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H_2 formation from Polycyclic Aromatic Hydrocarbon molecules

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Synopsis In this work we study statistical fragmentation of Polycyclic Aromatic Hydrocarbon (PAH) molecules following collisions with keV ions. Dissociation and transition state energies for H- and H_2-emissions from PAHs have been calculated and a simple electronic stopping model has been used to calculate collision-induced internal PAH temperatures. We find that H_2 may be formed efficiently from pristine PAHs for internal ion temperatures above 2200 K.

Polycyclic Aromatic Hydrocarbons (PAHs) and molecular hydrogen (H_2) are present in many astrophysical environments [1, 2]. Broad emission features in the mid-infrared spectrum are observed in space and are in general attributed to infrared fluorescence of PAHs excited by ultraviolet radiation [3]. H_2 is the most abundant molecule in the universe and influences interstellar chemistry and star formation [1]. It is therefore of great interest to find the connection between PAHs and molecular hydrogen.

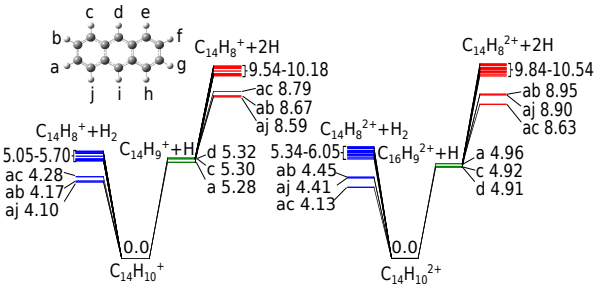

Figure 1. The adiabatic dissociation energies (in eV) for losses of H, H_2 and H+H from singly (left) and doubly (right) charged anthracene ($C_{14}H_{10}$) calculated with Density Functional Theory (B3LYP/6-311++G(2d,p)). The hydrogen atoms are labelled a-j.

We present experimental results for keV energy collisions between atomic ions and PAHs. We observe rich fragment mass spectra with peaks corresponding to the loss of e. g. H and 2H (H_2 or H+H) from singly charged PAHs. It is difficult to distinguish between H_2 and H+H contributions to $[PAH\text{-}2H]^+$ peaks by simple experimental techniques. In order to be able to discuss the origin of the $[PAH\text{-}2H]^+$ peaks, we have calculated dissociation energies and reaction barriers for H-, H_2- and H+H - emission from PAHs by means of quantum chemistry methods (B3LYP\6-311++G(2d,p)). Figure 1 shows the calculated adiabatic dissociation energies for H-, H_2- and H+H - emissions from singly and doubly charged anthracene ($C_{14}H_{10}$) [4].

We find that reaction barriers decrease the H_2-formation rates. As a consequence, this process is only effective for internal PAH temperatures exceeding, roughly, 2200 K, a temperature which is not reached for absorption of single photons below the Lyman limit (13.6 eV). In contrast, by using a simple model [5] for collision-induced electronic excitation, we find that PAHs may be strongly heated in collisions with ions and atoms such that H_2 molecules may be formed directly from pristine PAHs.

References

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