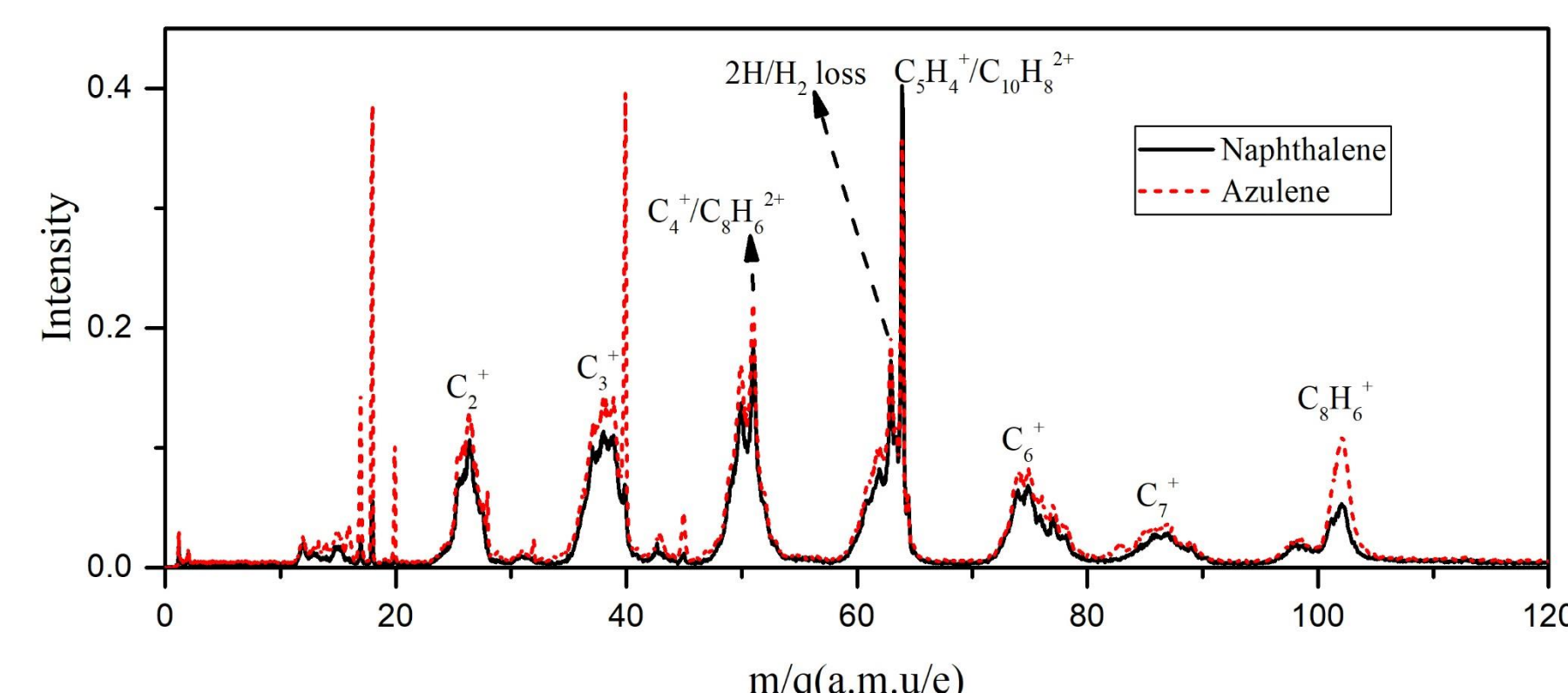
Motivation

- PAHs under higher impact energies show diverse fragmentation pattern
- Kinetic energy release in charge separation reactions is connected to state and PES of parent ion
- Multiple ionization and subsequent isomerization dynamics of PAHs
- Comparison of PAHs and PANHs at higher excitation energies.

