Stability of polycyclic aromatic hydrocarbons and polycyclic nitrogen heterocycles under electron impact

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Synopsis Stability against high energy electron impact is investigated in the case of naphthalene and two of its nitrogen containing derivatives namely, quinoline and isoquinoline. We observe that C_2H_2 and HCN loss show identical decay time constants in the microsecond time scale indicates the presence of plasmon excitation in these molecules.

Polycyclic aromatic hydrocarbons (PAHs) are a group of organic compounds consisting of two or more fused aromatic rings. Polycyclic aromatic nitrogen heterocycles (PANHs) are species with one or more CH groups substituted by a nitrogen atom in PAHs [1]. It is the proposed widespread existence of PAHs and PANHs in the interstellar medium (ISM) that has largely driven recent investigations of their spectroscopic and photo physical attributes [2]. Naphthalene($C_{10}H_8$) is one of the smallest PAH, but it exhibits many general spectroscopic and structural properties of larger PAHs [3] and hence is a good test candidate for PAHs. Small PANHs like quinoline(C_9H_7N) and its isomer isoquinoline(C_9H_7N) readily dissociate under exposure to interstellar radiation and thus an interest in their photochemistry, as they produce reactive photo products that may contribute to the composition of the ISM [4]. Particularly of significance is the HCN loss mechanism in these systems. The main focus of the present work is to compare fragmentation process under high energy electron impact on naphthalene with its nitrogen derivatives

Generally for PAHs and PANHs, the loss of H and C_2H_2/HCN are the most dominant statistical dissociation channels. Astro-biologically important statistical dissociation channels of the naphthalene and its nitrogen containing derivatives are probed using delayed extraction time of flight mass spectrometry technique (DEToF) [5]. Statistical decay channels show increasing yield of daughter ions as a function of extraction delay in the order of 10^6 s^{-1} decay constant, whereas the yields due to fast dissociation channels were observed to decrease as a function of extraction delay. On the basis of projectile beam energy dependence of the yield, the effect of plasmon excitation in quinoline and isoquinoline is shown for the first time. A strong dependence of the statistical dissociation yield on the location of nitrogen atom in the two molecules is observed [Figure 1]. And the decay time evolution was found to be exactly same for the same channels. A detailed analysis of HCN loss showed identical time scales in quinoline and isoquinoline but nearly twice the yield in favor of isoquinoline. An attempt is made to correlate these observations with the various structure parameter obtained using structure calculations.

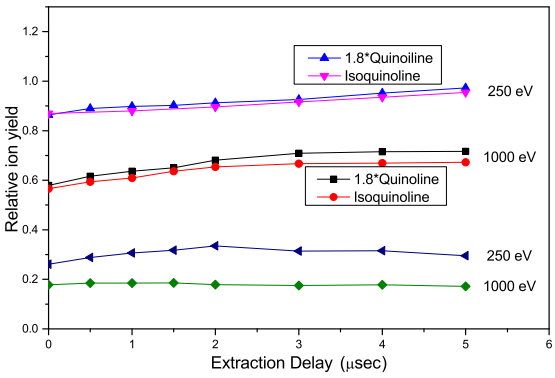

Figure 1. HCN/C2H2 loss channel in naphthalene, quinoline and isoquinoline at various energies of electron impact

References

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