ESF EXCHANGE GRANT REPORT

PROJECT WORK:

Studies of biomolecular cluster formation in the presence of ionising electrons

Researcher:	Dr. Samuel Eden, Open University, UK
Exchange grant reference:	1783
ESF activity unit:	PESC
ESF activity title and acronym:	
Exchange visit dates:	10 th of February – 29 th of March 2008
Host researcher:	Dr. Hdr Bernadette Farizon
Host address:	Institut de Physique Nucléaire de Lyon, Bâtiment Paul Dirac,
	4 rue Enrico Fermi, Villeurbanne F69622 cedex, France

Purpose of visit:

In addition to their relevance to fundamental aspects of molecular and statistical physics, experiments on neutral and ionic biomolecular clusters can help to bridge the "complexity gap" between the current understanding of radiation effects in the gas phase and in a biological medium. This represents a major current research challenge for physicists, chemists, and biologists, with important applications in quantifying the effects of radiation exposure.

The principle aim of this visit was to participate in the optimization of an apparatus to accelerate and mass-select dipole-bonded cluster ions formed in an expansion of gas comprising sublimated biomolecules, water, and a buffer gas in the presence of ionising electrons. This represents a novel variation of the classic technique to produce cluster ions by condensation in a supersonic expansion *followed by* ionisation in a beam of electrons or photons. In the Lyon methodology, electron impact ionisation of biomolecules in the expansion aids the formation of aqueous clusters due to the permanent dipole moments of the water molecules.

An additional aim of my visit was to contribute to the design of an original multi-coincidence position-sensitive detection system to observe the fragmentation patterns of biomolecular cluster ions following collisions with protons and neutral hydrogen atoms, including electron capture by the incident cluster ion.

Furthermore, the visit was planned to enable me to work with Dr. Bernadette Farizon to prepare manuscripts reporting absolute ionization cross sections for electron capture in proton collisions with gas phase nucleobases and associated fragmentation patterns.

Description of the work carried out during the visit:

I participated in a series of mass spectrometry measurements characterising ion beams formed by electron collisions with atoms and molecules in a supersonic expansion of a buffer gas (helium or argon) seeded with water vapour. Ions were accelerated to 6-8 keV, focused, energy-selected in an electrostatic sector field, and then mass-analysed by scanning a magnetic sector field in front of a channeltron detector. Development work on the experimental system focused on improving the intensity of the ion beam and optimizing the conditions for cluster ion formation. A number of technical modifications were carried out, in particular changing the position of *ioniser* filaments with respect to the supersonic expansion.

Description of the main results obtained:

The cluster ion source has been tested in different regimes. Further development work is currently being carried out to address certain technical problems encountered.

The design of the multi-coincidence detection system has advanced significantly, notably through the group's decision to purchase a specific set of ADC units for data acquisition from a microchannel plate - delay-line anode detector assembly. Following collisions between cluster ions and protons, this system will the enable time-of-flight identification of fragment ions to be combined with the characterisation of neutral fragments on the basis of the detection position and the distinct form of the signal.

Two manuscripts have been prepared reporting nucleobase fragmentation patterns following 20-150 keV proton impact induced ionisation. The experimental data enables mass spectra to be compared for *electron capture* (with projectile neutralisation) and for *direct ionisation* (with the emission of an electron into the continuum). This distinction is significant for the molecular-scale understanding of radiation damage in biological material as the *Bragg Peak* (the phenomenological basis for cancer therapy techniques utilizing ion beams) is understood to result from the interplay between ionisation, excitation, and charge exchange processes as incident ions slow down in an absorbing medium. These manuscripts will be discussed with our collaborators and submitted to international journals in the near future.

Future collaboration with the host institution:

As stated above, I am currently working with the IPM group in order to finalize a series of scientific communications. We plan to extend this collaboration through my participation in further experimental work exploiting the unique compatibilities of the experimental system under development at the IPNL (autumn 2008).

Projected scientific communications:

• 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, 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, B. Farizon, M. Farizon, S. Ouaskit, and T. D. Märk For submission to *J. Chem. Phys.*
- I have been invited to present a talk on behalf of the IPM group at the LEEMI (*Low-Energy Electron Molecule Interactions*) EIPAM conference, Roscoff (France) 7th 11th May 2008. The title of this presentation is *Electron transfer in proton collisions with DNA bases*

Travel Costs:

- € 148.50 for the return journey from London St. Pancras to Lyon Part Dieu (changing at Lille Europe)
- € 130 for a return journey to the Open University in the middle of my exchange period in order to coordinate my student's activity in the ongoing neutral cluster ionization experimental programme (Lyon Part Dieu to Milton Keynes, changing at Lille Europe and London St. Pancras)

Total = \notin **278.50** *See pages 4-7 for the scanned original tickets*

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

Samuel Eden's EIPAM visit was carried out successfully. We plan to extend this collaboration through Samuel Eden's participation in further experimental work at the IPNL in the autumn of this year.

Dr. Hdr Bernadette Farizon Head of the IPM group Institut de Physique Nucléaire de Lyon Lyon, 28th of April, 2008

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