

NEWSLETTER JULY 2003

EPIC Network makes a swift impact

The EU Framework V Network Electron and Positron Induced Chemistry (EPIC) is a network of internationally renowned research teams in Europe dedicated to the study of electron and position interactions with molecules. Its research may be broadly divided into two sub-topics based upon the type of molecular target involved.

Studies of interactions with halogenated targets are relevant to industrial plasmas, in particular those used in the semiconductor industry.

Studies of interactions with biological molecules and in particular the nucleotide based research that is linked to study of radiation damage in DNA.

Participating institutions are;

Centre of Molecular and Optical Sciences, The Open University, United Kingdom Department of Physics and Astronomy, University College London, United Kingdom Institut fur Ionenphysik, Leopold Franzens Universitaet Innsbruck, Austria Department of Physical Chemistry, Freie Universitaet Berlin, Germany

Department of Chemistry, Universita di Roma 'La Sapienza', Universita di Roma 'La Sapienza', Italy

Department of Physics, Trento University, Italy

Department of Physics, University of Aarhus, Denmark

J Heyrovsky Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, The Czech Republic.

Laboratoire des Collisions Atomiques et Moléculaires Université Paris-Sud, Paris, France

Together with collaborators within:

Department of Physics, University of Bonn, Germany

Department of Physics, Charles University, Prague, Czech Republic

Institute of Physics Belgrade, Serbia

Department of Physics, Comenius University, Slovakia

CSIC, Madrid, Spain

The Network officially started in September 2002 and within the first nine months has shown itself to be a dynamic and rapidly evolving Network of the leading scientists in Europe. The study of electron impact with biomolecules has received particular attention with a recent PRL publication from Institut fur Ionenphysik, Leopold Franzens Universitaet on dissociative attachment to nucleotide bases receiving coverage in the international media.

Network members have also been successful in developing research links with other members of the academic community and with applied/industrial partners. Three further networks based upon the core research in the EPIC network have been awarded.

An EU COST Action RADAM (Physics P9) to study radiation damage at the molecular level. This action links the electron/positron community with those studying ion and photon damage of biological molecules and brings EPIC network members together with radiation chemists and medical researchers. Joint meetings between EPIC and RADAM are planned for 2004.

An ESF Funded Programme entitled Electron Induced Processing at the Molecular level (EIPAM) bringing EPIC members together with researchers in the Scanning Tunnel Microscopy (STM) community to study how nanoscale physics and chemistry may be developed using STM techniques. This five year programme will start in 2004.

An ESF Network entitled 'Collisions in Atom Traps (CATS)' will bring together member of the cold atom community and members of EPIC to investigate electron/positron interactions with cold atoms and cold molecules, while also exploring the new world of ultracold plasmas ! A three year programme commencing in summer of 2003.

In addition, EPIC research in electron interactions with halocarbons is being applied to the development of next generation of plasma reactors for the semiconductor industry. We are developing links with Japanese industry, with a special workshop (organised by EPIC members) being held in Stockholm July 21-22, 2003 between European and Japanese researchers.

Thus EPIC is definitely fulfilling the hopes of its participants in acting as a forum and focus for development of electron and positron research within the European Community. In the next two years EPIC will seek to develop still further and explore links with research groups worldwide to ensure that a truly international research programme in electron and positron physics is developed with applications exploited from astrophysics to life sciences.

The development of such a vibrant research community is ideal for the training of young research scientists. The major goal of EPIC is to train the next generation of researchers such that research in electron and positron research will continue to grow and develop in the next decade. The network has been fortunate to recruit a unique set of talented younger researchers whose work in the next two years will provide much of the momentum and creativity of the research programme. Training of these younger researchers will require a set of workshops, the first of which is to be held in the UK in September 2003 and is dedicated to training researchers in the study of biological systems and will include practical courses in DNA extraction and analysis. A Vacuum training course will be held in December and a theoretical methods school is also planned. Presentation skills will be developed at the Network meetings when younger researchers will be able to present their work to the Network members and other senior researchers.

Thus the network has made an impressive start to its activities and will continue to develop as our younger researchers make their mark. This Newsletter reports on the research undertaken by the Network members in the last nine months for further details please see the Network webpage and those of the partners (http://physics.open.ac.uk/epic/EPIC%20home.html)

GROUP REPORTS

UCL Theory Group

Prof Jonathan Tennyson Dr Jemina Gorfinkiel Dr Natalia Vinci Ms Iryna Rozum Mr Chiara Piccarreta

Work being performed at UCL theory at present:

Electron collisions with CF3 and characterising the bound state CF3-.

Extending the R-matrix to deal with intermediate energies and the ab initio treatment of electron impact ionisation.

Dissociative recombination of CO++ (the CO dication).

Electron collisions with LiH.

