

**Electron and Positron Induced Chemistry
(EPIC)**

EU Network contract no. HPRN-CT-2002-00179

Commencement September 2002 (Funds received December 2002)

Duration 39 months

Period covered by this report: September 2002 to December 2005

Network coordinator:

Professor N J Mason

Dept of Physics and Astronomy

The Open University

Walton Hall

Milton Keynes

MK7 6AA

UNITED KINGDOM

Telephone; 44 1908 655132

Telefax; 44 1908 654192

Email; n.j.mason@open.ac.uk

Network home page: <http://www.isa.au.dk/epic>

Part A: Research Results

A1 Scientific Highlights:

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

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

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

Participating institutions were;

1. Centre of Molecular and Optical Sciences, The Open University, United Kingdom
2. Department of Physics and Astronomy, University College London, United Kingdom
3. Institut für Ionenphysik, Leopold Franzens Universität Innsbruck, Austria
4. Department of Physical Chemistry, Freie Universität Berlin, Germany
5. Department of Chemistry, Università di Roma 'La Sapienza', Università di Roma 'La Sapienza', Italy
6. Department of Physics, University of Aarhus, Denmark
7. J Heyrovsky Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, The Czech Republic.
8. Laboratoire des Collisions Atomiques et Moléculaires Université Paris-Sud, Paris, France

Together with collaborators within:

Department of Physics, Trento University, Italy
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
Department of Physics, Nuovo University of Lisbon

The Network officially started in September 2002 although funds were only received in December 2002 accordingly permission was granted to extend the Network until December 31 2005 Most younger researchers staff were appointed in 2003 and 2004 ensuring that the volume and pace of research accelerated throughout 2004 and 2005 with over journal publications and over 400 conference abstracts etc being generated by members during the Network. The Network proved to be a dynamic entity, rapidly evolving an innovative and unique research programme that has gained international recognition amongst leading scientists in Europe, the USA and Japan. The research programme has led to further funding both National and International, including European COST and ESF Programme funds.

During the course of the Network the scientific direction of the Network shifted with increasing emphasis towards the study of biomolecules a topic which is now regarded as one of the 'hot topics' of modern molecular physics/chemical physics research and one within which the Network has emerged as the International leader. Several partners (UIBK,FUB,ULRS,OU) have produced pioneering results that provide 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. Many papers have been published in internationally leading journals (PRL, J Chem. Phys.) and Network members invited to present their results at several prestigious International meetings. Collaborations with the radiation chemistry community have developed and several new avenues of research opened allowing Network partners to foster new research ties with the clinical community. Indeed such is the rapid development of this research topic that several new research programmes have developed to include ion and photon interactions with biomolecules.

The second highlight concerns the potential of slow electrons to act as a soft tool to control chemical reactions in the condensed phase. By setting the energy of a well defined electron beam to values below 3 eV it has been shown that it is possible to initiate chemistry at very low incident energies - energies less than that predicted to rupture chemical bonds. This low energy chemistry is driven by the process of dissociative electron attachment (DEA). DEA fragments may initiate further chemical reactions. For example in a CH₃Cl/NF₃ cluster F⁻ from NF₃ reacts with CH₃Cl by $F^- + CH_3Cl \rightarrow CH_3F + Cl^-$. An identical process may occur on a multilayer of co-deposited CH₃Cl and NF₃. Cl⁻ desorbs from the film leaving CH₃F so a multilayer may be chemically converted into pure film of another chemical species. Electron reactions can also bind *specific functional groups* to a surface in a controlled way. DEA of acetonitrile $CH_3CN + e^- \rightarrow CH_2CN^- + H$ being used in the functionalization of hydrogenated diamond to attach organic groups to surfaces. Such experiments suggest that it is possible to manipulate molecular reactions on surfaces using low energy electrons, such research has great significance in the nanotechnology area where 'nanoscale lithography' may be induced by electron patterning (perhaps using scanning tunnel microscopes) Such DEA induced processing has been entitled *Electron induced chemical lithography* and is the topic of a European Science Foundation Programme with member of this RTN joining the nanotechnology community and in particular researchers using scanning tunnel microscopes to manipulate chemical reactions on surfaces. A further COST action in this area (to commence in 2007) is currently being evaluated and was ranked as the leading proposal in the Chemistry domain.

