Ionization of biological molecules by multicharged ions

A M P Mendez, C C Montanari, and J E Miraglia

Instituto de Astronomía y Física del Espacio, CONICET–UBA

Introduction

The ionization of biological targets by the impact of heavy projectiles has become a field of interest due to its implementation in ion-beam cancer therapy. The study of such systems represents a challenge from the theoretical point of view; however, several approaches [1, 2] have been presented to deal with this process.

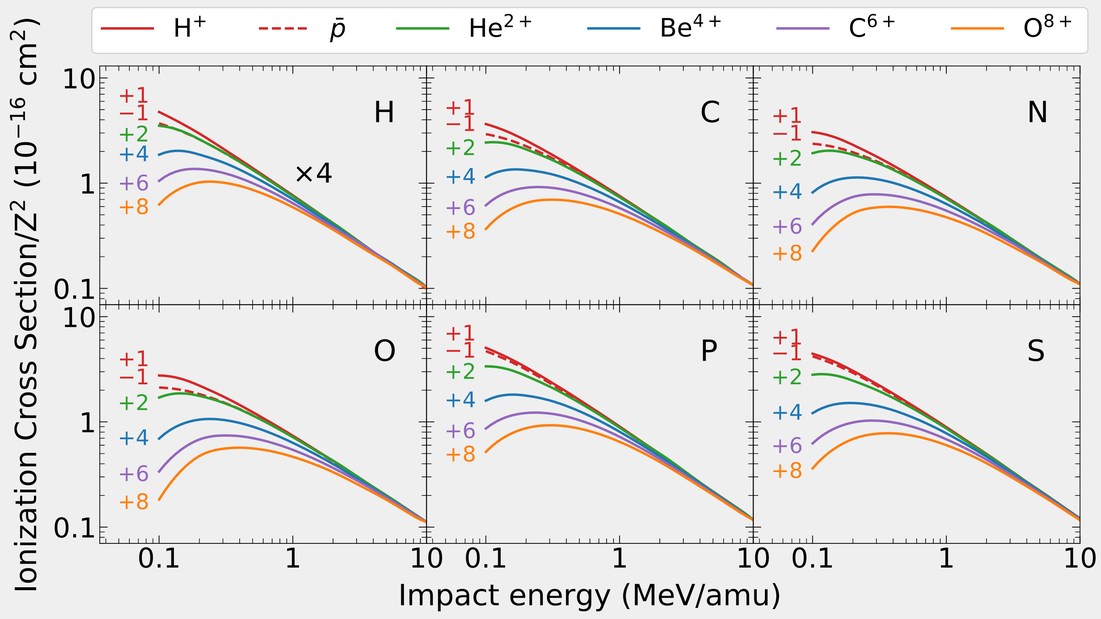
We investigate the ionization of several biological molecules of interest by the impact of multicharged ions in the intermediate to high energy range using the Continuum Distorted Wave-Eikonal Initial State method (CDW) [3] and the simple stoichiometric model (SSM) [4].

Ionization of atoms

We considered 36 collisional systems composed by

- targets: α = H, C, N, O, P, and S,
- projectiles: $\bar{p}$, H^+, He^{2+}, Be^{4+}, C^{6+}, and O^{8+}.

The total ionization cross section was calculated using the CDW [5].