Work has just started looking at electron water collisions as a function of geometry in all three vibrational degrees of freedom

OU/UCL Experiment Group

Prof Nigel Mason Dr Paulo Limão-Vieira Mr Sam Eden Ms Anita Dawes Mr Philip Holtom Mr Mike Davies Ms Sarah Webb Dr Stephen Brotton

Dr Dagmar Mayr Ms Eva Vasekova Mr Bobby Antony Ms Liz Drage

Current research has concentrated on the study of molecular systems relevant to semiconductor etching and halocarbons important in atmospheric physics and chemistry leading to ozone depletion and global warming. Particular emphasis is given to SF_5CF_3 , a newly discovered greenhouse gas. High resolution photo-absorption and electron energy loss spectroscopy (EELS) results further understanding of the molecules and their effects in the Earth's atmosphere. Analysis of electronic excitation into valence and Rydberg states is presented and accompanied by the assignment of many new structures. Photoelectron experiments are described, revealing detailed information on the ionisation pathways of SF_5CF_3 .

Further studies included low electron energy stimulated disorption experiments to investigate dissociative attachment and negative ion resonances of CCl_2F_2 and SF_5CF_3 at an Au (111) surface (with Freie University Berlin). The formation of transient negative ions via resonant electron capture at a particular energy in the unimolecular decomposition process from co-adsorption of water and Xenon sub-monolayer is presented and discussed. Reactions occurring on ice and dust surfaces at stratospheric altitudes are expected to have an important effect on global warming and ozone depletion processes. Analysis of the surface reactivity of gaseous SF_5CF_3 in order to understand how these mechanisms can affect the lifetime of the molecule in the atmosphere has been reported.

In a collaboration with a research group in Japan we are studying replacement gases for semiconductor plasma reactors. CF_3I and C_2F_4 have been the major focus as they provide a good source of CF_3 CF_2 radicals respectively. These experiments have been completed by theoretical calculations by UCL theoretical group.

Innsbruck Group

Prof.Tilmann Märk Prof.Paul Scheier Prof.Michael Probst Dr.Sara Matt Mag. Stephan Denifl Mag. Sylwia Ptasinska (EPIC young researcher) Mag. Peter Cicman Mag. Bruno Coupier Mag. Krysztof Gluch Mag. Stefan Feil

Using our two high resolution crossed beams machines (consisting of a hemispherical and trochoidal electron monochromator, respectively in combination with a quadrupole mass spectrometer) we have studied electron interaction (ionization and attachment) of a number of molecules relevant to biology (e.g., nuclear bases such as thymine, cytosine, uracil and substituted uracils, glycine, organic acids etc.) and to atmospheric chemistry. These measurements included the determination of ionization energies, cross sections, kinetic energy released and profuction and decay mechanisms of parent and fragment cations and anions involved. In addition we have carried out corresponding quantum mechanical and classical calculations about the electron and geometric structure of these ions and the cross sections involved.

Slovakia Group

Prof. Peter Lukac Prof. Jan D. Skalny Assoc. Prof. S. Matejcik Dr. Viktor Foltin Peter Cicman Michal Stano Lubomir Holubcik Linda Feketeova Tomas Mikoviny

Berlin Group

Dr. Hassan Abdoul-	Dr. Werner F. Schmidt	Richard Balog
Carime (EPIC)	Judith Langer	Michal Stano
Dr. Tihomir Solomun	Sascha Gohlke	Andrzej Rosa

Our current focus is directed towards probing gas phase biomolecules by low energy electrons (0-10 eV). We have demonstrated that the interaction of slow electrons (< 3eV) with the isolated nucleobases, (NB) Thymine (T), Adenine (A) Cytosine (C) and Guanine (G) leads to effective decomposition of the molecule via dehydrogenation. The reaction proceeds via resonance dissociative electron attachment (DEA) into $(NB-H)^- + H$ (NB = T, A, G, C) at cross-sections comparable to the geometrical cross section of the corresponding nucleobase. Experiments on Thymine deuterated at each of the carbon sites have demonstrated that the hydrogen radical is selectively abstracted from the nitrogen position. We have derived the value for the electron affinity of the N-dehydrogenated radical of Thymine as $EA(T-H)_N = 3.8 \pm 0.3 \text{ eV}$. In nucleic acids the nitrogen sites of the nucleobases connect to the DNA backbone and to the complementary base (in the A-T and C-G pairing). Our observation hence foreshadows significant consequences for the molecular description of genotoxic effects in living cells due to low-energy electrons, which are found to be the most abundant secondary species formed from ionizing radiation.

Paris Group

Dr. Roger Azria (permanent, CNRS) Dr. Daniel Caceres (post-doc since March 1st, 2003, EPIC funds) Dr. Jean-Pierre Gauyacq (permanent, CNRS) Jean-Pierre Guillotin (engineer) Dr. Anne Lafosse (permanent teaching and research position, Université Paris-Sud) Codruta Marinica (PhD student) Dr. Dominique Teillet-Billy (permanent, CNRS)

The monohydride hydrogenated Si(100) system has been studied and the H-Si(111) will be studied in the next future. The experimental work includes the study of energy loss spectra, elastic (reflectivity) and inelastic (vibrational) excitation functions by HREEL spectroscopy and electron stimulated H⁻ desorption. In the next step, the functionalisation (halogenation, oxidization) of silicon substrates and electron induced reactions on these modified surfaces will be studied.