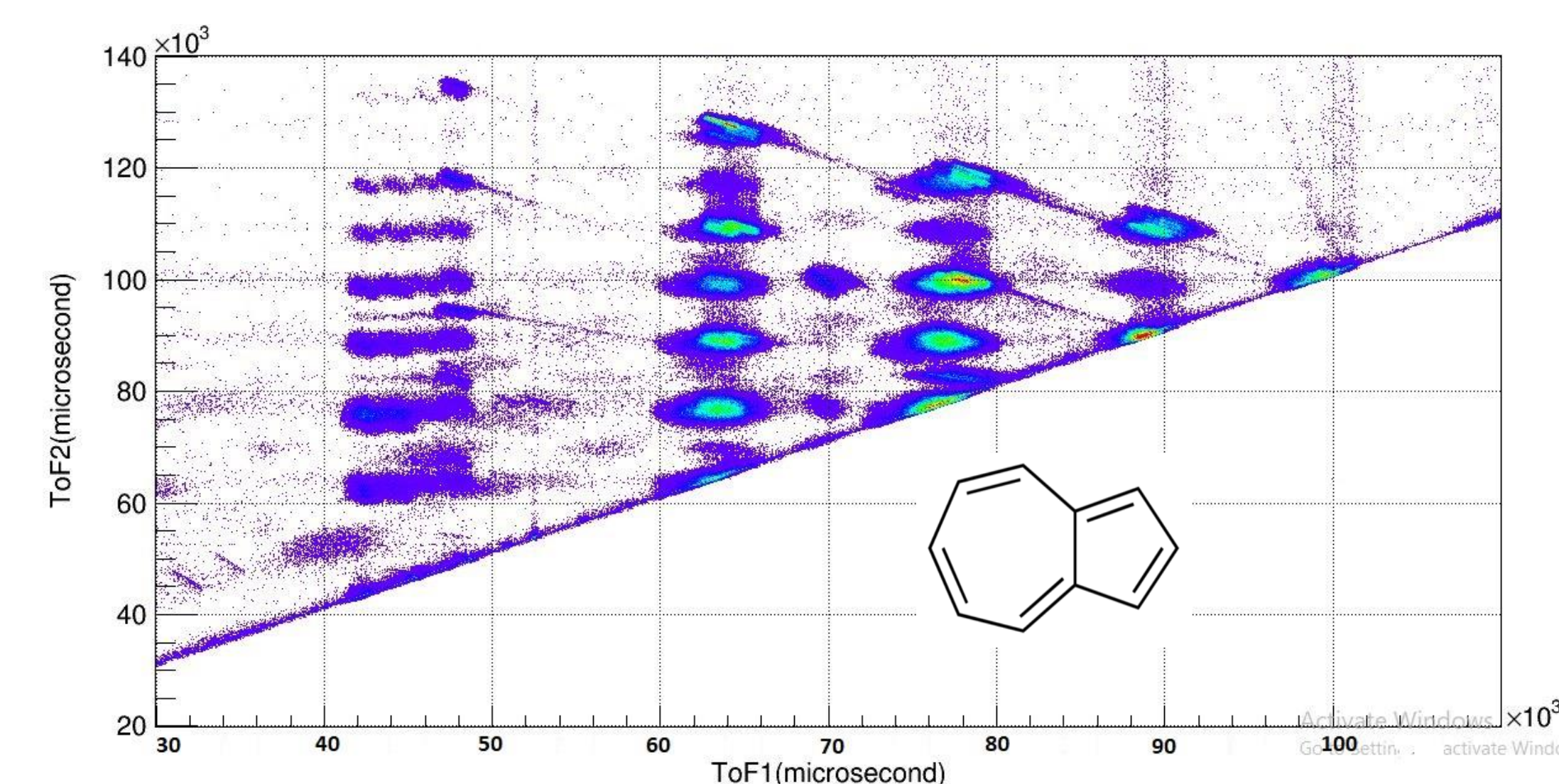
