STSM SCIENTIFIC REPORT

ESF COST Action CM0601:
Electron Controlled Chemical Lithography

Project: Experimental Studies of Fragmentation Processes in Molecular Cluster Ions

COST Action Number: CM0601
Beneficiary's Name and Institution: Dr Samuel Eden, The Open University
Host's Name and Institution: Bernadette Farizon, Institut de Physique Nucléaire de Lyon
Period: from 02/03/2009 to 31/03/2009
Place: Villeurbanne (FR)
Reference code: COST-STSM-CM0601-04480
Claimed amount of the grant: 2450.00 €

Purpose of visit:

The principle aim of this STSM was to participate in experiments probing the fragmentation of water cluster ions following collisions with atoms at impact velocities corresponding to large cross sections for electron transfer. Cluster-phase experiments of this kind provide a valuable intermediate model to relate information from studies of isolated molecules (e.g. fragment ion kinetic energies and electron capture cross sections) to observed surface chemistries. The potential of the experimental system for fragment anion detection following cluster-projectile collisions is expected to be of particular interest for the ECCL community.

In addition, the visit was planned to enable me to contribute to several manuscripts reporting fragment ion production branching ratios and electron capture cross sections for proton collisions with gas-phase nucleobases. This data will be invaluable for the analysis of future fragmentation pattern observations in proton collisions with mass-selected nucleobase-water cluster ions.

Description of the work carried out during the visit:

The IPM group's work focused on the optimization of the *DIAM* apparatus for experiments to study the fragmentation of mass-selected water cluster ions following 2-10 keV collisions with neutral atomic and molecular targets (notably He, Ar, and N_2). Charged and neutral fragments were detected in coincidence using a micro-channel plate (MCP) positioned opposite the incident cluster ion beam. The fragments passed through an electric field in order to separate ions and neutrals on the basis of their flight times to the detector, a technique which also enabled ion masses to be determined. During the STSM, a series of experiments were carried out and the data acquisition system was advanced considerably. Large volumes of data were thus gathered on an event-by-event basis in order to reconstruct fragmentation processes as a function of cluster size and thereby probe intermolecular effects.

As well as participating in the laboratory work described above, I contributed to drafts for three further publications based on previous gas-phase experiments which are of major significance for the IPM group's future research on biomolecular clusters exploiting the *DIAM* apparatus.

Description of the main results obtained:

Building upon the extensive progress made by the IPM group over the previous months, further optimization of the *DIAM* system was achieved during the period of the STSM. For example, the range of mass-selected $(H^+(H_2O)_n$ cluster ions produced by the source was extended (up to n = 39, reported in first article listed below). Moreover, the relative intensities of different cluster ion masses produced by the apparatus supported previous evidence for a *magic number* (a particularly stable configuration associated with a closed shell of H_2O molecules) at n = 21 [e.g. Castleman et al. *Chem. Phys.* **72** (1982) 185]. Various collision experiments were carried out, notably for *small* $(H^+(H_2O)_n$ (n < 10) impact upon helium atoms.

Future collaboration with the host institution:

I am currently collaborating with the IPM group and I aim to carry out further experimental work with the group, provisionally scheduled for autumn 2009. In particular, I am keen to contribute to planned developments of the *DIAM* system in order to carry out collision experiments using a pulsed incident cluster ion beam. This development will be particularly valuable for future studies of fragment anion production in cluster collision events.

Projected articles:

Production of intense beams of mass-selected water cluster ions and theoretical study of atom-water interactions
Z. P. Wang, P. M. Dinh, P.-G. Reinhard, E. Suraud, G. Bruny, C. Montano, S. Feil, S. Eden, H. Abdoul-Carime, B. Farizon, M. Farizon, S. Ouaskit, and T.D. Märk
Submitted to *Int. J. Mass Spectrom.*

Proton impact induced ionization of uracil: branching ratios and energy dependence of electron capture and direct ionization in the range 20-150 keV
J. Tabet, S. Eden, S. Feil, H. Abdoul-Carime, B. Farizon, M. Farizon, S. Ouaskit, and T.D. Märk
For submission to *Phys. Rev. A*

Mass spectrometry of adenine, cytosine, and thymine following 80 keV proton impact with separation of direct ionization and electron capture processes
J. Tabet, S. Eden, S. Feil, H. Abdoul-Carime, B. Farizon, M. Farizon, S. Ouaskit, and T.D. Märk
For submission to *Phys. Rev. A*

Absolute cross sections for electron capture in 80 keV proton collisions with gas-phase DNA and RNA base molecules
J. Tabet, S. Eden, S. Feil, H. Abdoul-Carime, B. Farizon, M. Farizon, S. Ouaskit, and T.D. Märk
For submission to *Phys. Rev. A*

The first article listed above contains data recorded during this STSM. The other articles in the list report experimental results measured over the period when I was a full-time member of the IPM group.

Confirmation by the host institution of the successful execution of the exchange grant visit:

Samuel Eden's ECCL visit was carried out successfully. We plan to extend this collaboration through Samuel Eden's participation in further experimental work at the IPNL provisionally scheduled for autumn 2009.

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Lyon, 20th of April, 2009