

## Electron transfer in potassium-tryptophan collisions: an experimental and theoretical fragmentation study

André Rebelo<sup>1</sup>, Guilherme Meneses<sup>1</sup>, Gustavo Garcia<sup>2</sup>, Adrià Gil<sup>3</sup>, Maria José Calhorda<sup>3</sup>, Filipe Ferreira da Silva<sup>1</sup>, Paulo Limão-Vieira<sup>1</sup>

<sup>1</sup> Laboratório de Colisões Atômicas e Moleculares, CEFITEC, Departamento de Física, FCT–Universidade Nova de Lisboa, Caparica, Portugal

<sup>2</sup> Instituto de Física Fundamental, Consejo Superior de Investigaciones Científicas, Serrano 113-bis, 28006 Madrid, Spain

<sup>3</sup> Univ Lisbon, Fac Ciencias, Ctr Quim & Bioquim, DQB, 1749-016 Lisbon, Portugal

afc.rebelo@campus.fct.unl.pt; f.ferreiradasilva@fct.unl.pt

It is known that ionizing radiation bring adverse effects to living cells. In the femtosecond regime, multiple ionizations may occur in the human body leading ultimately to the formation of radical and/or ionic species. In fact, for every MeV of radiation energy deposited in matter, about  $5 \times 10^4$  secondary electrons ( $< 100$  eV) are generated [1, 2]. In the  $10^{-15}$ - $10^{-12}$ s time window, these entities may propagate through nanometer distances in the biological medium, leading to several inelastic events [3]. Low energy electrons, with energy below 20 eV can be resonantly captured in unoccupied molecular orbitals (virtual orbitals) [4, 5]. This process results in an unstable excited transient negative ion, which can further decay via auto detachment, dissociation or, in a comparatively long time scale, via photon emission.

In the present communication electron transfer studies upon potassium collisions with tryptophan, are presented as well as theoretical DFT analysis. Experimental results have been obtained by means a crossed molecular beam apparatus coupled with Time-of-Flight mass spectrometer. It is clear that for energy collision below 75 eV in the lab frame, the main fragment corresponds to the scission of  $C_\beta$  indole bond, with hydrogen transfer. This has been also described by means to DFT calculations, CAM-B3LYP and BHandHLYP codes.

### References

- [1] V. Cobut, Y. Frongillo, J. P. Patau and T. Goulet, *Radiat. Phys. Chem.*, **3**, (1998), 229–243.
- [2] S. M. Pimblott, J. A. LaVerne, *Rad. Phys. Chem.*, **76**, (2007), 1244-1247.
- [3] S. Denifl, B. Sonnweber, G. Hanel, P. Scheier, T. D. Mark, *Int. J. Spect.*, **238**, (2004), 47-53.
- [4] R. Abouaf, J. Pommier, H. Dunnet, *Int. J. Spect.*, **226**, (2003), 397-403.
- [5] S. Ptasinska, S. Denifl, V. Grill, T. D. Mark, P. Scheier, S. Gohlke, M. A. Huels, E. Illenberger, *Angew. Chem.*, **44**, (2005), 1647-1650.