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Exploring metastable decay dynamics of polycyclic aromatic nitrogen containing hydrocarbons upon HCN evaporation

Exploring metastable decay dynamics of polycyclic aromatic nitrogen containing hydrocarbons upon HCN evaporation

P. K. Najeeb*[1], T. Sairam*, M. V. Vinitha*, Anudit Kala*, S. Vig*, Pragya Bhatt†, C.P. Safvan† and U. Kadhane*

* Department of Physics, Indian Institute of Space Science and Technology, Thiruvananthapuram-695547, India.
† Inter University Accelerator Centre, Aruna Asaf Ali Marg, New Delhi-110067, India.

Synopsis : Dicationic states of isoquinoline fragment is explored. A tail feature is observed in the coincidence map showing that $C_8H_6^{2+}$ has a metastable state. Using time of flight difference spectrum life time has been estimated to be ∼75ns.

Polycyclic Aromatic Nitrogen containing Hydrocarbons (PANHs) are known to be stable. In the interstellar regions photo or thermal processing may lead to dissociation of these species[1]. Earlier studies have focused on understanding the product formation from neutral and mono-cationic PANHs. However, the product formation from dicationic PANHs (present in interstellar) species has received far less attention. Moreover, understanding the dissociation of these metastable states may give us a hint regarding how the association reactions could have progressed to form these intact dications. Thus, to understand the mechanisms involved in the metastable dicationic species, simplest of PANHs quinoline ($C_9H_7N^+$) (and its isomer isoquinoline ($C_9H_7N^+$)) have been chosen. Even though, loss of C_2H_2 or HCN is feasible from these species, it has been shown that HCN is energetically favorable. In this article, we report metastable intermediate states that could be involved in the formation of $C_7H_3^+$, which belongs to $C_{2n+1}H_3$ class and unlike their analogues C_3H_3 and C_5H_3 less explored. We report $C_7H_3^+$ from quinoline and isoquinoline through an intermediate $C_8H_6^{2+}$ which possess a metastable state.

$$quinoline/isoquinoline \rightarrow C_8H_6^{2+} + HCN \quad (1)$$
$$C_8H_6^{2+} \rightarrow CH_3^+ + C_7H_3^+ \quad (2)$$

Earlier reports have obtained $C_8H_6^{2+}$ in the time of flight spectrum [2], since only a single hit information is obtained, it was attributed to be a stable species. Field et al.[3] have shown that the intensity variation of the difference of the time of flight(ToF) of the two ions in the tail region can give us an quantitative estimate regarding the lifetimes of the metastable species as shown in eqn.3.

$$I(t_2 - t_1) = Aexp(-\frac{m1+m2}{m1-m2}\frac{t_2-t_1}{2\tau}) \quad (3)$$

Here, m1 and m2 denotes the mass of the two fragments the metastable state is dissociating into, τ denotes the lifetime. It should be noted that the $C_7H_3^+$ molecule and its isomers are linear in their ground state. Moreover, removal of CH_3^+ is not energetically favored from the ring structures of $C_8H_6^{2+}$. The experiment was performed using ECR ion source based low energy ion beam facility (LEIBF) at Inter-University Accelerator Centre (IUAC), New Delhi, India [4].

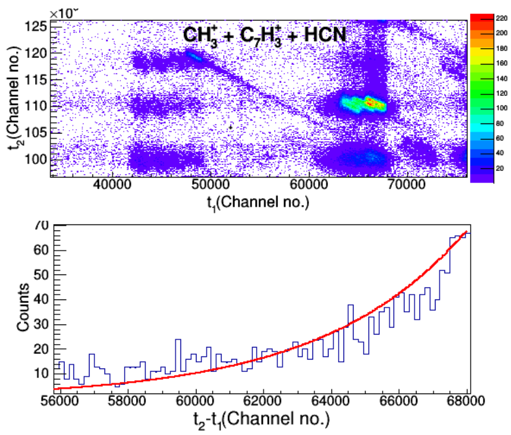

Figure 1. Top:The tail structure shown is formed when lifetime of parent $C_8H_6^{2+}$ has lifetime comparble to the time of flight of the fragments. Bottom: Shows the experimental intensity distribution as the function of ToF difference. This function is fit (red line) with eqn.3. giving lifetime (τ) of $C_8H_6^{2+}$ as ∼=75ns.

References

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[1]E-mail: najeeb.12@iist.ac.in