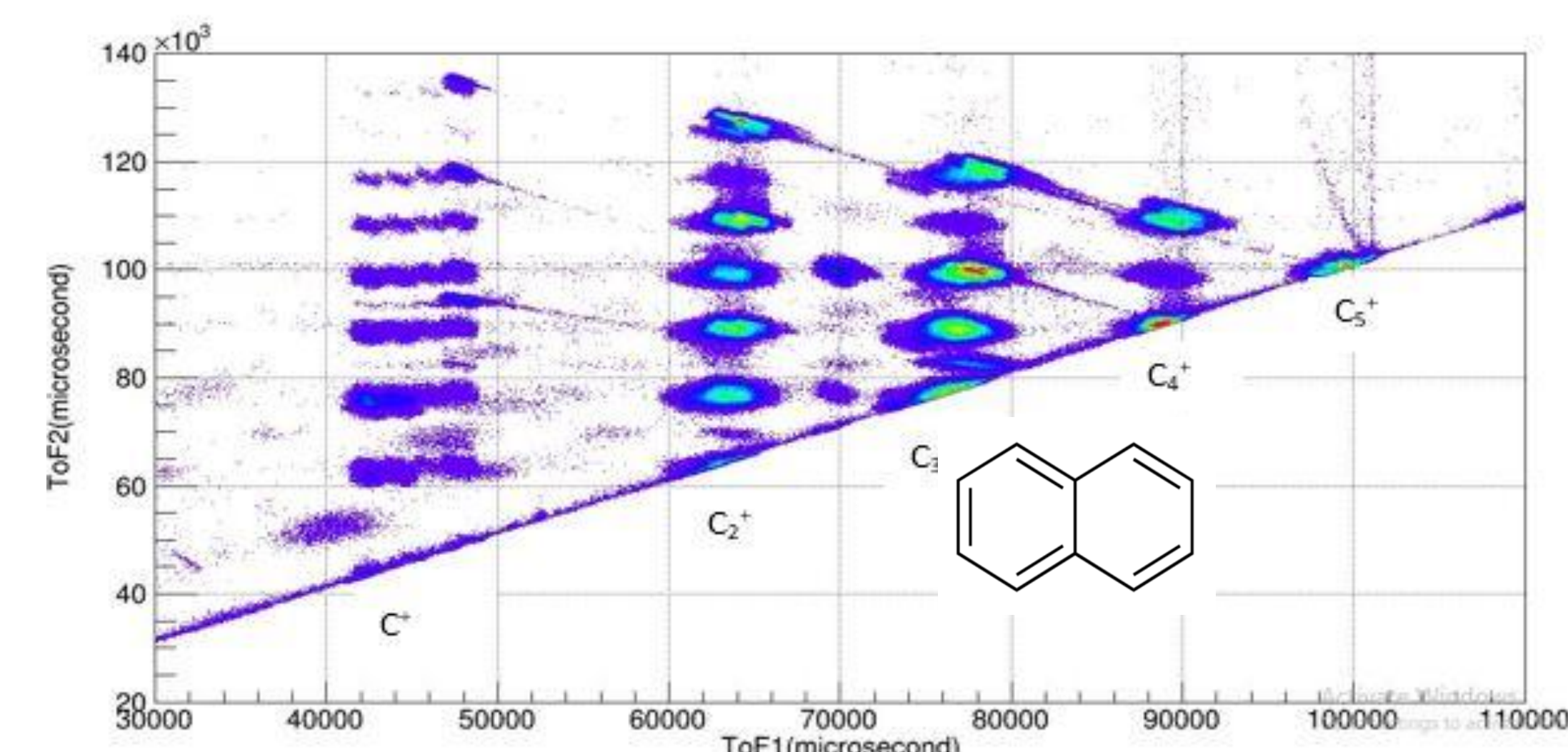