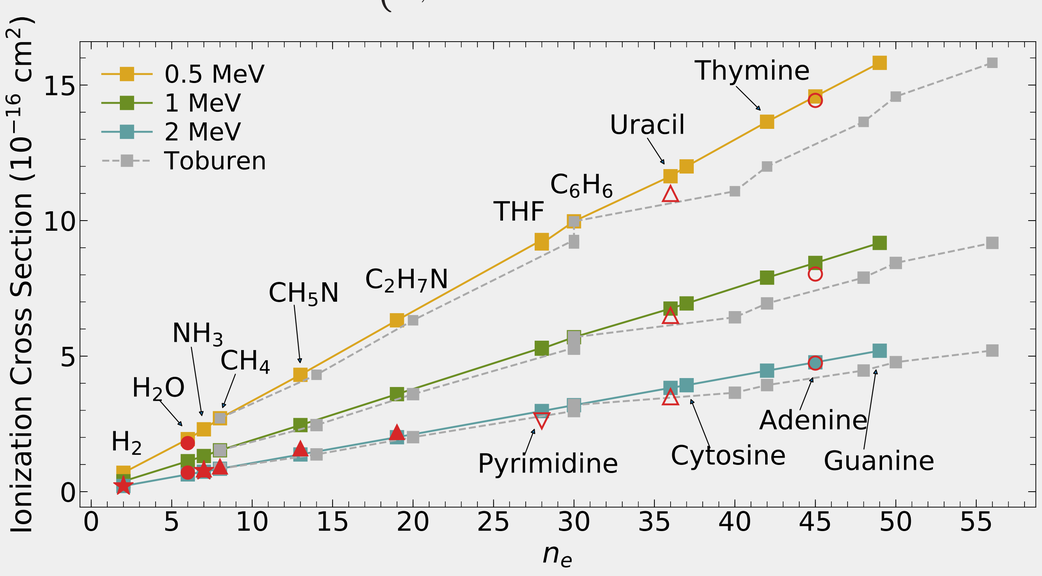
Scaling rules

Following [6], we define the scaled ionization cross section per weakly bound electron σ_e as

$$\sigma_e = \frac{\sigma_M}{n_e}, \tag{1}$$

where $n_e = \sum_\alpha n_\alpha \nu_\alpha$, and ν_α are the active electron numbers given by

$$\nu_\alpha = \begin{cases} 1, \to 1 & \text{for H,} \\ 4, \to 4 & \text{for C,} \\ 5, \to 4 & \text{for N and P,} \\ 6, \to 4.5 & \text{for O and S.} \end{cases} \tag{2}$$



The stoichiometric model

The SSM approaches the total ionization cross section of a molecule M as

$$\sigma_M = \sum_\alpha n_\alpha \sigma_\alpha \,. \tag{3}$$

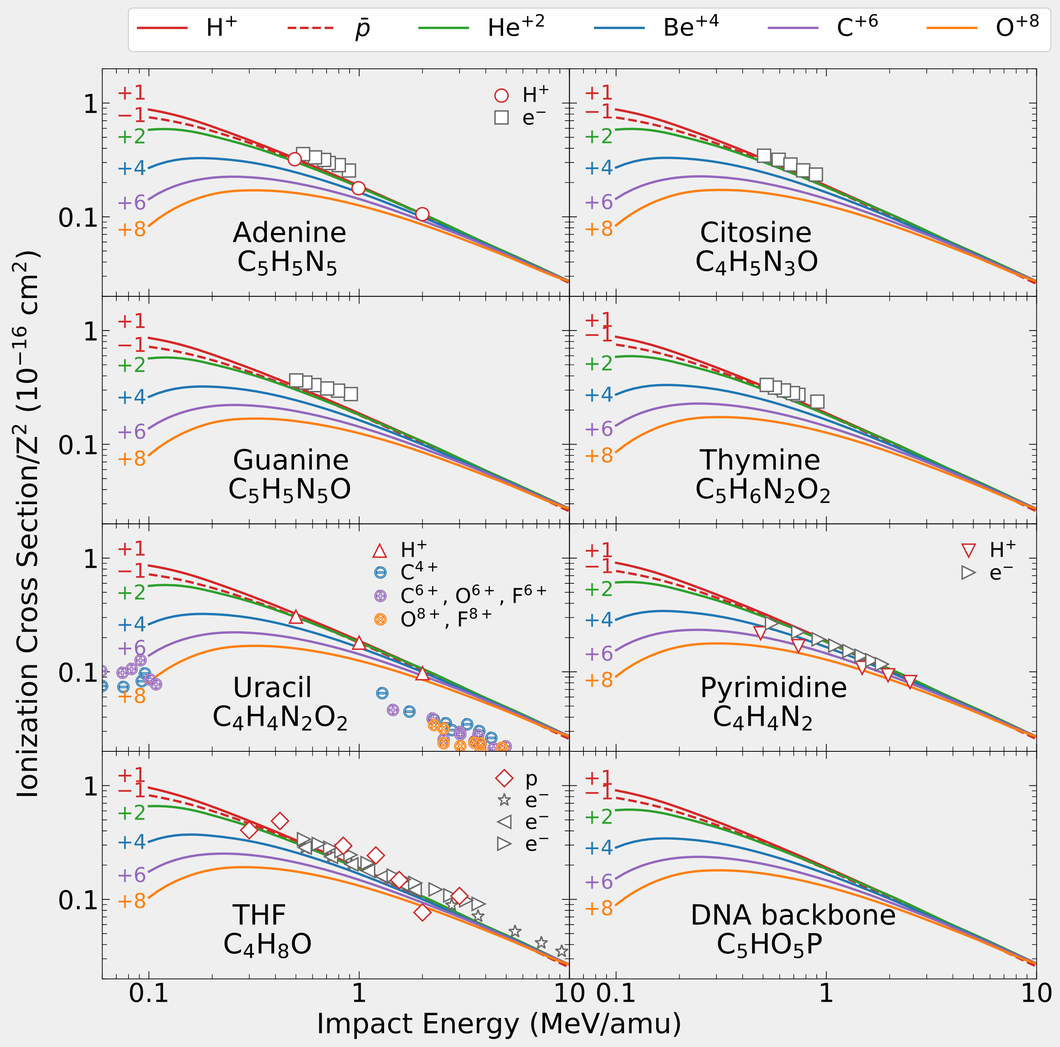
where n_α is the number of element α forming the molecule and σ_α is the ionization cross sections of the isolated atoms.