The interaction of an electron with an adsorbed molecule is modified by the environment. Thin insulating layers adsorbed on a metal surface have been considered. A microscopic modelling of the interaction of an electron with atomically thin Ar layers physisorbed on a metal surface has been developed. Their effect on the characteristics of the negative ion resonance of a probe molecule has been studied theoretically. Strong adsorption site effects have been observed for N₂ as probe molecule adsorbed on these layers.

Aarnus Group		
Prof David Field	Dr Jean-Pierre Ziesel	Mr Patrick Cahillane
Dr Nykola C. Jones	Dr Tom Field	Dr Soren Hoffmann
Mr Ingo Struve	Mr Andrew Slattery	Dr Lars Madsen

Low energy electron scattering.

The aim of our work in EPIC is to study the interactions of very low energy electrons with molecules of interest in man-made plasmas, as used in fabrication of microelectronic devices, and in natural plasmas, such as those of the atmosphere of the Earth and in the interstellar medium. We have concentrated recently on the halomethanes CH_xR_{4-x} R=Cl, I, CN. These polar species, which are part of the specified EPIC work programme, show very large cross-sections for scattering at energies below 50 meV (say). The events which lead to large cross-sections are rotationally inelastic scattering, and, in the case of CH_3I , a small contribution from electron attachment to form I⁻. We have also worked on the strongly electron attaching non-polar molecules CCI_4 and SF_6 , also part of the EPIC programme. In addition, we have started investigations on the chiral species D- and L-butan-2-ol.

The data for the CH_xR_{4-x} species have shown some surprising results. Cross-sections for CH_3CI rise to 3060 Å² at 13 meV impact energy, perhaps typical of a molecule with a moderate dipole moment (1.87D). CH_3I shows a scattering cross-section which rises to 4750 Å² at 8 meV impact energy, where the molecule has a slightly smaller dipole of 1.62 D. The

contribution from dissociative attachment is 160 Å² at 8 meV (Kaiserslautern group). CH₃CN, with a dipole moment of 3.92 D, shows a cross-section at 13 meV of 3350 Å², very similar to the much less polar species CH₃Cl. We are presently analysing these results in some detail, including data for backward scattering cross-sections.

Data on SF_6 and CCI_4 have drawn attention to the peculiar quantum behaviour of elastic scattering and chemical reaction (in CCI_4) occurring in superposition. Theoretical expressions developed to describe this have yielded an independent means of estimating attachment cross-sections, providing for the first time a method of measuring these cross-sections without recourse to rate data from swarm and other experiments.

The goal of work on the enantiomers of butan-2-ol is to try and establish whether the low energy scattering properties of these species showed dichroic effects. This is work in progress.

Rome Group

Prof Franco Gianturco Dr Tamio Nishimura Dr Enrico Bodo Dr Isabella Baccarelli Dr Alex Occhigrossi Mr Andrea Grandi Dr Nico Sanna

The activities of the URLS research node have been directed towards two distinct research lines:

A. <u>Positron-Molecule collisions at low energies</u>

The main aim of this work has been the setting up of a realistic computational model for the treatment of near threshold scattering of cold positrons from molecular gases containing polyatomic hydrocarbons, considering the dynamical couplings between the impinging e⁺ and the vibrational degrees of freedom of the target molecules. In particular, the work of the group has been directed at elucidating the possibility that threshold energy positrons could get temporarily bound to vibrationally "hot" gaseous polyatomic targets. The calculations have indeed shown that such species could form metastable virtual states that decay after trapping times longer than the vibrational periods of the modes involved. In some specific cases, like the C₂H₂, C₂H₄ and C₂H₆ systems, the calculations show that highly excited modes could bring the virtual state into the negative energy discrete.

B. <u>Temporary negative ions in molecular gases</u>

The URLS research group has been interested recently in generating from computational studies the structures of metastable precursors of biomolecules that are formed by attachment of low-energy secondary electrons, produced by primary radiation employed for biodegrading processes ("radiation damage" processes). The calculations have looked at the presence of ground state dynamical resonances in both biomolecules like Uracil, Thymine, Guanine and in clusters of carbon atoms like C_{20} , C_{60} and C_8H_8 . The results for biomolecules are the first examples of a nonempirical approach to the calculation of resonant states, resonance widths and resonant wavefunctions for the scattered electron.

Prague Group Prof Petr Carsky Dr Roman Curik

Mr Michal Kovacic Mr Peter Hrusc Mr Peter Papp

We succeeded to extend the discrete momentum representation (DMR) computational method to vibrationally inelastic electron scattering by polyatomic molecules. Originally the method was restricted to elastic scattering. Presently we are close to finish a paper on the vibrationally inelastic electron scattering on propane which will be a joint paper with experimentalists from the University of Colorado. We agreed on another paper with them in which we will study the effect of energy, scattering angle and the direction of the incoming electron on the individual vibrational modes. So far we are using the static-exchange approximation. Students from Bratislava, Hrusc and Papp, work on extension of DMR to also include polarization effects.

