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Innsbruck, 21<sup>th</sup> December 2008

REFERENCE: Short Term Scientific Mission, COST CM0601

Beneficiary: Filipe Ferreira da Silva, Inst. für Ionenphysik und Ang. Physik (AT)

Host: Paulo Limao-Vieira, New University of Lisbon (PT) Period: from 08/12/2008 to 19/12/2008 Place: Lisbon (PT)

Reference code: COST-STSM-CM0601-3439

#### SCIENTIFIC REPORT

#### PURPOSE OF VISIT

The scientific mission to the Atomic and Molecular Collisions Laboratory, New University of Lisbon was devoted to the experimental studies on the negative ion formation in electron transfer experiments in atom-molecule collisions by means of a crossed molecular beam machine. The expected molecular targets included nitromethane and d-nitromethene. Some experiments with thymine were also planned.

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

During this STSM, a part from the planned activities, it was necessary to build a new potassium ion source in order to improve its performance from the point of view of better ion current to the charge exchange oven, allowing a lower energy energy projectile beam (<20 eV) and also to avoid position sensitive differences with the pulsed potassium beam and the TOF delay to extract the negative ions formed in the interaction region. Some pending publications have been finished and expected to be submitted shortly.

#### DESCRIPTION OF THE MAIN RESULTS OBTAINED

A joint publication on pyrimidine has been finished (see a few details on appendix I) to be submitted to Phys. Chem. Chem. Phys. shortly and data on electron attachment to explosive related molecules, PETN – Pentaerythritol tetranitrate, RDX – cyclo trimethylnotrinitramine and SEMTEX were carefully analysed to be submitted to a international journal in collaboration with the Austrian colleagues from Innsbruck. Therefore, during this scientific misson was possible to:

- 1. compile and analyse the VUV data of pyrimidine;
- 2. discussion and comparison of the EELS data obtained by the Serbian group (B P Marinkovic) on pyrimidine under dipolar conditions and as a function of the scattering angle:
- 3. discussion on the recent assignments, both valence and Rydberg as well as for the hot bands of pyrimidine;
- 4. assignment of the anionic fragments for the PETN, RDX and SEMTEX was carefully done and the resonant energy profiles analysed;

### FUTURE COLLABORATION WITH HOST INSTITUTION

This research joint programme will continue, especially the joint collaboration work with the Innsbruck group on electron attachment. Due to the need of building a new potassium source, was not possible during this visit to performed the planned experiments. However, the new source was successfully assembled and tested, which will allow to perform the proposed experiments by the Lisbon group during the forthcoming weeks.

# PROJECTED PUBLICATIONS/ARTICLES RESULTING OR TO RESULT FROM THE GRANT

One joint publication is to be submitted to Phys. Chem. Chem. Phys. on the VUV spectroscopy of pyrimidine. Other two publications will emerge during the next months as a result of the interpretation and assignments of the DEA data recorded for the explosive related molecules, PETN, RDX and SEMTEX.

Innsbruck, 21<sup>st</sup> December 2008

Filipe Ferreira da Silva

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

Lisbon, 21st December 2008

Paulo Limao-Vieira

## APPENDIX I - Recent results and data analyses from the STSM to Lisbon.

Figure 1) – High resolution VUV photoabsorption spectrum of pyrimidine (3 – 11 eV)

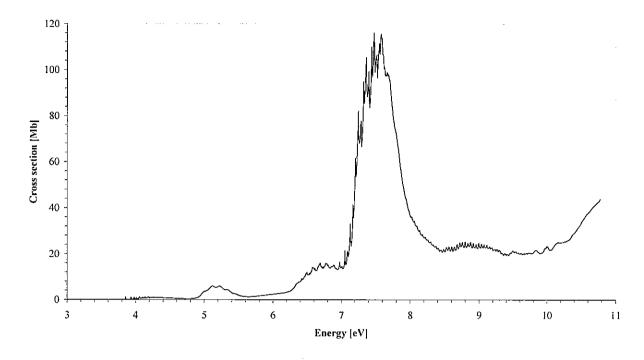


Figure 2) – High resolution VUV photoabsorption spectrum of pyrimidine (3.7 - 3.9 eV)

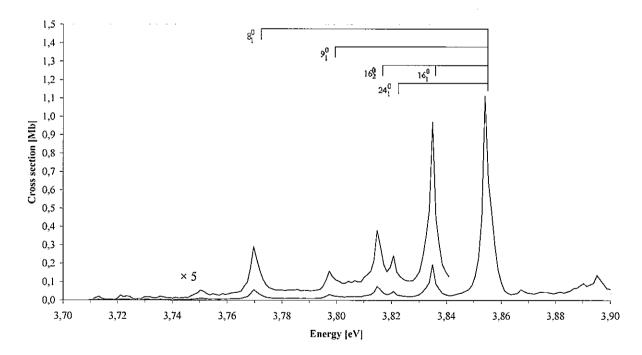


Figure 3) – High resolution VUV photoabsorption spectrum of pyrimidine (3.8 – 4.3 eV)

