Collision dynamics of PAH clusters with charged particles

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The polycyclic aromatic hydrocarbon (PAH) molecules are believed to be abundant in interstellar space. The collisions dynamics of charged particles with PAH clusters would play an important role in the chemical evolution in molecular clouds. Recently, there have been experimental studies for the collision of ions with PAH molecules and PAH clusters [1,2]. In the present work, we make an analysis for the experimental observation. In the collision with singly and doubly charged ^{3}He ions, doubly charged clusters of anthracene and coronene were detected for cluster size $n \geq 15$. To analyze the origin of this *appearance size*, we propose a stacked structure model [3]. In the model, it is assumed that a PAH cluster takes a layer structure of planar molecules. (See Fig. 1) The appearance sizes are calculated for doubly charged clusters of benzene, anthracene and coronene by the present model [3] and by the conventional liquid drop model [4]. They are shown in Table 1 together with experimental results [1-2,5]. For benzene cluster, the liquid drop model gives a considerably good agreement with the experiment [5] while the stacked structure model does not at all. For anthracene and coronene clusters, both models conspicuously underestimate the appearance sizes in comparison with the experimental results [1-2]. The origin of this discrepancy is discussed. The result was partly reported in [3].

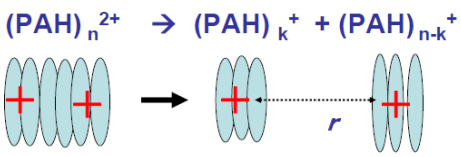

Fig. 1: Stacked structure model for stability for fragmentation of doubly charged PAH cluster.

Table 1. Appearance sizes of doubly charged clusters.

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

References

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