

## Positive ion desorption from frozen N-heterocycles stimulated by high-energy electron impact

Fabio Ribeiro\*<sup>1</sup>, Jessica Martins\*, Wania Wolff<sup>†2</sup>, Heloisa Boechat-Roberly<sup>‡</sup> and Maria Luiza Rocco\*

\* Instituto de Química, Universidade Federal do Rio de Janeiro, RJ, 21941-909, Rio de Janeiro, Brazil

† Instituto de Física, Universidade Federal do Rio de Janeiro, RJ, 21941-909, Rio de Janeiro, Brazil

‡ Observatório do Valongo, Universidade Federal do Rio de Janeiro, RJ, 20.080-090 Rio de Janeiro, Brazil

**Synopsis** Ion desorption measurements induced by the impact of electrons onto pyridine and pyrimidine ices will be presented. The data reported here is of relevance for chemical evolution models of astrophysical objects.

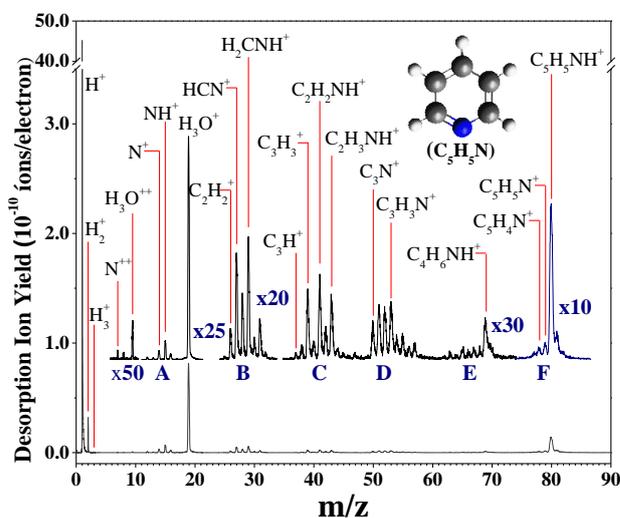
Nitrogen-Heterocyclic molecules (N-heterocycles) are one of most important biological class of molecules, since they make up the genetic material for all living organisms. Among them, pyridine ( $C_5H_5N$ ) and pyrimidine ( $C_4H_4N_2$ ) are prototypical aromatic molecules, in which the benzene ring is substituted by one and two nitrogen atoms, respectively. These molecules have also been the subject of intense radioastronomical surveys towards the interstellar-medium (ISM), although their detection was unsuccessful [1].

On the other hand, the presence of uracil traces in the organic extracts of the Murchison meteorite [2] may point to the incorporation of N-heterocycles into the solid component of the ISM, causing the molecular depletion observed in the gas-phase. Therefore, the desorption induced by photons and collisions with charge particles may be an important mechanism for leading neutral and ionic fragments into the gas-phase, acting as tracers for N-heterocycles.

In this work, we report the results of high-energy electron impact onto vapor deposited ices of  $C_5H_5N$  and  $C_4H_4N_2$  by means of the electron stimulated ion desorption (ESID) technique. Desorbed cations from the icy surface were analyzed by time-of-flight mass spectrometry (TOF-MS). Both  $C_5H_5N$  and  $C_4H_4N_2$  exhibit six distinct regions on their ESID spectra, containing ionic fragments bearing one to six members of the original heterocyclic ring. As reported in [3], five-membered fragment ions were observed for the first time in electron impact experiments for  $C_4H_4N_2$ .

Figure 1 shows several minor fragments from the ESID spectrum of  $C_5H_5N$  at 120 K, indicating strong fragmentation. Proton-transfer reactions also play an important role during desorption, as inferred by the intensity of the pro-

tonated parent ion ( $C_5H_5NH^+$ ) at  $m/z = 80$ . Cluster ions have also been identified and their formation is discussed on the basis of ion-molecule interactions.



**Figure 1.** ESID spectrum of positive ions from pyridine ice ( $C_5H_5N$ ) at 120 K due to 2.3 keV electron impact. Regions A to F are magnified in order to highlight the cracking pattern of solid pyridine.

The comparison between positive ion yields for  $C_5H_5N$  and  $C_4H_4N_2$  will be presented. Several of the detected ions in this work are in agreement with cometary observations, and thus may act as an indicative of the presence of N-heterocycles on astrophysical objects.

### References

- [1] S. B. Charnley *et al.* 2005 *Adv. Space Res.* **36** 137
- [2] Z. Martins *et al.* 2008 *Earth Planet. Sci. Lett.* **270** 130
- [3] F. A. Ribeiro *et al.* 2014 *J. Phys. Chem. C* **118** 25978

<sup>1</sup> E-mail: [fabioribeiro@iq.ufrj.br](mailto:fabioribeiro@iq.ufrj.br)

<sup>2</sup> E-mail: [wania@if.ufrj.br](mailto:wania@if.ufrj.br)