UCL Positron Group

Dr Gaetana Laricchia	Dr Marta Szluinska	Ms Cristiana Arcidiacono
Mr Simon Armitage	Ms Dawn Leslie	Dr Akos Kover

We plan to extend our techniques for the investigation of positron induced ionization (including positronium formation and annihilation) to water. Preparatory work is underway. On a longer time scale, we also aim to measure the total cross-section of positronium in collision with water molecules and to examine the methodology for extending to positrons pioneering studies, carried out within the network, of electron interactions with bio-molecules (and to targets consisting of a bio-molecule clustered either with water or simple organic molecules).

Institute of Physics Belgrade Group (joining as an associate member to collaborate in research programme)

(a)

Dr Bratislav Marinkovic - senior researcher Dr Jozo Jureta - senior researcher Dr Dragutin Sevic - researcher Dr Dusan Filipovic - associate prof. at Faculty of Physics, Univ. of Belgrade Aleksandar Milosavljevic - Ph.D. student Sanja Tosic - Ph.D. student Predrag Kolarz - Ph.D. student

Electron energy loss spectroscopy and electron threshold spectroscopy of H2S and H2O molecules. Measuring the concentration of negative air ions, developing the instrumentation.

(b) Gaseous Electronics Laboratory

Prof Dr Zoran PetrovicMs Dragan MaricDr Gordana MalovicMs Nevena PuacDr Aleksandra StrinicMs Olivera SasicDr Jasmina JovanovicMs Alexsandra Stojkovic

Ms Svetlana Zivanov Dr Slobodan Vrhovac Dr Zoran Raspopovic Mr Sasha Dujko Experimental device for measurement of excitation and ionization coefficients. The data may be converted to normalize sets of cross sections especially at higher mean energies. The procedures for swarm analysis of transport data and normalization of cross sections. Data bases for simulation of plasmas: cross section sets including dissociative attachment and ionization cross sections and tested by using the swarm technique.

Monte Carlo codes for simulation of electron transport in Time Of Flight and Steady State Townsend conditions, codes for simulation of transport in rf fields, simulations for complex temporal field transients and in complex spatial structures. Basic semi-analytic transport theory

Momentum Transfer Approximation. Detailed simualtion of swarm - surface interactions.

Experimental device for measurements of the properties of low ressure discharges. Modeling of basic properties of low pressure discharges. Modeling of breakdown in gases, modeling of secondary electron yields in gas breakdown. gas breakdown in complex structures and in microdischarges. Capacitively coupled plasma reactors for treatment of polymer surfaces, plasma etching and treatment of organic materials and biological samples. Modeling of plasmas. Modeling of charging in small nanostructures and development of etching in high aspect ratio structures. Modeling of production of beams of reactive fast neutrals for charging free etching. Studies of adsorption of atomic particles in low pressure discharges by breakdown kinetics. We also have corona and dielectric barrier discharges (with possible applications for air cleaning) and pseudo spark switch. We plan to develop additional drift tube for drift velocity (and possibly diffusion coefficient) measurements and possibly to activate Cavalleri diffusion cell depending on the funds that are available). But these items in the brackets are either not easily associated with the project or depend on the funds to complete the experimental devices.)

First EPIC (Electron and Positron Ion Chemistry) Network Meeting (Febr. 8-9, 2003, Parkside Hotel, Woughton-on-the Green, Milton Keynes, UK)

Report by Professor Loucas G. Christophorou, Academy of Athens, Greece

The first EPIC network group meeting has been a joy to attend. The network has identified and has brought together excellent research groups. The collective membership of the network puts the network at the very top of the field.

The group consists of some of the world's foremost experts currently working on the experimental and theoretical aspects of low-energy electron and positron interactions with matter. This field flourished in the USA for almost have a century and is now rejuvenated in Europe with a new outlook and vigor. It was gratifying to see at this meeting the strong emphasis on creating a European infrastructure in the field appropriate for basic and applied science, science education and training, and advanced technology stretching from nanotechnology and plasma science applications to single molecule engineering, controlled beam technology, and advanced instrumentation. In this regard it was pleasing to see the strong coupling and coordination of the various groups of the network, the extensive collaborations of the various groups, and the efforts being made to bring into this collaboration and field more young scientists.

The presentations at the meeting centered mostly on low-energy electron collision induced processes. Important new experimental data were presented on a number of molecules consistent with the network's planned activity, such as electron interactions with biomolecules and molecules of interest to plasma processing and electron and positron induced processes in the gaseous phase, molecular clusters, and the condensed phase. Foremost among these were the results on negative ion states and reactions both in the gaseous and the condensed phases of matter. These included data on electron scattering, differential electron scattering, attachment, ionization and relative as well as absolute measurements on simple molecules and more complex biomolecules such as Uracil and bases of DNA and RNA. Most interesting were also the new calculations that have been presented on the effect of the medium on negative ion resonances. It was gratifying to see the theoretical progress achieved in understanding these effects since this is an important step in our efforts to link our knowledge in the gas phase to that in the condensed phases of matter. Similarly, most interesting was the theoretical work on dissociative electron attachment and on the electron energy loss processes, especially those due to vibrational excitation, in collisions of low-energy electrons with small molecules. The work reported on positron-molecule interactions aimed at the understanding of positron-induced fragmentation of biomolecules and the differences between positron and electron molecule interactions.