A third highlight has been the development of industrial contacts with the Japanese semiconductor industry. The Network's research into electron interactions with halogenated targets relevant to industrial plasmas has received widespread interest amongst the industrial community particularly in Japan. This has led to the organization of an annual meeting entitled EU-Japan Symposium on Plasma Technology. The first was held under the auspices of EPIC in Stockholm in July 2003, the Second in Tokyo, Japan February 2003, the third in Slovakia in January 2005, the Fourth was held in Sendai in Japan in January 2005 and hosted by recently established Japanese Centres of Excellence in Plasma Technology. In 2006 the Fifth meeting will be held in Belgrade Serbia. In 2004 the Japanese Centres founded an International Network of Centres of Excellence in Plasma Technology (COE Plasma) inviting centres from Korea, USA, Germany, France and the Netherlands to join, The EPIC Network was given a special place as a distributed 'Network of Excellence'. The COEs were established with the intention of exchanging staff and students between such centres. It is expected that some of the Young Researchers employed by the Network will take advantage of these exchanges and travel to Japan to conduct further research, their training in the EPIC Network having made them highly suitable personnel for such a programme.

The success of the Network and the demand for other academic laboratories; institutes etc to participate in the research programmed evolving from the EPIC Network has led to EPIC members seeking further funding to build upon EPIC. These applications have met with success. An EU COST Action (Physics P9) on Radiation Damage (RADAM) was awarded

and commenced in November 2003 to study radiation damage at the molecular level (www.isa.au.dk/cost). This five year programme 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. A joint meeting between EPIC and RADAM was held in Lyons 24th to 27th June 2004 <http://costp9-radam.in2p3.fr/index.html> and brought together over 150 researchers. In March 2005 this was followed by an EPIC/COST Training Workshop held in Potsdam Berlin <http://www.radam05.org/> and EPIC and COST RADAM both participated in the International Miller conference on Radiation chemistry held in Nice in September <http://web.cnrs-orleans.fr/~webcbm/miller/index.htm> and the micordosimetry conference held in Venice in November <http://micros05.lnl.infn.it/>. The COST RADAM has to date allowed over 100 short visits (1 to 4 weeks) to be organized between different groups/institutes and laboratories many of which have involved EPIC partners either as hosts or travelling fellows including several of the Younger Researchers supported by EPIC who have thus been able to visit and collaborate with teams not in the EPIC Network.

A major achievement of the EPIC Network has been to demonstrate the ability of electrons (and positrons) to induce chemistry both in the gas phase, in clusters and on surfaces. By combining our knowledge with that of the nanotechnology community we have established new opportunities for electron induced processing. Accordingly we applied for and were awarded an ESF Funded Programme entitled Electron Induced Processing at the Molecular level (EIPAM) <http://www.isa.au.dk/eipam/>. This five year programme brings 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. The Programme commenced in July 2004 and the first meeting was held as part of the 332th Wilhelm and Else Heraeus Seminar, "Processes Driven by Low Energy Electron-Molecule Interactions" 1st-4th September, 2004 at Bad Honnef, Germany. 2002. The Programme supports short visits, conferences and workshops and *Fellowships*. The first EIPAM Fellows were appointed in October 2004 and included several from EPIC partners. In 2005 EIPAM and EPIC annual Meetings were combined into a single meeting held in Viterbo in Italy June 25 to 30 <http://www.isa.au.dk/eipam/>. EIPAM 3 allowed members of the EPIC Network to continue to meet at an annual meetign nad present results arising from research conducted under the RTN and was held in Malta September 16 – 20 2006. Many EPIC younger researchers presented their results at this meeting.

Another aspect of the research conduced under EPIC that was not initially foreseen was the relevance of such research to the cold atom community. Much of the research now developing with cold atoms and molecules involves the interaction of particles including electron-atom and electron-molecule collisions. Therefore members of the EPIC network were approached by members of the cold atom/molecule collision community to discuss areas of mutual interest. An ESF Network entitled 'Collisions in Atom Traps (CATS)' was applied for and granted and will bring members 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 ! This three year programme commenced in October of 2003. In February 2005 a special ESF 'Exploratory Workshop' on ultracold chemistry was held in Mulhouse, France that brought several younger EPIC members together with younger researchers in cold atom/molecules and in April a meeting on ultracold plasmas was held in Gif Sur Yvette Near Paris. These meetings led to the establishment of an ESF Eurocore programme on the Properties of Cold Quantum Matter, *the only one in physical sciences to be so approved*, in 2006.