Molecules studied

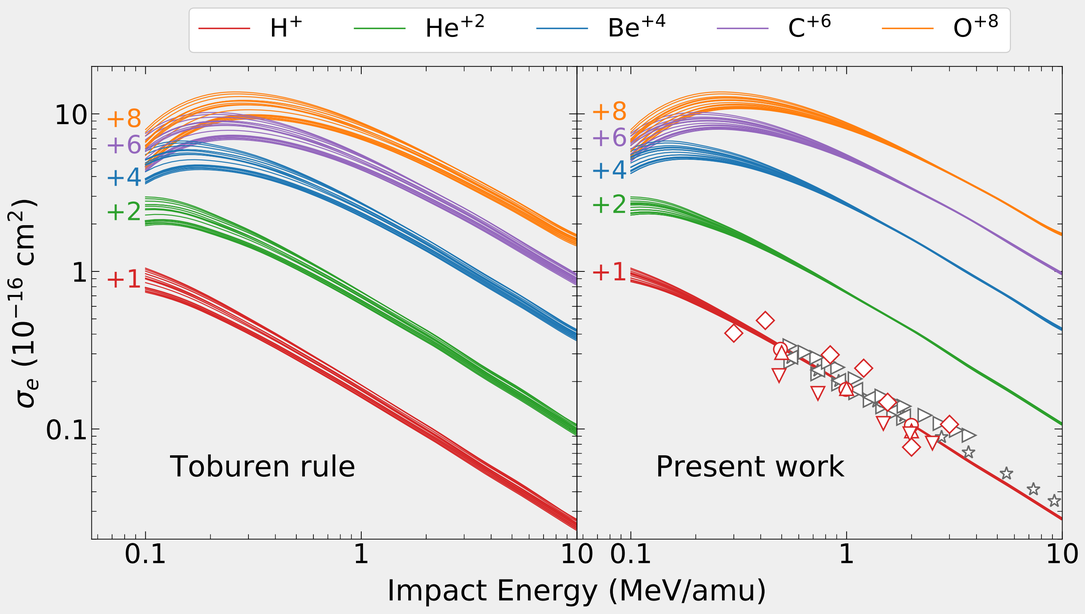
We considered the following molecules:

- CH: CH_4, C_2H_2, C_2H_4, C_2H_6, C_6H_6
- CHN: C_5H_5N, $C_4H_4N_2$, C_2H_7N, CH_5N
- DNA: $C_5H_5N_5$, $C_4H_5N_3O$, $C_5H_5N_5O$, $C_5H_6N_2O_2$, $C_4H_4N_2O_2$, C_4H_8O, $C_5H_{10}O_5P$, $C_{20}H_{27}N_7O_{13}P_2$

Ionization of DNA and RNA bases



CDW–based scaling



References

[1] M. E. Galasssi, R. D. Rivarola, M. Beuve, G. H. Olivera and P. D. Fainstein, Phys. Rev. A **62**, 022701 (2000).

[2] H. J. Lüdde, A. Achenbach, T. Kalkbrenner, H.-C. Jankowiak and T. Kirchner, Eur. Phys. J. D **70**, 82 (2016).

[3] Fainstein P.D., Ponce V. H. and Rivarola R. D. J. Phys. B: At. Mol. Opt. Phys. **21** 287 (1988).

[4] A. M. P. Mendez, C. C. Montanari and J. E. Miraglia, arXiv:1909.13847 [physics.atm-clus]

[5] J. E. Miraglia, https://arxiv.org/abs/1909.13682 [physics.atom-ph]

[6] W. E. Wilson and L. H. Toburen, Phys. Rev. A **11**, 1303 (1975).

* alemendez@iafe.uba.ar