As the activity of the EPIC network progresses, the group may consider emphasizing the following.

Quantitative data on the various processes investigated Experimental and theoretical work on Transient species (radicals)

Energy rich (excited) targets

Physical methods to quantify radiation damage by low-energy electrons

Development of new experimental techniques for fundamental studies in the bio and nano areas

- Review, synthesis, and assessment of knowledge on molecules of recognized generic significance (e.g., H_2O)

Training how to handle DNA and other biomolecules.

I, finally, wish to thank Professor Nigel Mason for the invitation to attend the EPIC meeting and for his hospitality.

EPIC NETWORK MEETING PRAGUE Wednesday 30 JULY 2003

9:00	Nigel Mason	Welcome and introduction
	The Open University	
9:10	Gustavo Garcia	Secondary electron interactions and radiation
	University of Madrid	damage
9:40	Nykola Jones	Low energy electron-molecule scattering experiments
	University of Aarhus	
10:00	Franco Gianturco	Low energy resonances and temporary negative ions
	University of Rome	from electron/positron scattering off polyatomic
		molecules and carbon clusters
10:20	Jimena Gorfinkiel	Progress report: H2O and CFx
	University College London	
10:40	Bobby Antony	Calculation of ionization cross-sections of free
	The Open University	radicals
11:00	Coffee	
11:30	Paul Scheier	Reactions of slow electrons with molecules of
	University of Innsbruck	biological relevance
12:00	Peter Cicman	Dissociative electron attachment to N2O5
	University of Innsbruck	
12:15	Sylwia Ptasinska	Dissociative electron attachment to glycine by low
	University of Innsbruck	energy electron impact
12:30	Sam Eden	Electronic excitation of C ₂ F ₄
	University College London	
12:45	Paulo Limao-Vieira	Environmental impact of SF ₅ CF ₃
	University College London	
1:00	Lunch	
2:30	Daniel Caceres	Electron Induced Reactions on Hydrogenated Silicon
	University of Paris	and Diamond Surfaces
2:45	Anne Lafosse	Electron Interaction with Hydrogenated Si(100) and
	University of Paris	Diamond surfaces: H-
		Desorption and Surface Vibration
3:15	Richard Balog	Surface processing with low energy electrons
0.00	University of Berlin	Other a shareful and the station of DNA because here
3:30	Hassan Abdoul-Carime	Site selective dissociation of DNA bases by
4:00		
4:00	Tea Deter Denn	Development of the Discrete Memoritum
4:30	Acc. Of Sciences, Drague	Development of the Discrete Momentum
4.45	Aca. Of Sciences, Plague	Accessment of the Discrete Memontum
4.40	Acc. Of Sciences, Drague	Assessment of the Discrete Momentum
	Aca. Of Sciences, Prague	
5:00	Simon Armitage	Positronium beam production and scattering
	University College London	
5:15	Marta Szluinska	Positron Induced Ionization Processes
	University College London	
6:00	EMS RECEPTION	
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PUBLICATIONS

UCL Theory Group

- 1. JD Gorfinkiel, LA Morgan and J Tennyson. "Electron impact dissociative excitation of water within the adiabatic nuclei approximation" *J. Phys. B: At. Mol. Opt. Phys.*, 35, 543-555 (2002)
- 2. I Rozum, NJ Mason and J Tennyson. "Electron collisions with the CF2 radical using the R-matrix method" *J. Phys. B: At. Mol. Opt. Phys.*, 35, 1583-1591 (2002).
- 3. A Faure and J Tennyson. "R-matrix calculations for polyatomic molecular ions: electron scattering by H3+ and H3O+" *J. Phys. B: At. Mol. Opt. Phys.,* 35, 1865-1873 (2002).
- 4. CS Trevisan and J Tennyson. "Calculated rates for the electron impact dissociation of molecular hydrogen, deuterium and tritium" *Plasma Phys. Controlled Fusion*, 44, 1263-1276 (2002).
- 5. A Faure and J Tennyson. "Electron-impact rotational excitation of symmetric top molecular ions" *J. Phys. B: At. Mol. Opt. Phys.*, 35, 3945-3956 (2002).
- 6. CS Trevisan and J Tennyson. "Calculated rates for the electron impact dissociation of molecular hydrogen: mixed isotopomers and scaling laws" *Plasma Phys. Controlled Fusion*, 44, 2217-2230 (2002).
- 7. A Faure and J Tennyson. "Rate coefficients for electron-impact rotational excitation of H3+ and H3O+" *Mon. Not. Roy. astr. Soc.*, 340, 468-472 (2003).
- 8. I Rozum, NJ Mason and J Tennyson. "Electron collisions with CF radicals using the R-matrix method" *J. Phys. B: At. Mol. Opt. Phys.*, (in press)
- 9. J Tennyson, JD Gorfinkiel, I Rozum, CS Trevisan and N Vinci. "Electron molecule collisions calculations using the R-matrix method" *Radiation Phys. Chem.*, (in press).
- 10. A Faure, J Gorfinkiel and J Tennyson. "Electron-impact rotational excitation rates for the water molecule" *Mon. Not. Roy. astr. Soc.*, (submitted).