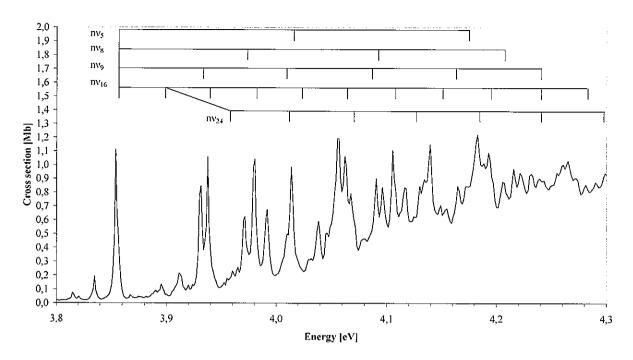


Figure 4) – High resolution VUV photoabsorption spectrum of pyrimidine (4.5 - 6.0 eV)

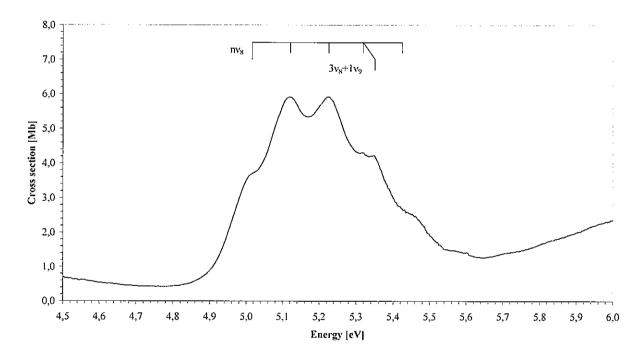


Figure 5) – High resolution VUV photoabsorption spectrum of pyrimidine (6.0 – 7.0 eV)

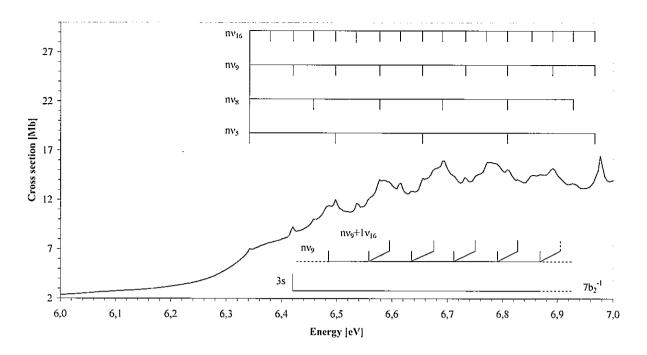


Figure 6) – High resolution VUV photoabsorption spectrum of pyrimidine (6.9 – 7.8 eV)

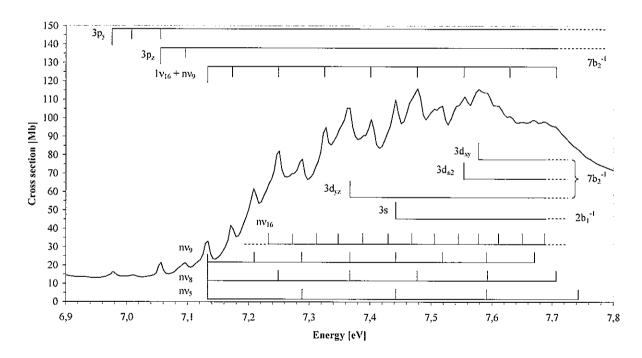


Figure 7) – High resolution VUV photoabsorption spectrum of pyrimidine (7.8 – 9.6 eV)

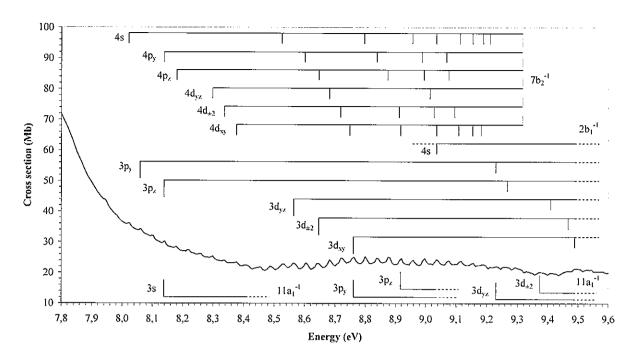


Figure 8) – High resolution VUV photoabsorption spectrum of pyrimidine (9.5 – 10.8 eV)