Oil sands contributing to PAH deposition in lakes in Northern Alberta

Energetic fragments of C₁₀H₈ isomers at first hit



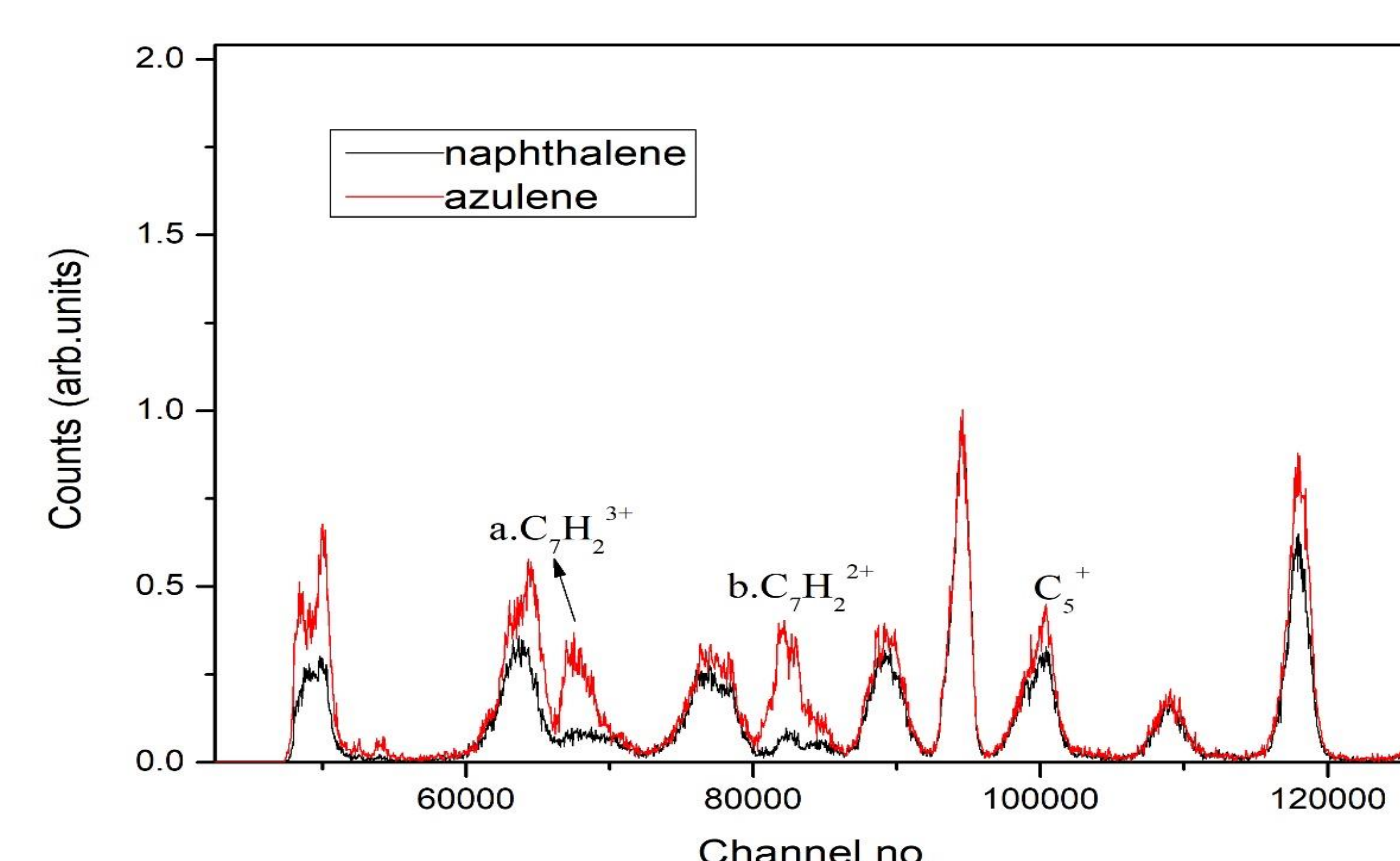
Ion-ion coincidence plot of C₁₀H₈ isomers