OU/UCL Experimental Group

- 1. S Eden, P Limão-Vieira, N J Mason and S V Hoffmann. "VUV spectroscopy of CF₃Cl, CF₃Br, CH₃I and CH₃Cl" (2003) in preparation.
- 2. S Eden, P Limão-Vieira, N J Mason and S V Hoffmann. "VUV photo-absorption of hexafluoropropene C₃F₆" *Chem. Phys. Lett.* (2003) submitted.

- 3. S Eden, P Limão-Vieira, P Kendall, N J Mason, J Delwiche, M-J Hubin-Franskin, M Kitajima, H Tanaka, H Cho, S Hoffmann and S Spyrou. "Electron excitation of tetrafluoroethylene, C₂F₄" *Chem. Phys. Lett.*, (2003) submitted.
- I C Walker, M H Palmer, J Delwiche, S V Hoffman, P Limão-Vieira, N J Mason, M F Guest, M-J Hubin-Franskin, J Heinesch and A Giuliani. "The electronic states of isoxazole studied by VUV absorption, electron energy-loss spectroscopies and ab initio multi-reference configuration interaction calculations" *J. Chem. Phys.*, (2003) submitted.
- 5. P Limão-Vieira, S Eden, N J Mason and S V Hoffmann. "High resolution VUV photoabsorption of acetaldehyde, CH₃CHO" *Chem. Phys. Lett.* (2003) 376, 737-747.
- 6. A Giuliani, I Walker, J Delwiche, S V Hoffmann, P Limão-Vieira, N J Mason, M-J Hubin-Franskin. "Electronic spectroscopy of fufuryalcohol" *J. Chem. Phys.* (2003) submitted.
- A Giuliani, J Delwiche, S V Hoffmann, P Limão-Vieira, N J Mason, M-J Hubin-Franskin. "2-methylfurane: An experimental study of the excited electronic levels by electron energy loss spectroscopy, UV-VUV photo-absorption spectroscopy" *J. Chem. Phys.* (2003) in press.
- 8. P Limão-Vieira, S Eden, N J Mason. "Absolute photo-absorption cross sections and electronic state spectroscopy of selected fluorinated hydrocarbons relevant to the plasma processing industry" *Radiat. Phys. Chem.* (2003) 68, 187-192.
- P Limão-Vieira, P A Kendall, S Eden, N J Mason, J Heinesch, M-J Hubin-Franskin, J Delwiche, A Giuliani. "Electron and photon induced processes in SF₅CF₃" *Radiat. Phys. Chem.* (2003) 68, 193-197
- 10. P Limão-Vieira, S Eden, P A Kendall, N J Mason, A Giuliani, M-J Hubin-Franskin, J Delwiche and S V Hoffmann. "Electronic excitation and oscillator strength of SF₅CF₃ by high resolution VUV photo-absorption, electron energy loss and He(I) photoelectron spectroscopy" *Chem. Phys. Lett.* (2003) submitted.
- 11. A Pelc, W Sailer, P Limão-Vieira, N J Mason, J Limtrakul, P Scheier, M Probst and T D Märk. "Low energy electron attachment to CH₃CN" Chem. Phys. Lett., (2003) submitted.
- 12. S Eden, P Limão-Vieira, P Kendall, N J Mason, S V Hoffmann, S M Spyrou. "High resolution photo-absorption studies of acrylonitrile, C₂H₃CN, and acetonitrile, CH₃CN" *Eur. Phys. J. D*, (2003) in press.
- 13. S Eden, N J Mason, P Limão-Vieira, M Kitajima, M Okamoto, H Tanaka, D Newnham and S Hoffmann. "Electron and Photon Impact Studies of CF₃I" in *Electron Scattering from Atoms, Nuclei, Molecules and Bulk Matter*, Ed.C T Whelan and N J Mason, Plenum Press, (2003) pp. 33-44.