Conclusions on the EPIC Network: The EPIC Network has more than fulfilled the hopes of its participants in acting as a forum and focus for development of electron and positron research within the European Community. We believe that it has played a key role in fostering a new dynamism and excitement in electron and positron research that has led a renaissance in electron and positron physics is developed with applications exploited from astrophysics to life sciences. The Network has been widely admired outside Europe and acted as a catalyst for similar collaborative projects most notably in Australia, where a 'Centre of Excellence' in electron and positron physics has been established by the Government involving all the major Australian research universities. This Centre has recently signed a formal memorandum of understanding with the major EU groups (including all the EPIC partners) for staff and student exchanges, to begin in 2007

After the end of the network the research community it has engendered will continue to develop its activities not least due to the superb set of younger researchers we have been able to recruit and train, several of which have now received further funding and some permanent academic positions. For the latest news request you view the Network webpage and those of the partners (<http://www.isa.au.dk/epic>) This Network will be updated even after the official end of the Network to report on progress of the research groups and their members.

Difficulties encountered

No major difficulties were encountered. The Network being judged a great success by its participants and by the wider academic research community.

Recruitment was slow for some groups with delays in obtaining the funding from the EC (received only in December 2002) leading to the loss of two young researchers who had in principle agreed to join the network but who took other posts in October 2002 where funds were *immediately* available. This led to a slower than expected start for positron based research at UCL (partner 2) and for partner 5 (ULRS, Rome). However all posts were filled by late 2003 although some staff only started their training in January 2004. This staggered appointment schedule has required some alteration in the order of training courses with the experimental programme being accelerated and theoretical slightly retarded reflecting the appointment of experimental researchers ahead of theoretical appointees. *These difficulties in appointing staff has however led to some groups not being able to match the training months in the period Sept 2002 to August 2005, therefore we requested (and obtained) a formal extension to December 2005 (the date on which funds for the Network were actually received) – this allowed all partners to complete their training and ensure no younger researcher's appointment is curtailed.*

In October 2002 the Network co-coordinator left University College London to take up a new post as Professor of Physics and Director of Research at the Open University. Since the original application involved a joint experimental and theoretical training programme at UCL this required some alteration in the training arrangements between UCL and OU with UCL continuing training in theoretical aspects of the programme and OU undertaking the experimental. For this reason Postdoc appointments were not made until July 2003 (for experiment) and January 2004 (for theory). The two institutes are only an hour travel time apart so the two teams were in weekly contact. Some rearrangement of funds between OU and UCL was necessary to meet these arrangements with the funding for the younger researcher involved in theoretical work being transferred from the OU to UCL

However, the largest 'difficulty' of the network has been its success ! Many other European groups as well as US, Japanese, Australian, Brazilian and Indian groups have requested

observer status to allow them to integrate with the research programme. We have been pleased to welcome them to our meetings (unpaid) and are delighted by the subsequent research that has evolved from these links. The success in obtaining support for two ESF Networks an ESF programme and most recently an ESF Eurocore has shown that the EPIC Network is achieving its stated goal of integrating European research in Electron and Positron Chemistry making Europe the international leader in this area. Our links with Japanese Industry is also a notable achievement. *We therefore thank the EU for their support.*

Younger Researchers Employed by the Network

The development of such a vibrant research community has proven to be ideal for the training of young research scientists. The major goal of EPIC was 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 coming years will provide much of the momentum and creativity of the EU research programme. Training of these younger researchers was organised through a mixture of personal research and a series of training workshops, the first of which was held in the UK in September 2003 dedicated to training researchers in the study of biological systems and included practical courses in DNA extraction and analysis. A Vacuum training course was held in December 2003 and was repeated in December 2004. A theoretical methods workshop was held in Prague February 14 to 18 2005. This meeting was organized by the YRs themselves and provided them with a unique opportunity to discuss the future development of theoretical modeling of electron/positron interactions with molecules. The meeting specifically precluded more senior staff since they may have preconceptions as to which methodology to follow. Two younger researchers from India and Brazil also attend the meeting (funded by non EPIC Funds).

Presentation and communication skills have been developed by their attendance at Network meetings where younger researchers present their work to the Network members and other senior researchers. All younger researchers employed by July 2003 gave presentations at the EPIC network meeting in Prague in July 2003 and again at the Mid-term review meeting in June 2004 in Obergurgl Austria. At the combined EPIC EIPAM Meeting in Viterbo June 2005 all EPIC YRS then employed presented their research orally and in posters, the wider interests of the audience ensured a lively discussion ! The standard of the presentations was uniformly high. In 2006, post the closure of the network, several of the younger scientists presented their work at the EIPAM meeting in Malta.