Importance of PAHs

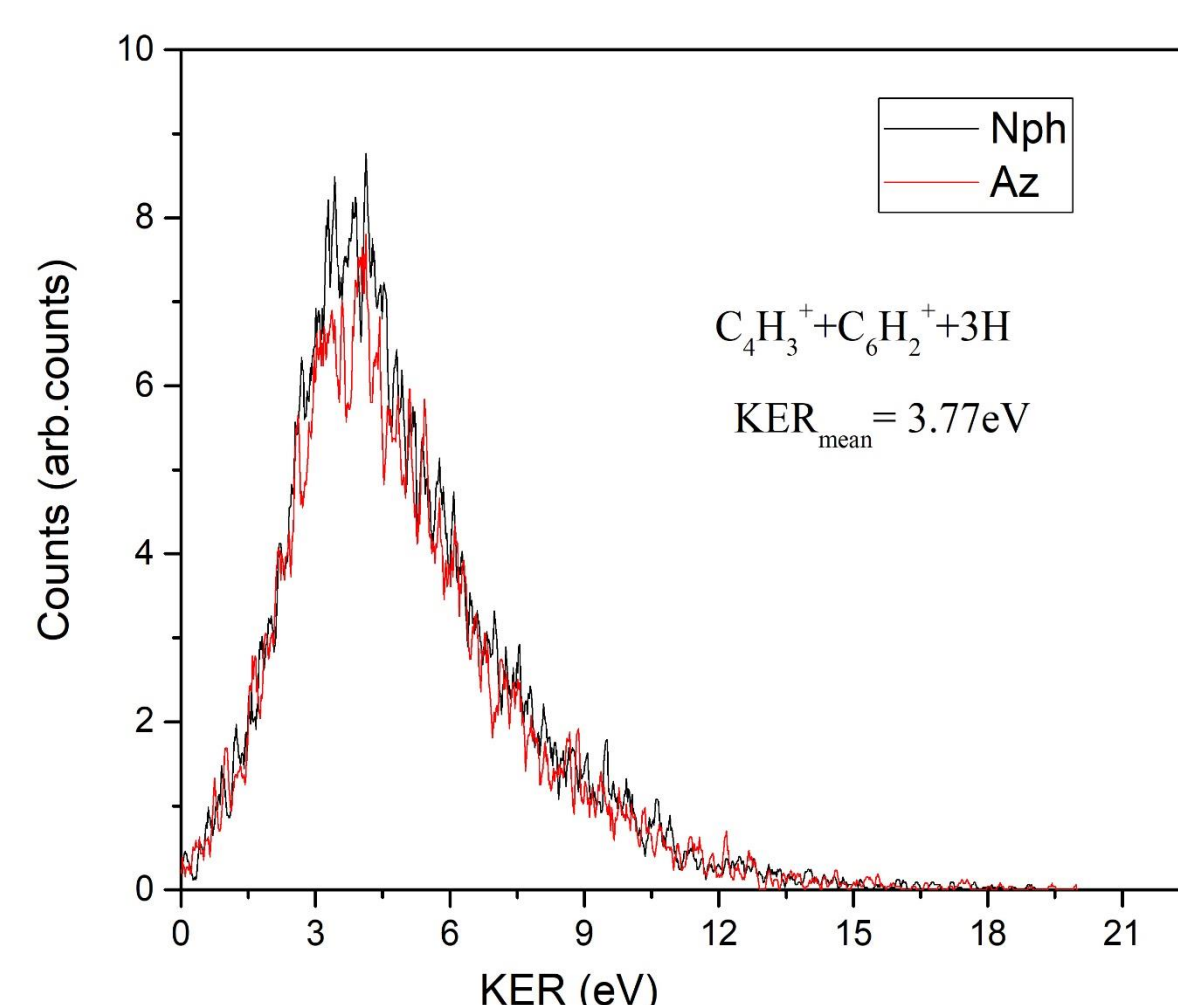
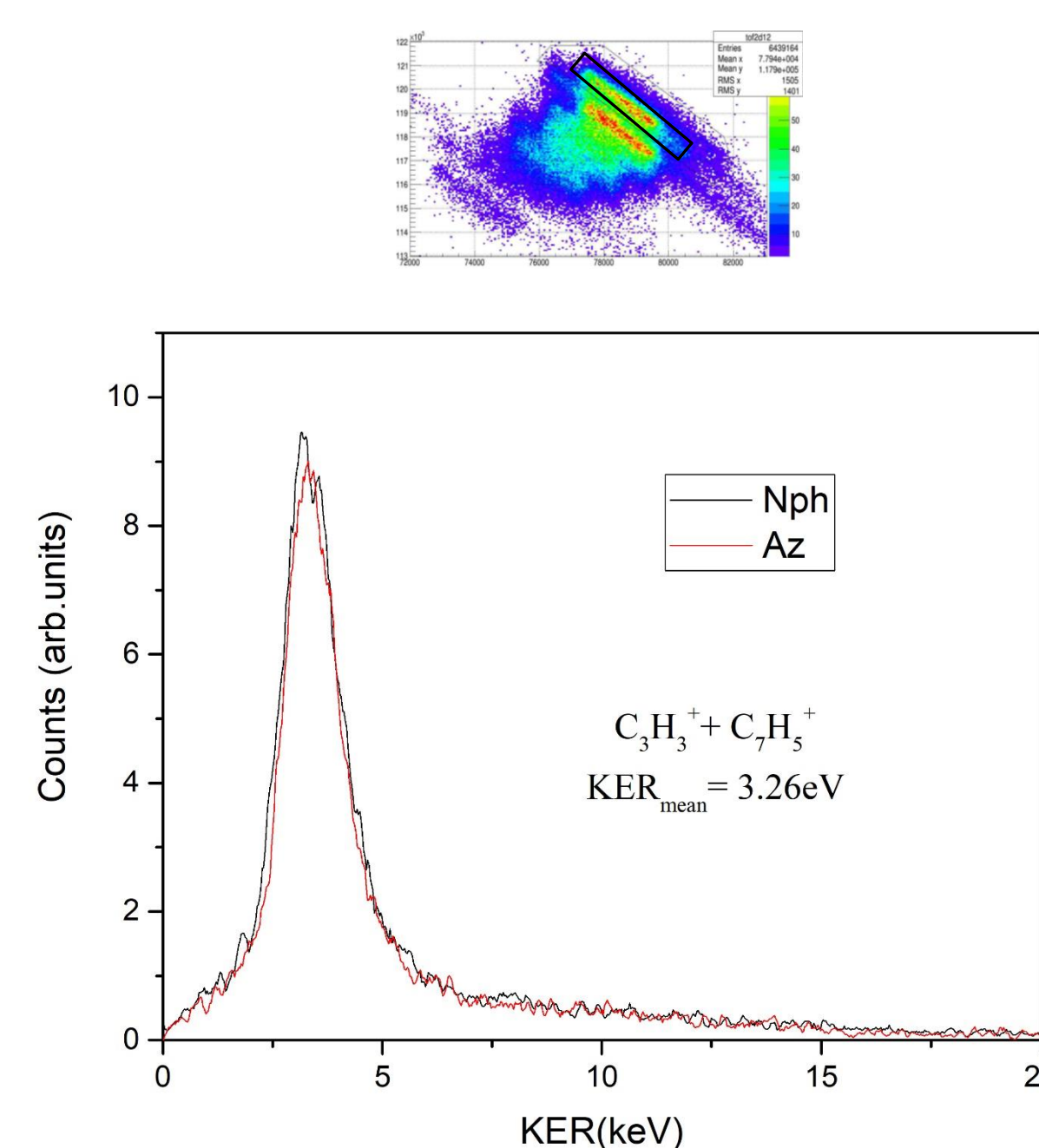
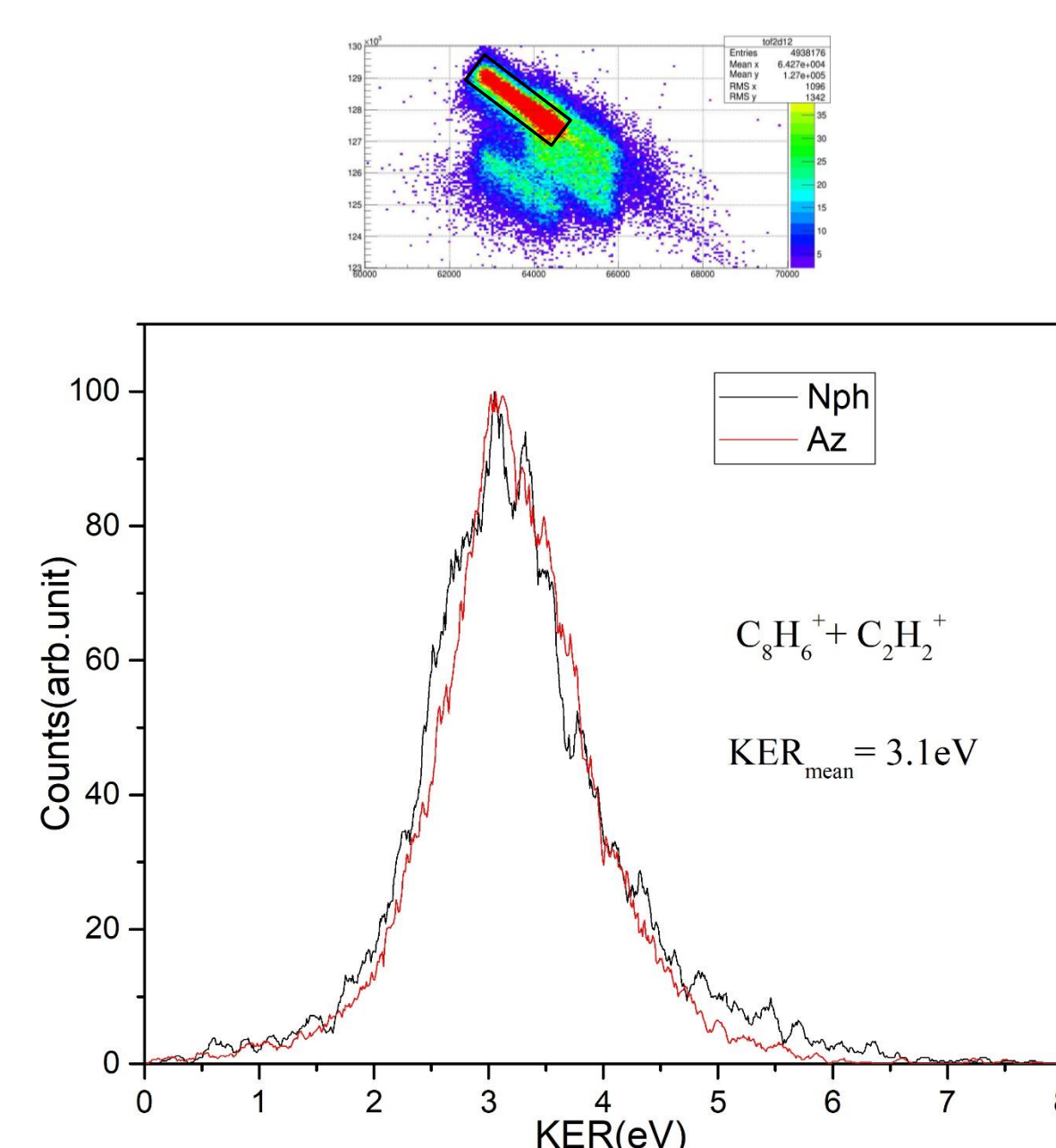
