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REFERENCE: Short Term Scientific Mission, COST P9
Beneficiary: Dr. M-J Hubin-Franskin, University of Liège, Liège, Belgium
Host: Paulo LIMAO-VIEIRA, New University of Lisbon
Period: from 15/11/2004 to 19/11/2004 Place: Lisbon - Portugal
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SCIENTIFIC REPORT

PURPOSE OF VISIT

This visit was devoted to the interpretation and analysis of the spectroscopic data of biomolecules that Paulo LIMAO-VIEIRA, *New University of Lisbon* has got during his visit in the *Laboratoire de Spectrsocopie d'Electrons Diffuses, University of Liège*, Belgium. The Portuguese group has a proved quite large expertise in the data treatment and assignment of electronic states.

DESCRIPTION OF THE WORK CARRIED OUT DURING THE VISIT

This five days stay at the physics department of the New University of Lisbon gave me the opportunity to have long and fruitful discussions with Paulo Limao-Vieira on recent measurements carried out on acetic acid during the visit of Paulo Limao-Vieira in Liège.

The spectroscopic results on the molecule of acetic acid were obtained by means of different and complementary experimental methods :

1. the high resolution electron energy loss spectrum (HREELS) recorded in electric dipolar excitation conditions at the University of Liège in collaboration with Dr Alexandre Giuliani ;

2. the high resolution HeI photoelectron spectrum in collaboration with Jacques Delwiche;

3. the UV absorption spectrum measured at VUV beam line of ISA the Århus University synchrotron radiation facility in collaboration with Dr Søren Vrønning Hoffmann and Alexandre Giuliani;

Analysis has shown that there is a very good agreement between the UV absorption measurements and the HREELS spectrum, showing there are no saturation effects in the absorption.

The valence shell electronic spectrum has been shown to be largely dominated by valence excited states of n-π^*, n-σ^* and π-π^* type. Very few of them exhibit fine features. Most of the valence sates are very likely predissociated into two neutral radicals. The electron impact spectrum confirm all the bands and fine features observed by photoabsorption. As it extends up to 14 eV it shows that there is still absorption around 13 eV, this with a rather large cross section

A careful analysis of the Rydberg series converging to the first ionisation limit of the molecule has been performed. New series have been observed. They correspond to new values for the quantum defect, compared to literature data. The analysis of the Rydberg series was greatly facilitated thanks to the availability of the high resolution HeI photoelectron spectrum. For the first time, this spectrum having been recorded with an energy resolution of about 15 meV new vibrational features are observed and analysed in terms of at least three progressions. There is also an indication that the first electronic band of the spectrum could be predissociated. Unfortunately, it appeared that there is some disagreement between our photoelectron spectrum and the data from the literature regarding to the first ionisation energy. The discrepancy on the value of the first ionisation limit is quite large so that it is very difficult to compare our data with those from the literature, the resolution of our spectrum being much better. In order to clarify the problem, the first photoelectron band will be reinvestigated and special attention will be payed to the calibration of the energy scale. As soon as the new measurements will be finished, the paper on acetic acid already well advanced in his redaction, will be terminated and sent for publication.

I wish to thank the management of the COST action P9 for the financial support.

FUTURE COLLABORATION WITH HOST INSTITUTIONS

Joint collaboration is ongoing with the host institution and is planed for the near future the study of the electronic state spectroscopy of atmospheric interest molecules and biomolecules. Quantum chemical calculations on the electronic excitation energies for the molecules studied during my visit are planned in close collaboration with a theroretical research group. The first results have been just obtained for acetic acid and will be included in he publication.

PROJECTED PUBLICATIONS/ARTICLES RESULTING OR TO RESULT FROM THE STSM

At this moment at least two joint publications are being prepared to be submitted to international journals shortly.

Prof. Marie-Jeanne Hubin-Franskin

Liège, 22th November, 2004.

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

The scientific mission of Marie-Jeanne Hubin-Franskin to the New University of Lisbon has been quite successful.

Dr. Paulo Limao-Vieira

Liège, 22 th November 2004.