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Collision-induced dissociation of 2- and 3-dimensional polycyclic aromatic hydrocarbon cations in a modified ion-trap detector

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Abstract

A modified Finnigan MAT ion-trap detector has been employed in a systematic examination of the collisional dissociation of the cations of selected 2- and 3-dimensional polycyclic aromatic hydrocarbons (PAH) with a carbon content ranging from 10 to 24 carbon atoms: naphthalene, acenaphthylene, acenaphthene, phenanthrene, anthracene, pyrene, corannulene and coronene. The cations were produced by electron impact, excited for 50 ms using monopolar resonant excitation, and then dissociated by collisional activation with argon collision gas. A comparison of the results obtained in this way for the naphthalene cation fragmentation with results obtained by photodissociation show that appreciable amounts of internal energy, $\geq$ 7.3 eV, could be deposited in the ion using the ion-trap method. C–H bond cleavage was favoured over C–C bond cleavage for all PAH cations. Significant C–C cleavage with elimination of (2C,2H), (2C,3H) and (2C,4H) was observed with anthracene, phenanthrene and corannulene. With the exception of the cations of acenaphthylene and corannulene, larger PAH cations were observed to be more stable against fragmentation. The acenaphthylene cation was the most stable. The cation of the 3-dimensional, strained corannulene molecule exhibited an enhanced fragmentation efficiency relative to the cations of the related 2-dimensional pyrene and coronene molecules. Mechanistic pathways are proposed for the dissociation of this cation. © 1997 Elsevier Science B.V.

Keywords: Ion trap; PAH cations; Corannulene cation; Collision induced dissociation (CID)

1. Introduction

The first synthesis of corannulene in 1966 [1] stimulated a number of theoretical and experimental studies of 3-dimensional hydrocarbons containing only sp^2-hybridized carbon atoms and led to the theoretical prediction that a 3-dimensional hollow carbon cluster should be stable [2]. This carbon cluster, known today as buckminsterfullerene, was proposed to contain 60 sp^2 carbon atoms. It is noteworthy that the experimental discovery [3] and the first laboratory production [4] of C_{60} resulted from the work of physical chemists and astrophysicists who had long been curious about the importance of carbon-containing molecules, such as carbon

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