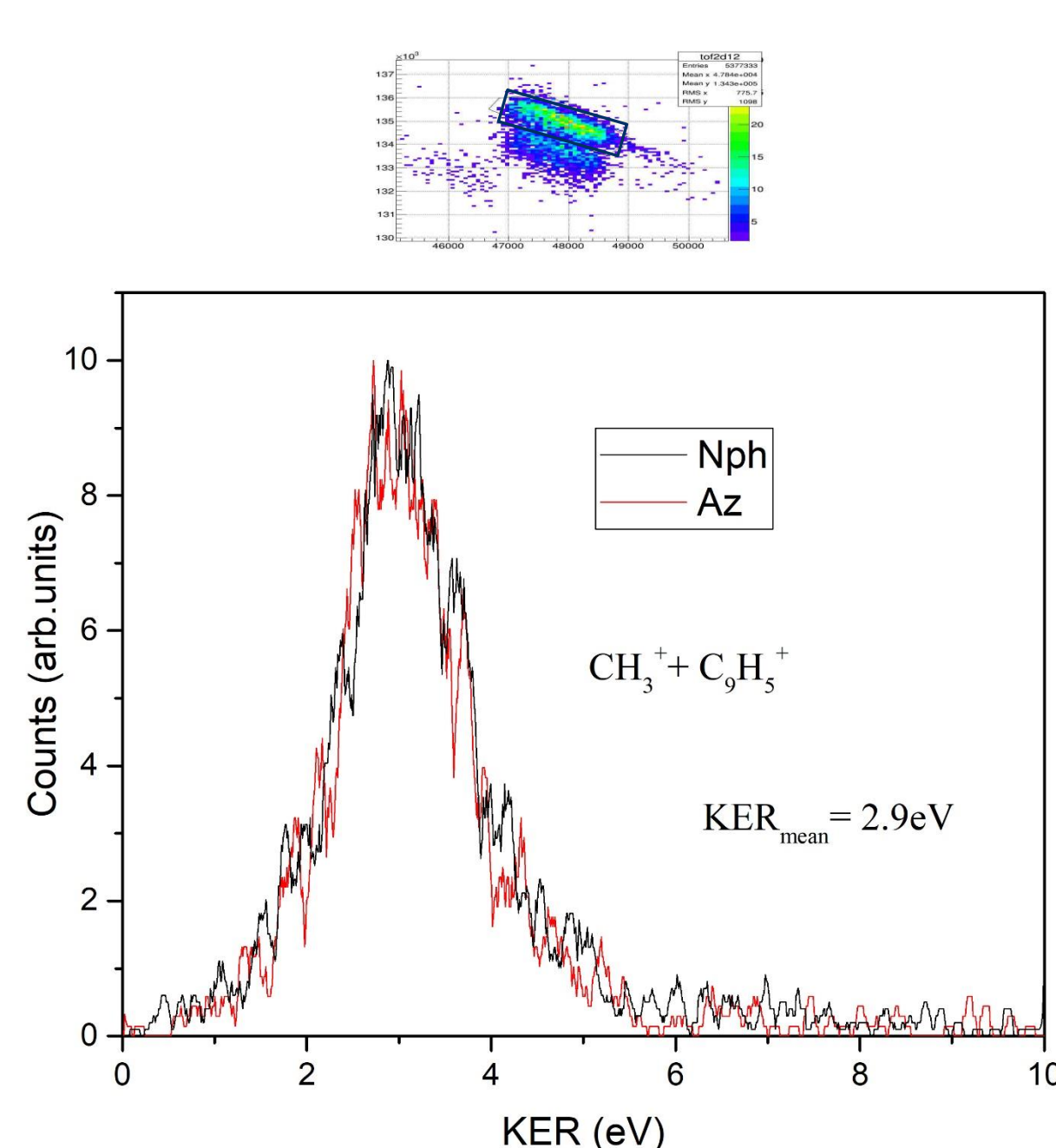
- PAHs and their cations are proposed as carriers of unidentified IR emission bands from ISM
- Ionization balance, energetic and chemical history of ISM can be gained from PAH model
- Well-known class of environmental pollutants