We are particularly delighted by the success of several of the younger researchers employed by the Network in being appointed to longer term posts that ensures they will be members of the 'EPIC' community for many years to come. Dr N Jones (UAR) has been appointed to a senior research post at the Aarhus Storage Ring Facility commencing October 2004, testimony to the impact she has made during her time there as an EPIC Younger Researcher. Dr Dagmyr Jaksch (nee Mayr) has been employed as a lecturer at the Open University before starting maternity leave from December 2005, she will return initially part-time on November 2006. Dr Zoran Pesic employed in positron physics at UCL is now a research fellow at Institut des Nano Sciences de Paris, Campus Boucicaut, 75015 Paris, France. Dr Simone Taioli has taken up a post-doc position working in Earth Sciences at UCL working with Dr Dario Alfe who is a holder of a EURYI award. Simone is working on calculations of the properties and composition of the centre of the of the earth using density functional methods. Ms Cristiana Arcidiacono at UCL is now preparing her PhD thesis for submission in late 2006. Dr Sylwia Ptasinska (UIBK) submitted her thesis (within the three year period) and graduated in November 2004, employed as an EPIC postdoc in Innsbruck in 2005 in 2006 she

has recently held a Postdoctoral in the University of Sherbrooke Canada before taking up a prestigious three year UK University Research Fellowship at the Open University in the UK in 2007. Dr. Linda Feketove (UIBK) was employed as a postdoc in another partner laboratory (UAR) before taking up a three year post in University of Monash, Australia, with whom network partners signed a formal agreement as part of EU-Australia collaboration. Dr Michal Stano also employed at UIBK returned to Comenius University, Slovakia to continue research as a research fellow before being appointed a Visiting Fellow in the Department of Physics University of Iceland. Dr Hasan Abdoul-Carime employed in FUB has returned to Paris. Mr Tibor Sadlako (FUB) has returned to Poland to continue his predoctoral studies. Dr. Jan Franz employed ULRs Dec. 1st, 2004 to June 31, 2005 now has a three year postdoctoral post with another EPIC Network partner (UCL) to develop a positron scattering code to support EPIC led research. Dr. Slawomir Telega (ULRS Jan 2005 – November 2005) continued his research in the group in Rome for another 9 months. He will carry out further studies on the threshold behaviour of electron and positron beams at low energies. Dr. Kai Willner (ULRS May 2005 – November 2005) intends to continue his research activities at the ULRs Node and will be supported by another research grant. His interests will be on the asymptotic behaviour of phaseshifts in gaseous molecular systems. Dr. L. Gonzalez-Sanchez (ULRS May 2005 – Dec 2005) intends to continue her present research in the same group in Rome for another year and will be supported by another research grant. Joining somewhat late in the programme she had less opportunity to visit other groups or participate in meetings but attended the follow up meetings funded by the EIPAM Programme in 2006 Her work will be focussing on the dynamical study of quantum collisional excitations of OH, OH⁺ and OH⁻ molecular polar targets by collisions at ultralow energies, with the aim of establishing clear propensity rules that could be exploited by experimental studies of the same systems in magneto-optical traps. Within the Prague group Dr Vincent Brems exploited his training skills by joining industry as a computational physicist and modeller. Michal Tarana is now a doctoral student in the Institute of Theoretical Physics, Charles University in Prague. Peter Papp will defend his PhD dissertation shortly and will be postdocing at the Department of Plasma Physics, Comenius University, Bratislava. Dr Daniel Caceres. After 12 and after 6 months as an EPIC post-doc in the Paris research team (UPSO) has been appointed a lecturer at the University Carlos III in Madrid. Dr Damian Pliszka has a permanent teaching position in Poland and continues to develop his EPIC based research through sabbatical and collaborations.

A2 Publications:

Those in italic are publications involving one or more network partners. (Brackets indicate partner numbers collaborating in the work with numbers as listed in A1). Underscore indicates younger member of the network. For further details please see the Network webpage and those of the partners (<http://www.isa.au.dk/epic>)

Partner 1; Open University (2002-2005)

