Stacked structure model for stability of doubly charged clusters of polycyclic aromatic hydrocarbon molecules

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The polycyclic aromatic hydrocarbon (PAH) molecules and PAH clusters are responsible for the structure in the infrared spectra of interstellar medium. Collisions of charged particles with PAH clusters are expected to play important roles in the chemical evolution in molecular clouds. Recently an experiment was carried out for the collision of PAH clusters with slow ions [1,2]. In these collisions, doubly charged clusters of anthracene and coronene were detected for cluster size $n \geq 15$. To analyze the origin of this appearance size for doubly charged PAH clusters, we have proposed a stacked structure model [3]. We assume that a neutral PAH cluster takes a layer structure of planar molecules The inter-molecular distances are commonly taken to be the equilibrium distance of a neutral dimer. As a result of double ionization, one of the distances r is supposed to be elongated while the other distances are retained (see Fig. 1). The total interaction potential for fragmentation is given as a sum of the Morse potential between the nearest molecules and the Coulomb potential between the singly charged fragments. The parent cluster is judged to be stable if the total interaction potential has an energy barrier as a function of distance r . The calculated appearance sizes with the present model [3] and the liquid drop model [4] for doubly charged clusters of benzene, anthracene and coronene are shown in Table 1 together with experimental results. For benzene cluster, the liquid drop model gives a considerably good agreement with an experiment [5] while the stacked structure model does not. For anthracene and coronene clusters, both models conspicuously underestimate the appearance sizes in comparison with the experimental results [1-2]. The origin of this descrepancy is discussed.

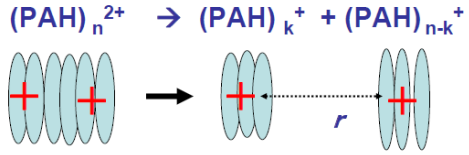

Fig. 1 Stacked structure model for stability against for fragmentaion of doubly charged PAH cluster.

Table 1. Appearance sizes of doubly charged clusters.

constituent	experiment	present model	liquid drop model
benzene	23	9	18
anthracene	15	6	6
coronene	15	3	3

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