CH₃⁺ emission channels of azulene and naphthalene

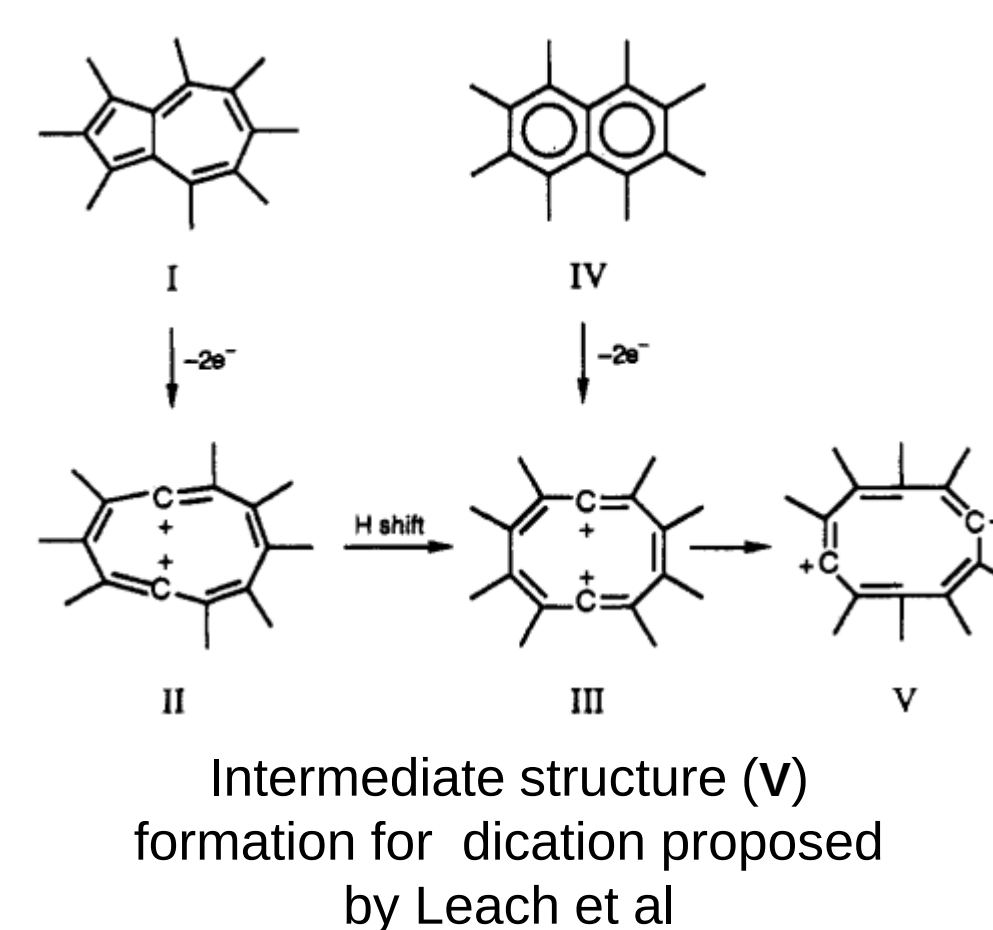


- ❑ In figure fragment a and b is specific to azulene. i.e quadruply and triply charged fragment of azulene quickly eliminates CH₃⁺ and become stable in microsecond time scale

Kinetic energy release of binary fission channels

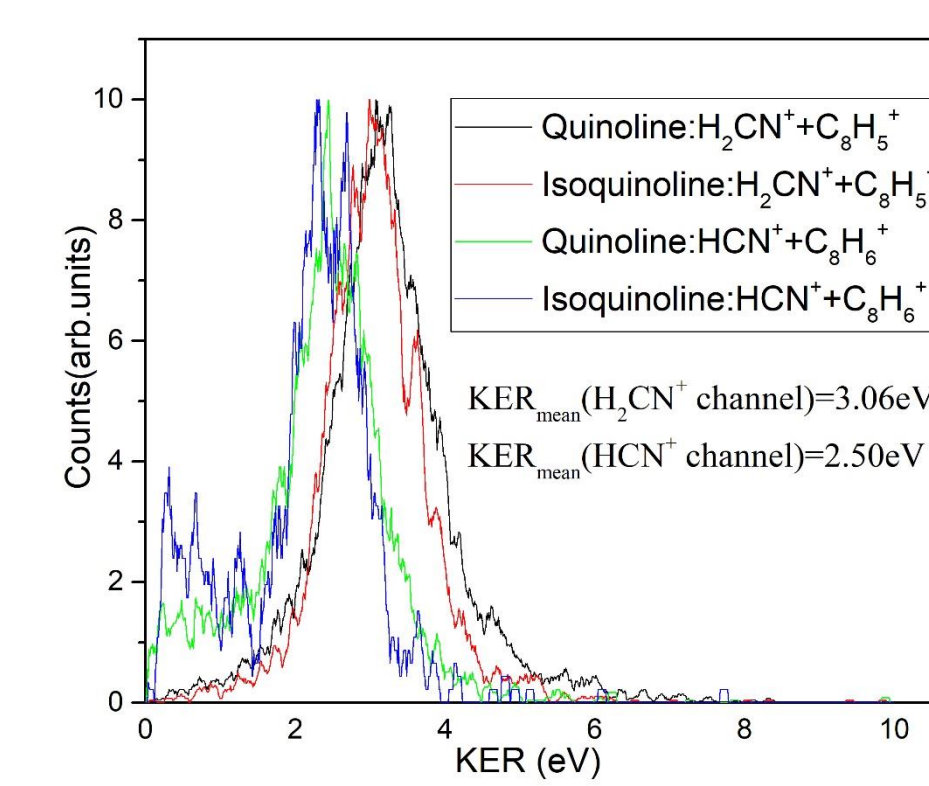


- A remarkable similarity is observed between KER spectra of azulene and naphthalene,
- It indicates both molecules have same dication precursors in double product reactions
- KER is measured upto 3.26eV for carbon conserving channels



- ❑ Major dication channels show a clear binary fission and associated statistical decay
- ❑ The lifetimes of the larger dication fragments are of the order of micro second
- ❑ Most of the charge separation reactions are identical to both molecules. It indicates a common intermediate multiply charged precursor ion formation

Fragmentation and KER of C₉H₇N isomers



- Identical KER spectra is obtained for quinoline and isoquinoline for the two binary channels
- Unlike other channels, HCN⁺ emission has low energy component
- KER distribution of H₂CN⁺ channel and C₂H₂⁺ emission channel of C₁₀H₈²⁺ are found to be identical

Conclusion

- Similarity in ion-ion coincidence map and KER spectra of different energetic excitation channels of PAH (PANH) isomers suggests fast isomerization in multiply charged ions
- In contrast to naphthalene certain triply and quadruply charged azulene ion have higher propensity to decay via CH₃⁺ elimination
- Emission of H₂CN⁺ from PANH dication is observed as one of the strongest channels among binary fission, corresponding molecule (amidogen) is a newly detected interstellar molecule

References

- [1] Leach, S., J. H. D. Eland, and S. D. Price. J.Phys.Chem,93.22 (1989): 7575-7583.
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