- 1 *Electron and photon induced processes in SF₅CF₃*
P Limão-Vieira, P A Kendall, S Eden, N J Mason, J Heinesch, M-J Hubin-Franskin, J Delwiche and A Giuliani (2003) Radiation Physics and Chemistry 68 193-7 (1,6)
- 2 *Low Energy Electron Attachment to CH₃CN*
A Pelc, P Limao-Vieira, W Sailer, N J Mason, P Scheier, M Probst and T D Mark Chem Phys Lett (2003) (1,3)
- 3 Theoretical total ionization cross sections of CH_x, CF_x SiH_x SiF_x (x =1 – 4) and CCl₄ targets by electron impact
K.N. Joshipura, M. Vinodkumar, B.K. Antony and N.J. Mason
Eur. Phys. J. D **23**, 81-90 (2003)
- 4 Electron Driven Processes; Scientific challenges and technical opportunities
N J Mason (2003) Proceedings of 17th International Conference on the Application of Accelerators in Research and Industry 885-8
- 5 Study of condensed phase molecules and molecular synthesis in astrophysical environments. A Dawes, P Holtom and N J Mason Recent Developments in Chemical Physics 4 (2003) 519-3
- 6 *Dissociative electron attachment to formic acid (HCOOH)*
A Pelc, W Sailer, P Scheier, M Probst, N J Mason, E Illenberger and T D Maerk Chem. Phys Lett 361 277-84 (2002) (1,3,4)
- 7 *Electron attachment to simple organic acids*
A Pelc, W Sailer, P Scheier, N J Mason, E Illenberger and T D Maerk Vacuum 20 (2003) 429-33 (1,3)
- 8 Temperature Dependent high-resolution infrared photoabsorption cross sections of trifluoromethyl sulphur pentafluoride
P A Kendall, N J Mason, G A Buchanan, G Marston, P Tegeder, A Dawes, S Eden, P Limao Vieira and D A Newnham
Chemical Physics **287** 137 – 142 (2003)
- 9 *Low energy electron attachment to formic acid*
A. Pelc, W. Sailer, P. Scheier, N.J. Mason and T.D. Märk
Eur. Phys. J. D 20, 441-444 (2002) (1,3)
- 10 Shrinking Ozone layer; Global Perspectives and Remedial Measures
S K Pathak and N J Mason Resonance Indian Journal of Science Education **7** 71-80 (2002)
- 11 *Corona discharge in gaseous mixtures: Generation of ozone*
JD Skalny, N J Mason and T Mikoviny
Romanian Reports in Physics 54 117- 133 (2002) (1,3)
- 12 *2-methyl furan: An experimental study of the excited electronic levels by electron energy loss spectroscopy, VUV photoabsorption and photoelectron spectroscopy*
A Giuliani, M J Hubin- Franskin, J Delwiche , P Limao Vieira and N J Mason J. Chem. Phys. 119 (2003) 3670 (1,6)
- 13 Inelastic scattering and stopping power for electrons in O₂ and O₃ at intermediate and high energies, 0.3-5 keV
A. Williard, P. A. Kendall, F. Blanco, P. Tegeder, G. García, and N. J. Mason
Chem. Phys. Lett. (2003)

