Charge communication, molecular growth, and fragmentation processes involving fullerenes and polycyclic aromatic hydrocarbons

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Polycyclic aromatic hydrocarbons (PAHs) are widespread atmospheric pollutants and omnipresent in many astrophysical environments. Recently, fullerenes have also been identified in space [1], but only in hydrogen poor environments where there are no signs of PAHs being formed. These observations raise important questions about the formations, stabilities, and reactions of PAHs and fullerenes in *cold* environments. In the present work [2-5], we have studied keV-ions (e.g. He^{+}, He^{2+}, and Xe^{20+}) colliding with isolated molecules and weakly bound clusters of PAHs (cf. Fig. 1) and fullerenes, partly inspired by the importance of such interactions in space [6] and to shed light on e.g. charge communication, molecular growth and fragmentation processes involving complex molecules in general. In order to guide the interpretations of our experimental results we have performed Density Functional Theory calculations, which yield information on e.g. the charge state dependent ionization and dissociation of isolated PAHs and clusters of PAHs, and the size dependent stabilities and formations of C_n-fullerenes with $60 \leq n \leq 112$. Many of the intriguing issues revealed in the present work, and as of yet unexplored PAH and fullerene features, will be studied in more detail by means of the double electrostatic storage ring DESIREE which is designed for merged beams reactions between internally cold cations and anions.

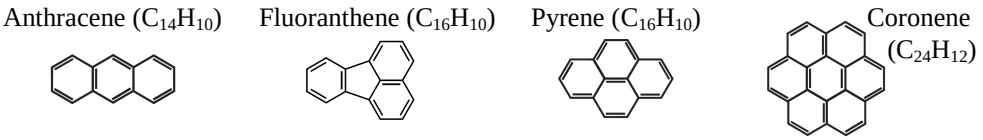

Figure 1. Molecular structures of polycyclic aromatic hydrocarbons (PAHs) studied in the present work.

References

[1] J. Cami *et a al*, Science, **329**, 1180 (2010)

[2] A. I. S. Holm *et al*, Phys. Rev. Lett., **105**, 213401 (2010)

[3] A. Lawicki *et al*, Phys. Rev. A, **83**, 022704 (2011)

[4] A. I. S. Holm *et al*, J. Chem. Phys., **134**, 044301 (2011)

[5] H. Zettergren *et al*, J. Chem. Phys., **133**, 104301 (2010)

[6] J. Postma *et al*, Astrophys. J. , **708**, 435 (2010)

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