- 14. P A Kendall, N J Mason, G A Buchanan, G Marston, P Tegeder, A Dawes, S Eden, P Limão-Vieira, D A Newnham. "Temperature dependent high-resolution infrared photoabsorption cross sections of trifluoromethyl sulphur pentafluoride" *Chem. Phys.*, 287 (2003) 137-142.
- 15. N J Mason, P Limão-Vieira, S Eden, P Kendall, S Pathak, A Dawes, J Tennyson, P Tegeder, M Kitajima, M Okamoto, K Sunohara, H Tanaka, H Cho, S Samukawa, S V Hoffmann, D Newnham and S M Spyrou. "VUV and Low Energy Electron Impact Study of Electronic State Spectroscopy of CF₃I" *Int. J. Mass Spectrom.*, 223-224 (2003) 647-660.
- 16. P Limão-Vieira, S Eden, P A Kendall, N J Mason and S V Hoffmann. "High resolution VUV photo-absorption cross-section for dimethylsulphide, (CH₃)₂S" Chem. Phys. Lett., 366 (2002) 343-349.
- 17.P Limão Vieira, S Eden, P A Kendall, N J Mason and S V Hoffmann. "VUV photoabsorption cross section for CCl₂F₂" *Chem. Phys. Lett.*, 364 (2002) 535-541.
- 18. P Limão-Vieira, S Eden, N J Mason, R Balog, C König, I Bald and E Illenberger.
 "Negative ion formation by low electron energy to condensed SF₅CF₃ molecules" 13th Int. Symposium on Electron-Molecule Collisions and Swarms, Prague, Czech Rep. (2003).
- 19. S Eden, P Limão-Vieira, P Kendall, N J Mason, M Kitajima, H Tanaka, H Cho, M-J Hubin-Franskin, J Delwiche and S Hoffmann. "Spectroscopic studies of valence, Rydberg and ionic states of tetrafluoroethylene, C₂F₄" 13th Int. Symposium on Electron-Molecule Collisions and Swarms, Prague, Czech Rep. (2003).
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- P Carsky, R Curik, FA Gianturco, RR Lucchese and M Polasek. "Computing the Exchange Interaction in Electron Scattering from Polyatomic Molecules" *Phys. Rev. A* <u>65</u> (2002) 052713
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- 9. A Occhigrossi and FA Gianturco. "Low-energy positron dynamics in small hydrocarbon gases" *J. Phys. B* <u>36</u> (2003) 1383
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UCL Positron Group

1. G Laricchia, S Armitage, DE Leslie and P Van Reeth. "Positron and positronium interactions with atoms and molecules" *Radiation Physics and Chemistry* (2003) in press

- 2. DE Leslie, S Armitage and G Laricchia. "Positronium Beam Production and Scattering" contributed paper, *Positron03 Workshop*, Denmark
- 3. C Arcidiacono, A Kover and G Laricchia. "Electron ejection from collisions of positrons with helium" contributed paper, *Positron03 Workshop*, Denmark
- 4. M Szluinska and G Laricchia "Ionization processes induced by positrons" contributed paper, *Positron03 Workshop*, Denmark
- 5. M Szluinska, P Van Reeth and G Laricchia. "Empirical scaling of positron- and electron- impact ionization cross-sections" contributed paper, *Positron03 Workshop*, Denmark
- 6. G Laricchia, S Armitage and DE Leslie "Positronium induced collisions" invited paper, *Positron03 Workshop*, Denmark
- 7. A Kover, C Arcidiacono and G Laricchia. "Experiment on positron-atom scattering" invited paper, *Positron03 Workshop*, Denmark
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- 9. S Armitage, DE Leslie, AJ Garner and G Laricchia. "Fragmentation of positronium in collision with He atoms" *Physical Review Letters* **89** (2002) 173402-1
- 10. M Szluinska, P Van Reeth and G Laricchia. "Empirical scaling of positron- and electron-impact ionization cross sections" *J Phys B* **35** (2002) 4059
- 11. G Laricchia, P Van Reeth, M Szluinska and J Moxom. "Total positron-impact ionization and positronium formation from the noble gases" *J Phys B* **35** (2002) 2525
- 12. G Laricchia. "Scattering of positrons and positronium by atoms and molecules" in *"The Physics of Electronic and Atomic Collisions"* (Rinton Press, New York) (2002) 329
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- 14. P Van Reeth, M Szluinska and G Laricchia. "On the normalization of the positronimpact direct ionization cross-section in the noble gases" *Nucl. Instr. Meth. B* 192 (2002) 220
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- 16. M Szluinska, P Van Reeth and G Laricchia. "Energy dependence of the total ionization and positronium formation cross-sections in e+ - Xe collisions" *Nucl. Instr. Meth. B* 192 (2002) 215

17. JW Humberston, P Van Reeth and G Laricchia. "Correlations between cross sections and threshold energies for positronium formation and direct ionization" *Nucl. Instr. Meth. B* **192** (2002) 44

Belgrade Group

AR Milosavljevic, D Sevic and BP Marinkovic "Investigation of transmission of four-element analyzer electron lenses on the apparatus 'UGRA' by simulations in the 'SIMION' program" *Proc. 21st SPIG, Contributed Papers and Abstracts of Invited Lectures, Topical Invited Lectures and Progress Reports, 26-30 August 2002, Soko Banja, Yugoslavia*, Eds. M.K.Radovic and M.S.Jovanovic (Dept. of Physics, Faculty of Sciences and Mathematics, Univ. of Nis) Contributed Paper, p.22-25