- 14 *The Electronic states of 2-Furanmethanol (Furfuryl alcohol) studied by photon absorption and electron impact spectroscopy.*
A. Giuliani, I. C. Walker, J. Delwiche, S. V. Hoffmann, P. Limão-Vieira, N. J. Mason, B. Heyne, M. Hoebeke and M. -J. Hubin-Franskin
J. Chem. Phys. **119** (2003) 7282. (1,6)
- 15 The Physics of a Thunderstorm B J Mason and N J Mason
Eur J Phys (2003) **24** S99
- 16 *Electron collisions with the CF radical using the R-matrix method*
I Rozum, N J Mason and J Tennyson *J. Phys B* **36** 2419-32 (2003) (1,2)
- 17 *Electron Scattering from Atoms, Molecules, Nuclei and Bulk Matter*
C T Whelan and N J Mason Plenum Press published 2003
- 18 *Electron and Photon impact excitation of CF₃I*
S Eden, P Limao Vieira, N J Mason, M Katijma, M Okomoto, D Newnham and S Hoffmann in *Electron Scattering from Atoms, Molecules, Nuclei and Bulk Matter* ed by C T Whelan and N J Mason Plenum Press 33 - 44 (2003)
- 19 *Electron Energy Loss spectroscopy of Trifluoromethyl Sulphur Pentafluoride*
P A Kendall and N J Mason in *Electron Scattering from Atoms, Molecules, Nuclei and Bulk Matter* ed by C T Whelan and N J Mason
Plenum Press 99-110 (2003)
- 20 *Electron Driven process: Scientific Challenges and Technological opportunities* N J Mason in *Electron Scattering from Atoms, Molecules, Nuclei and Bulk Matter* Ed by C T Whelan and N J Mason
Plenum Press 179-190 (2003)
- 21 *The electronic states of isoxazole studied by VUV absorption, electron energy loss spectroscopies and ab initio multi-reference configuration interaction calculations.* I C Walker, M H Palmer, J Delwiche, S V Hoffman, P LVieira, N J Mason, M F Guest, M J Hubin-Franskin, J Heinsch and A Giuliani *J. Chem. Phys.* (2003) in press
- 22 *Electron Scattering from Ozone. What do we know ?* N J Mason
Physica Scripta (2003) **68** C37-43
- 23 *VUV photoabsorption of hexafluoropropene*
S. Eden and P. Limão-Vieira, S.V. Hoffmann and N. J. Mason
Chem Phys Lett (2003) **379** 170-176 (1,6)
- 24 *Low energy (0-18eV) electron interaction with free and bound SF₃CF₃: Negative ion formation from single molecules, clusters and nanofilms*
R Balog, M Stano, P. Limão-Vieira, C Konig, I Bald, N J Mason and E Ilenberger *J. Chem Phys* (2003) **119** 10396 (1,4)
- 25 *Electronic State spectroscopy of acetaldehyde, CH₃CHO by high resolution VUV photo-absorption*
P Limao Vieira, S Eden, N J Mason and S V Hoffmann
Chem. Phys. Lett **376** 737-47 (2003) (1,6)
- 26 *High resolution photo-absorption studies of acrylonitrile, C₂H₃CN and acetonitrile, CH₃CN* *Electronic State spectroscopy of acetaldehyde, CH₃CHO by high resolution VUV photo-absorption*
S Eden, P Limao Vieira, P Kendall, N J Mason, S V Hoffmann and S M Spyrou
Eur. Phys. J D **26** 201-210 (2003) (1,6)
- 27 *Electron collisions with the CF₃ radical using the R-matrix method*
I Rozum, N J Mason and J Tennyson *New Journal of Physics* (2003) **5** 155 (1,2)
- 28 *Electronic Excitation of Tetrafluoroethylene, C₂F₄*
S. Eden, P. Limão-Vieira¹, Paul Kendall, N. J. Mason, J. Delwiche, M.-J. Hubin-Franskin, M. Kitajima, H. Tanaka, H. Cho and S.V. Hoffmann (2003)
Chem Phys **297** 257-269 (2003) (1,6)

- 29 *Complex study of negative corona discharge in pure carbon dioxide and its mixtures with oxygen.*
T Mikoviny, M Kocan, S Matejcik, N J Mason and J D Skalny
J Phys D (2004) **37** 64-73 (1,3)
- 30 *Ozone generation in a negative corona discharge fed with N₂O and O₂*
J D Skalny, S Matejcik, T Mikoviny, S Eden and N J Mason
J Phys D; Applied Physics (2004) **37** 1052-57 (1,3)
- 31 *An experimental study of SF₅CF₃ by electron energy loss spectroscopy, VUV photo-absorption and photoelectron*
P. Limão-Vieira, S. Eden, P. A. Kendall, N. J. Mason, A. Giuliani, J. Heinesch, M. -J. Hubin-Franskin, J. Delwiche and S. V. Hoffmann
Int J Mass Spec. (2004) **233** 335-41 (1,3)
- 32 *Electron impact ionization studies with aeronomic molecules*
B K Anthony, N J Mason and K Joshipura
International J Mass Spec. (2004) **233** 207-214
- 33 *An analysis of mass spectrometric study of negative ions extracted from negative corona discharge in air.*
Jan D. Skalny, Tomas Mikoviny, Stefan Matejcik, Nigel J. Mason
Int J Mass Spec. (2004) **233** 317-24
34. *R-matrix calculation of low-energy electron collisions with LiH*
B K Antony, N J Mason and J Tennyson *J Phys B* (2004) **37** 1689 - 1697.(1,2)
- 35 *On the valence shell electronic spectroscopy of 2-vinyl furan*
A Giuliani, I C Walker, J Delwiche, S V Hoffman, C Kech, P L Vieira,
N J Mason and M J Hubin-Franskin *J. Chem Phys* (2004) **120** 10972-10982 (1,3)
- 36 *Cross Sections for electron collisions with water molecules*
Y Itikawa and N J Mason *J Chem Phys Ref Data* in press
37. *Sensitization of 5-bromouridien by slow electrons*
H Abdoul-Carime, P Limao-Vieira, S Gohlke, I Petrushko, N J Mason and E Illenberger
Chemical Physics Letters **393** 442-7 (2004)(1,4)
38. *Dissociative Electron Attachment to dinitrogen pentoxide N₂O₅*
P Cicman, G A Buchanan, B Gulejova, J D Skalny, N J Mason, P Scheier
and T D Maerk
J. Chem Phys. **121** 9891-9897 (2004) (1,3)
- 39 *The effect of ozone treatment on the microbial contamination of pork meat measured by detecting the emissions using PTR-MS and by enumeration of microorganisms*
D. Mayr, T. Mikoviny, R. Margesin, F. Schinner, J.D. Skalny, T.DMärk and N. J. Mason
Int J Mass Spec. **239** 209-14 (2004) (1,3)
- 40 *. Cross Sections for electron collisions with water molecules*
Y Itikawa and N J Mason *J. Phys. Chem. Ref. Data* **34** 1-22 (2005)
41. *Electron scattering cross sections for SF₆ and SF₅CF₃ at intermediate and high energies (100-10000 eV)*
P. Limão-Vieira, F. Blanco, J. C. Oller, A. Muñoz, J. M. Pérez, M. Vinodkumar, G. García, and N. J. Mason
Phys Rev A **71** 032720 (2005)
- 42 *A combined experimental and theoretical study on the formation of the aminoacid glycine (NH₂CH₂COOH) and its isomer (CH₃NHCOOH) in extraterrestrial ices*
P D Holtom, C J Bennett, Y Osamura, N J Mason and R I Kaiser
ASTROPHYSICAL JOURNAL **626** 940-952 (2005)
- 43 *Electron stimulated desorption of Cl⁻ from absorbed and condensed Cl₂; Effects of environment and orientation.*

