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Photoprocessing of large PAH cations

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Abstract. In cosmic environments, polycyclic aromatic hydrocarbons (PAHs) strongly interact with vacuum ultraviolet (VUV) photons emitted by young stars. Trapped PAH cations ranging in size from 30 to 48 carbon atoms were irradiated by tunable synchrotron light (DESIRS beamline at SOLEIL). Their ionization and dissociation cross sections were determined and compared with TD-DFT computed photoabsorption cross sections. Evidence for radiative cooling is reported.

Keywords. Astrochemistry, ISM: molecules, methods: laboratory, ultraviolet: ISM

1. Introduction

Interstellar polycyclic aromatic hydrocarbons (PAHs) are processed by the interaction with vacuum ultraviolet (VUV) photons emitted by young stars (Montillaud *et al.* 2013). After absorption of a VUV photon, an isolated PAH can undergo different relaxation processes: ionization, dissociation and radiative cooling, including infrared fluorescence which results in the aromatic infrared bands observed in many astronomical objects (Joblin & Tielens 2011, Peeters 2011). In this study we extend the work of Zhen *et al.* (2016) to large PAH cations (between 30 and 48 carbon atoms) in order to quantify their photofragmentation and photoionization cross sections over the $9-20\,\mathrm{eV}$ range.

2. Experimental Method

The PAH cations were isolated in the Thermo Scientific$^{\mathrm{TM}}$ LTQ XL$^{\mathrm{TM}}$ linear ion trap of the DESIRS beamline (Milosavljević *et al.* 2012) at the synchrotron SOLEIL and energized by VUV photons in the range of $9-20\,\mathrm{eV}$. All resulting photoproducts were mass-analyzed and recorded as a function of photon energy in steps of 0.1 to 0.5 eV and with irradiation times of 0.2 or 0.8 s. The main channels observed were the doubly ionized parent cations and the fragments corresponding to the loss of H and $2\mathrm{H}/\mathrm{H}_2$.

3. Photoproduct Cross Sections

From the recorded peak intensities and for monochromatic radiation the ionization and dissociation cross sections, σ_{I} and σ_{D}, respectively, can be derived using

$$\sigma_{\mathrm{I,D}}(h\nu) = \sigma_{\mathrm{Abs}}(h\nu)\, Y_{\mathrm{I,D}}(h\nu) = \frac{1}{\Gamma_{\mathrm{Dico}}\phi t} \ln\left(\frac{P_0}{P(t)}\right) \frac{S_{\mathrm{I,D}}(t)}{S_{\mathrm{I}}(t)+S_{\mathrm{D}}(t)}, \qquad (3.1)$$

where $\sigma_{\rm Abs}$ is the total photoabsorption cross section, $Y_{\rm I,D}$ is the ionization/dissociation yield, $\Gamma_{\rm Dico}$ is a proportionality factor that allows us to refine the actual photon flux seen by the ions, ϕ is the photon flux in $[{\rm s}^{-1}{\rm cm}^{-2}]$, and P_0 are the parent ions before irradiation with $P_0 = P(t)+S_{\rm I}(t)+S_{\rm D}(t)$, where $P(t)$ are the parents and $S_{\rm I}(t)$ and $S_{\rm D}(t)$ the secondary ions from ionization and dissociation after irradiation, respectively. The results are depicted in Fig. 1 and compared with the theoretical photoabsorption cross sections, $\sigma_{\rm Abs}$, which have been computed using the real time, real space implementation of TD-DFT from the Octopus code (Malloci *et al.* 2004). A significant fraction of the absorbed energy appears to be relaxed radiatively even at high energies.

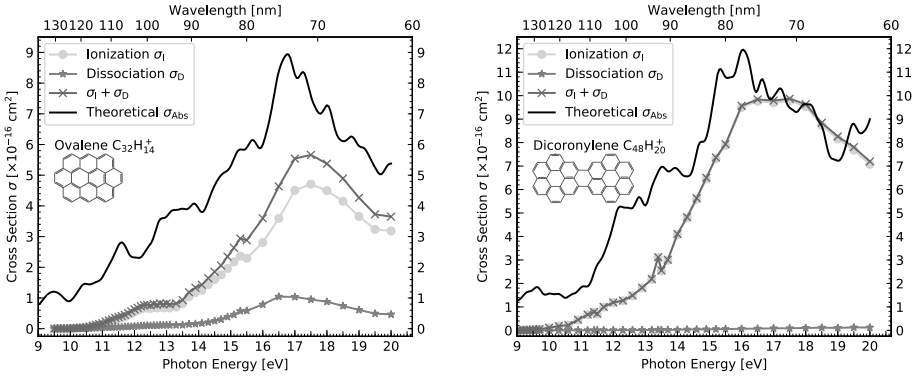

Figure 1. Experimentally determined cross sections for ionization, $\sigma_{\rm I}$, and dissociation, $\sigma_{\rm D}$, compared to the theoretically computed photoabsorption cross sections, $\sigma_{\rm Abs}$, for ovalene (left panel) and dicoronylene (right panel).

4. Conclusion & Outlook

The photoionization process is found to strongly dominate and almost no dissociation is observed for our largest PAH cation, $C_{48}H_{20}^+$. Please note that these results depend on $\Gamma_{\rm Dico}$ which is determined by assuming $Y_{\rm I} + Y_{\rm D} \approx 1$ at 18 eV for the case of $C_{48}H_{20}^+$. We conclude that $Y_{\rm I}$ increases with increasing number of carbon atoms. In order to further probe the impact of the excitation scheme on the photoionization and the dissociation yield, additional experiments under multiple photon absorption will be performed at the PIRENEA setup available in Toulouse (Useli-Bacchitta *et al.* 2010).

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