Paulo LIMAO-VIEIRA
Atomic and Molecular Collisions Laboratory
Department of Physics, New University of Lisbon
2829-516 Caparica, Portugal
plimaovieira@fct.unl.pt

REFERENCE: ESF Exchange Grant, 1336
Beneficiary: Paulo LIMAO-VIEIRA, New University of Lisbon
Host: Prof. Dr. Marie-Jeanne Hubin-Franskin University of Liège, Bekgium
Period: from 13/02/2007 to 06/03/2007 Place: Liège - Belgium

SCIENTIFIC REPORT

PURPOSE OF VISIT

The main purpose of the visit was to bring together both applicants' and host expertise on the VUV electronic state spectroscopy of several molecular targets, including plasma processing molecules and mainly those Volatile Organic Compounds (VOCs) and some biological molecular species as well. The other main goal of this stay was to establish a series of other near future experimental measurements (both EELS and He(I) photoelectron) to study model systems in the initiation reaction of the lipidic peroxidation that takes place in the double layer of the cellular membrane and as parts of DNA adenine substitution that are substantial parts of DNA, which should lead to better understanding of effects linked to chemical and structural changes of biomolecular systems connected with radiation damage induced by low energy electrons.

DESCRIPTION OF THE WORK CARRIED OUT DURING THE VISIT

He(I) photoelectron spectroscopy (in close link with Prof. Jacques Delwiche) of some of the VOCs (e.g., limonene and isoprene) have been recorded and data analyses is on going. Electron Energy Loss Spectra analysis of c-C_5F_8, and the theoretical ab initio calculations obtained by two different computational methods (TDDFT and EOM-CCSD) have been discussed.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

- He(I) photoelectraon spectra on c-C_5F_8, pyrimidine, isoprene and limonene;
- Ab initio calculations to compute vertical excitation energies have been obtained together with the Lille – France – group, and discussed during the applicants' stay.

FUTURE COLLABORATION WITH HOST INSTITUTION

Due to the link with the Liège group, the study of other relevant molecular targets are on going, with the special attention to other VOCs like limonene, 2 methyl-3-buten-2-ol. Molecules due to their relevance as a model to study the initiation reaction of the lipidic peroxidation that takes place in the double layer of the cellular membrane and as parts of DNA adenine substitution are planned to be studied as well.

PROJECTED PUBLICATIONS/ARTICLES RESULTING OR TO RESULT FROM THE GRANT

There are two publications to be submitted shortly:

1. "c-C_5F_8 VUV electronic state spectroscopy by high-resolution synchrotron radiation, electron impact, He(I) photoelectron and *ab initio* calculations";
2. "On the valence shell electronic state spectroscopy of monoterpene limonene".

Other publications will emerge during the next months as soon as we compile and analyse the relavant data recorded. We expect 2 – 3 more papers to be submitted to international journals as part of the present grant.

Paulo Limao-Vieira

Lisbon, 7th March 2007.

CONFIRMATION BY THE HOST INSTITUTE OF THE SUCCESSFUL EXECUTION OF THE MISSION

The visit of Paulo Limao-Vieira was accomplished with success and according to the planed activities.

Prof. Dr. Marie-Jeanne Hubin-Franskin

Liège, 7th March 2007.