- P Tegeder, R Balog, N J Mason and E Illenberger
Phys Chem Chem Phys 7 685-690 (2005) (1,4)*
- 44 Relaxation processes in a negative corona discharge fed by air, oxygen and carbon dioxide
J Orszagh, J D Skalny and N J Mason
Proceedings of WDS conference (2005)
- 45 Atmospheric Chemistry with Synchrotron Radiation
N J Mason, A Dawes, R Mukerji, E A Drage, E Vasekova, S M Webb, D Jaksch
and P Limão-Vieira *J Phys B* (2005) **38** S893
- 46 FTIR spectroscopy and estimation of the global warming potential of CF₃Br and C₂F₄
E A Drage, E Vasekova, S M Webb, D Jaksch, R McPheat, K Smith and N J Mason
Journal of Quantitative Spectroscopy and Radiative Transfer (2005) in press
- 47 Rotational excitation of molecules by low energy electrons
Yukikazu Itikawa and Nigel Mason *Physics Reports* **414** 1- 41 (2005)
- 48 *Water; VUV electronic state spectroscopy by synchrotron radiation P. Limao-Vieira, Raquel Mota, Rui Parafita, Alexandre Giuliani, Joao Lourenco, Gustavo Garcia, Soeren Hoffmann, Nigel Mason, Paulo Ribeiro, PhD; Maria Raposo
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61. S. Ptasinska, S. Denifl, S. Gohlke, P. Scheier, E. Illenberger, T. Märk, *Fragmentierung von Thymidin durch niederenergetische Elektronen. Implikationen für den Mechanismus von Einzelstrangbrüchen in DNA. Angewandte Chemie* 12/**118** (2006), 1926-1930 (3,4)
62. S. Ptasinska, S. Denifl, P. Scheier, E. Illenberger, T. D. Märk, *Bindungs- und ortsselektive Abspaltung von H-Atomen aus Nucleobasen, induziert durch Elektronen sehr niedriger Energie (<3 eV). Angewandte Chemie* 42/**117** (2006), 7101-7103 (3,4)
63. P. Sulzer, S. Ptasinska, F. Zappa, B. Mielewska, A. R. Milosavljevic, P. Scheier, T. Märk, I. Bald, S. Gohlke, M. Huels, E. Illenberger, *Dissociative electron attachment to furan, tetrahydrofuran, and fructose. The Journal of Chemical Physics* 4/**125** (2006), 044304-6 [PDF](#); [doi:10.1063/1.2222370](https://doi.org/10.1063/1.2222370); IF:3.138; selected for the *Virtual Journal of Biological Physics Research* **12** (2006) issue 3 (3,4)