PIA Sanchez, P Kolarž, I Periæ, BP Marinkoviæ and DM Filipoviæ "Photonic, electronic and atomic collisions in front of charged metallic tips" *Proc 23rd ICPEAC 2003, Stockholm,* Abstract of Contributed Paper, Th176

Invited Talk at National Conference

P Kolarz, BP Marinkovic, DM Filipovic and A Stamatovic "Instruments for UV radiation measurement" in *Proc. 2nd Symposium "Sun protection - fashion or necessity?"* VMA, Belgrade, 6-7 Jun 2002, CD of Abstracts, Ed. Z.Nidzovic, p.6 (in Serbian)

GRANTS and OTHER NEWS

UCL Theory Group

Dr Alexandre Faure (ex Marie Curie Fellow at UCL) has been awarded a CNRS position in Grenoble. He will continue to collaborate on electron collision processes of astronomical importance and is at present studying electron-water collisions in collaboriation with UCL.

Cynthia Trevisan was awarded her PhD at UCL for a thesis entitled "Near-threshold electron impact dissociation of molecular hydrogen" She is now a post-doc with Ann Orel (UC Davis) and is working on electron collisions with ethylene.

OU/UCL Experimental Group

P Kendall (PhD) Paul Kendall was awarded his PhD in April. The thesis was entitled "Spectroscopic studies of atmospheric molecules related to global warming".

COST Action Physics P9; Radiation damage (RADAM)

Consortia to investigate radiation damage in biomolecules including DNA. The consortia involve physicists, chemists and biologists. The programme will run three years from November 2003.

ESF Network Collisions in Atom Traps (CATS)

A Network that involves over a dozen of Europe's leading cold atom groups to study the interaction of cold atoms to form molecules; the comparison of cold atoms in optical lattices with solid state phenomena and the collisions of cold targets with electrons, photons and ions. The OU research will see the restoration of the cold atom lab and the commencement of studies to form ultracold plasmas (that is superposition of cold ions and meV electrons). A three year programme to start in September.

ESF Programme on Electron Induced Processing (EIPAM)

A major programme to study how electrons may be used to manipulate atoms and molecules on surfaces and induced chemical processing. It will be the first time that the Scanning Tunnel microscopy community and electron physics community will work together in a common programme. This is to last 5 years starting in early 2004.

Innsbruck Group

Dr.Gernot Hanel has received for his PRL on uracil the student award 2003 from the science faculty of the university of Innsbruck.

Prof. Paul Scheier has received for his work the Lichtenstein price 2003 of the University of Innsbruck.

The PRL on electron attachment to uracil (G.Hanel, B.Gstir, S.Denifl, P.Scheier, M.Probst, B.Farizon, M.Farizon, E.Illenberger and T.D.Märk, Electron attachment to uracil: effective destruction at subexcitation energies, Phys.Rev.Letters, 90 (2003)188104, 1-4) has stirred quite some excitement in the scientific and common press, e.g. see the US press article below:

We are pleased to inform you that your article, "Electron Attachment to Uracil: Effective Destruction at Subexcitation Energies", published in Physical Review Letters 90, 188104 (2003), has been selected for the May 15, 2003 issue of the Virtual Journal of Biological Physics Research. The Virtual Journal is an edited compilation of links to articles from participating publishers, covering a focused area of frontier research. You can access the Virtual Journal at <u>http://www.vjbio.org</u>. Thank you for your contribution.

Berlin Group (grants)

Electron Attachment to Excited Molecules (DFG)

Activation of Polymer surfaces by Fluorination (Ministry of Technology / Industrial Support Modification of Molecular films by low energy electrons (DFG)

Aarhus Group (grants)

Electron Induced Processing at the Molecular Level (EIPAM). Funded through the European Science Foundation (ESF)

ESF Network: Collisions of Atoms in Traps (CATS)

EU funded: Cooperation in Science and Technology (COST) "Radiative Damage in Biomelcular Systems"

Funding from the Danish National Science Foundation for running costs over 3 years. Funding from the Danish National Science Foundation for major apparatus requirements. Funding from the Carlsberg Foundation for major apparatus.

Rome Group (grants)

The National Institute of the Physics of Matter (INFM) in Italy has given to the URLS group a computational grant for the support of the modelling research in biomolecules.

Two students have completed their Master Thesis in this area of research during the Academic Year 2002-2003.

UCL Positron Group (grants)

The Engineering and Physical Sciences Research Council project grant "Positron and positronium collisions with atoms and molecules" £418,356; PI G. Laricchia. This proposal was selected for a highlight by EPSRC in Newsline.

The recent work by UCLP on the fragmentation of positronium in collisions with helium atoms (S. Armitage, D.E. Leslie and G. Laricchia Physical Review Letters 89, 2002, 173402-1) has been selected for highlights by the American Institute of Physics/American Physical Society news team in Physics News Update, Physical Review Focus and Physics Today.

Belgrade Group (grants)

One month grant from Franch govermant for Bratislav Marinkovic to stay one month at LCAM (Laboratoire des Collisions Atomiques et Moléculaires) at Orsay, France.