PHOTOSTABILITY OF ORGANIC MOLECULES IN CIRCUMSTELLAR ENVIRONMENT

T. Monfredini¹, W. Wolf², E. Mendoza¹, M. L. Rocco³, A. Lago⁴, and H. M. Boechat-Roberty¹

Aromatic Infrared Bands, the footprint of molecules like neutral and ionic Polycyclic Aromatic Hydrocarbons (PAHs), have been observed in several astrophysical environments. We present the experimental results of the photoionization and photodissociation of the methyl-benzene (or toluene) molecule, a basic unit for the methylated PAHs, using synchrotron radiation at C1s resonance, $\sim 285 \text{ eV}$ (soft X-ray) and time-of-flight massspectrometry. Absolute photoionization and photodissociation cross sections have been determined. Then the ionization and destruction rates and half-life of the toluene molecule were also obtained for the X-ray photon flux of the pre-planetary nebula CRL 618.

The measurements were performed at the Brazilian Synchrotron Light Source (LNLS) using X-ray photons from the spherical grating monochromator (SGM) at energies around the C1s resonance (280-320 eV). The experimental set-up has been described in detail by Boechat-Roberty et al. (2005) and Pilling et al. (2006). Briefly, soft X-ray photons intersects perpendicularly the effusive gaseous sample inside a high vacuum chamber (base pressure around 10^{-8} Torr). Mass spectra of the ionic fragments were obtained using the photoelectron photoion coincidence method. From these spectra, partial ion yields (PIYs) were obtained by

$$PIY_i = \left(\frac{A_i}{A_t^+} \pm \frac{\sqrt{A_i} + A_i \times ER/100}{A_t^+}\right) \times 100\%, \quad (1)$$

Where A_i is the area of each peak and A_t^+ is the total area of the peaks. The estimated error factor (ER) due to the data treatment is about 2-3 % (Pilling et al., 2007). We have determined the absolute photodissociation, σ_{ph-d} (Equation 2), and photoionization (σ_{ph-i}) cross sections.

$$\sigma_{ph-d} = \sigma^+ \left(1 - \frac{PIY_{C_7 H_8^+}}{100} \right), \tag{2}$$

where σ^+ is the absolute photoabsorption cross section (from Hitchcock, A., 2013).

The photon flux of the pre-planetary nebula CRL 618 at 285 eV is 4.7×10^5 photons cm⁻² s⁻¹ (Boechat-Roberty et al., 2009). We have determined the photodissociation (k_{ph}) and photoionization (ς_i) rates and the half-life $(t_{1/2})$ of toluene using Equations 3 and 4, and have compared with previous results for the benzene molecule (Boechat-Roberty et al., 2009).

$$k_{ph} = \sigma_{ph-d}(E)f(E), \qquad (3)$$

$$t_{1/2} = \frac{ln2}{k_{ph}}.$$
 (4)

The results show that methyl-benzene is more stable than benzene, surviving more to stellar X-ray photons.

TABLE 1

Molecule	Cross Section (cm^2)			
	σ_{ph-d}	σ_{ph-i}	σ^+	
C_6H_6	3.7×10^{-16}	1.7×10^{-17}	4.2×10^{-16}	
$\mathrm{C}_{6}\mathrm{H}_{5}\mathrm{CH}_{3}$	$1.7{ imes}10^{-17}$	1.8×10^{-19}	$1.9{\times}10^{-17}$	

TABLE 2

Molecule	$t_{1/2}$ (years)	$k_{ph} ({\rm s}^{-1})$	$\varsigma_i (\mathrm{s}^{-1})$
C_6H_6	1903	1.2×10^{-11}	7.9×10^{-12}
$\mathrm{C}_{6}\mathrm{H}_{5}\mathrm{CH}_{3}$	2751	8.0×10^{-12}	$2.7{\times}10^{-13}$

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¹Observatório do Valongo, Universidade Federal do Rio de Janeiro (UFRJ), Postal: 20080-090, Ladeira Pedro Antônio, 43, Rio de Janeiro - RJ, Brasil (monfred@astro.ufrj.br).

²Instituto de Física/UFRJ.

³Instituto de Química/UFRJ.

⁴Centro de Ciências Naturais e Humanas/UFABC.