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REFERENCE: Short Term Scientific Mission, COST P9

Beneficiary: Paulo Limao-Vieira, New University of Lisbon

Host: Prof. Dr. Paul Scheier, University of Innsbruck, Innsbruck, Austria

Period: from 09/06/2007 to 15/06/2007 Innsbruck - Austria

Reference code: COST-STSM-P9-02863

## **SCIENTIFIC REPORT**

### ***PURPOSE OF VISIT***

The main purpose of the visit was to join the current investigations on electron interactions with amino acids embedded in helium and water clusters and electron attachment to gas phase amino acids, as an extension work of the Innsbruck earlier studies on gas phase biomolecules. However, and for technical purposes at the moment was not possible to fully perform those experiments. Meanwhile, the recent electron harpooning experiments on nitromethane carried out in my laboratory in Lisbon by the atom-molecule collision technique, have revealed the formation of several anionic species that have not been reported in the recent publication on dissociative electron attachment experiments from the Innsbruck team. Though, the mechanism of formation of the newly discovered fragments have not yet been understood and some complementary studies were needed. So, we took advantage of an apparatus equipped with an electric field sector and a magnetic mass selector (CH5), to look at free-electron attachment experiments with nitromethane. The ion yields were obtained as a function of the electron energy. The present configuration of the set-up allows also MIKE scans to be taken.

### ***DESCRIPTION OF THE WORK CARRIED OUT DURING THE VISIT***

The set of experiments carried out in the CH5 set-up for dissociative electron attachment (DEA) in nitromethane, in an energy range of 0 – 15 eV, has allowed a mass scan and the possibility to spot new anionic fragments which seem to be mostly in agreement with the present results obtained in Lisbon. Negative ion resonances have been extended from the previous DEA work up to 15 eV. The observed ionic yields showed that the neutral molecule upon electron attachment, must undergo a considerable intramolecular rearrangement in order to produce some of the observed structure. Another interesting investigation has been focused on the MIKE scans for metastable decays measurements of some of the fragments.

## **DESCRIPTION OF THE MAIN RESULTS OBTAINED**

During this visit to Innsbruck, it was possible to get a complete set of nitromethane negative ion formation mass scans and DEA studies in the electron energy region of 0 – 15 eV. These spectra include MIKE scans for some of the fragments:

- Negative ion yields of nitromethane;
- Mass, appearance energy and also MIKE scans for some of the nitromethane molecular fragments were obtained.

## **FUTURE COLLABORATION WITH HOST INSTITUTIONS**

As part of the international joint collaboration kept over the years with the Innsbruck laboratory, the above mentioned work will be explored regarding a publication and other molecular targets are being evaluated for future exchange programs.

## **PROJECTED PUBLICATIONS/ARTICLES RESULTING OR TO RESULT FROM THE STSM**

The results obtained to nitromethane will be evaluated and prepared in a joint publication, to be submitted to an international journal in due time.

Paulo Limao-Vieira

Lisbon, 3<sup>rd</sup> July 2007.

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



Prof. Dr. Paul Scheier

Innsbruck, 3<sup>rd</sup> July 2007.