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Dissociation of doubly charged Coronene as a function of internal energy

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Synopsis We report on the dissociation of doubly charged Coronene ($C_{24}H_{12}{}^{2+}$) as a function of internal energy. The mass spectra were obtained for internal energy measured up to 50 eV using the CIDEC method in collisions with F^+ and H^+ at 3 keV. The dehydrogenation processes of the molecule were observed over this large range of energy as well as the other weaker channels, loss of C_2H_n, $2C_2H_n$ and ionization. The branching ratios for the fragments $C_{24}H_{12-n}{}^{2+}$, $C_{22}H_{12-n}{}^{2+}$, $C_{20}H_{12-n}{}^{2+}$ and $C_{24}H_{12-n}{}^{3+}$ (n=0-6) were measured.

Polycyclic aromatic hydrocarbons (PAHs) are extensively studied since many decades due to their relevance e.g. in astrophysics in the attempt of explaining the observation of the unidentified infrared bands. The important role of PAHs as catalyst in the formation of H_2 in the photodissociation regions of the interstellar medium has also been suggested. The numerous photodissociation and collision experiments as well as theoretical investigations have shown that the main dissociation channels are the loss of H, H_2 and small hydrocarbon molecules such as C_2H_2. With a highly symmetric structure coronene ($C_{24}H_{12}$) is considered as a model PAH system. The emission of an even number of H atoms is in general favored but the related process whether the direct H_2 emission or the sequential H loss is still under debate [1].

In this work, the fragmentation of coronene induced by collision with F^+ and H^+ at 3 keV is investigated using the CIDEC method [2]. In this method the excitation energy of the doubly charged coronene ion is determined by measuring the kinetic energy loss of the negative scattered ion formed in the collision $F^+ + C_{24}H_{12} \longrightarrow F^- + C_{24}H_{12}{}^{2+}$. The measurements are performed in coincidence with time-of-flight mass spectrometry leading to mass spectra resolved in internal energy of the $C_{24}H_{12}{}^{2+}$ parent ion (Figure 1). As expected the dehydrogenation of coronene (loss of H, H_2) is the dominant process. Internal energy up to 50 eV have been measured. Over this wide range of energy the branching ratios for the fragments $C_{24}H_{12-n}{}^{2+}$, $C_{22}H_{12-n}{}^{2+}$ (C_2H_n loss), $C_{20}H_{12-n}{}^{2+}$ ($2C_2H_n$ loss) and $C_{24}H_{12-n}{}^{3+}$ (n=0-6) were measured to be about 90%, 4%, 1% and 5% respectively. These branching ratios are also presented in table 1 as a function of selected energy ranges. Stable

$C_{24}H_{12}{}^{2+}$ parent ions are observed with internal energy of about 10 eV but it is noticeable that a small fraction of $C_{22}H_{12-n}{}^{2+}$ fragment is also observed at this energy. This may indicate a strong competition between the loss of H and C_2H_2 at low excitation energies while H/H_2 loss dominate at higher excitation energy as already observed for doubly charged anthracene ions [3].
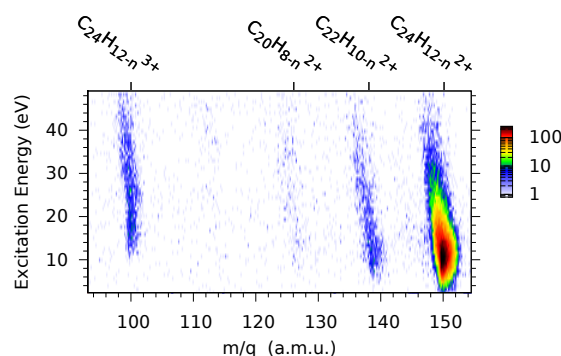

Figure 1. Excitation energy of $C_{24}H_{12}{}^{2+}$ as a function of the mass spectrum. $C_{24}H_{12}{}^{2+}$ are formed in 3 keV $F^+ + C_{24}H_{12} \longrightarrow F^- + C_{24}H_{12}{}^{2+}$ collisions.

Table 1. Branching ratios (%) as a function of the excitation energy of $C_{24}H_{12}{}^{2+}$ parent ion. Energy range in eV.

	1.5-10	10-19	19-27	27-49
$C_{24}H_{12-n}{}^{2+}$	97.5	94.5	80	50
$C_{22}H_{12-n}{}^{2+}$	2.5	3	7	14
$C_{20}H_{12-n}{}^{2+}$		< 1	2	7
$C_{24}H_{12-n}{}^{3+}$		2	11	29

References

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