Conference participations - invited lectures

1. T.D.Märk, Fundamental properties of multiply charged ions, Invited Lecture, Int. Summer School Multiply Charged Ions, Trest, 2003
1. T.D.Märk, Phase transitions in multiply charged ions, Invited Lecture, Int. Summer School Multiply Charged Ions, Trest, 2003
2. S.Denifl, J.Fedor, B.Gstir, G.Hanel, Z.Herman, E.Illenberger, J.Limtrakul, M.lezius, N.J.Mason, S.Matejcik, C.Mair, T.D.Märk, A.Pelc, P.Scheier; W.Sailer, M.Probst, Invited lecture, EMS 2003, Prag, 2003.
3. S.Matt-Leubner, J.Fedor, F.Hagelberg, R.Parajuli, K.Gluch, A.Stamatovic, O.Echt, P.Scheier, T.D.Märk, Invited lecture, Spontaneous decay reactions of molecular or rare gas dimer ions studied by high resolution mass spectrometry, ICPEAC Satellite meeting on e₂e, Frankfurt, 2003

4. T.D.Märk, Invited lecture, Electron interactions with atomic and molecular clusters: excitation, ionization and dissociation, Int. Symp. Atomic Cluster Collisions, St.Petersburg, 2003
5. T.D.Märk, Invited special report, Site selective electron attachment to RNA and DNA bases, XXIII Int. Conf. on photonic, electronic and atomic collisions, Stockholm, 2003
6. T.D.Märk, Invited lecture, Molecular processes, IAEA Atomic and Molecular Data for Fusion Energy Research, Int.Center Theoretical Physics Trieste, 2003.
7. T.D.Märk, Invited lecture, Electron Impact Ionization, IAEA Atomic and Molecular Data for Fusion Energy Research, Int.Center Theoretical Physics Trieste, 2003.
8. S.Denifl, S.Ptasinska, G.Hanel, M.Probst, P.Scheier, T.D.Märk, Invited lecture, Radiation damage in molecules of biological relevance, Asutian-Hungarian workshop on charged – particle transport through nanostructures and solids, Debrecen, 2003.
9. J.Fedor, K.Gluch, R.Parajuli, S.Matt, O.Echt, F.Hagelberg, A.Stamatovic, M.Probst, P.Scheier, T.D.Märk, Invited plenary lecture, Electron interactions with atomic and molecular clusters: excitation, ionization and dissociation, Int. Symposium for Atomic and Surface Physics 2004, Aosta, 2004.
10. P.Scheier, S.Denifl, S.Ptasinska, M.Probst, S.Yoon, T.D.Märk, Dissociative electron attachment to biologically relevant molecules, invited lecture, ECAMP 8, 2004, Rennes
11. S.Ptasinska, S.Denifl, M.Probst, P.Scheier and T.D.Märk, Invited plenary lecture, Inelastic interaction of low energy electrons with molecules of biological relevance: attachment and ionization, 332. WE Heräus Seminar on Processes Driven by Low energy electron molecule interactions, Bad Honnef, 2004
12. S.Denifl, S.Ptasinska, M.Probst, P.Scheier and T.D.Märk, Invited plenary lecture, Low energy electron interaction with biomolecules, XVth MOLEC, Nunspeet, 2004.
13. P.Scheier, S.Ptasinska, S.Denifl, P.Candori, M.Probst, T.D.Märk, Inelastic interaction of low energy electrons with biologically relevant molecules, invited lecture, SPIG, 2004.
14. P.Scheier, S.Ptasinska, S.Denifl, P.Candori, M.Probst, T.D.Märk, Inelastic interaction of low energy electrons with biologically relevant molecules, invited lecture, 1st International COST Conference Radiation damage in biomolcular systems, Lyon 2004.
15. S.Denifl, J.Fedor, K.Gluch, S.Feil, S.Matt-Leubner, A.Stamatovic, F.hagelberg, M.Probst, O.Echt, P.Scheier, T.D.Märk, Experimental and theoretical study of metastable decays of rare gas (Ar,Ne, Kr, Xe and He) cluster ions, invited lecture, Vth Intern. Conf. Ion implantations and other applications of ions and electrons, Kazimierz Dolny, Poland, 2004
16. T.D.Märk, Probing electronic states of rare gas dimer ions by sector field mass spectrometry: achieving spectroscopic accuracy in the determination of potential energy curves, Invited lecture, 6.Igler MS Tage2005 Perspectives in Mass Spectrometry, Igls, 2005.
17. J.Fedor, K.Gluch, R.Parajuli, S.Matt-Leubner, O.Echt, P.Scheier, T.D.Märk, Electron induced metastable decay of diatomic ions: probing electronic states by sector field mass spectrometry to obtain high accuracy potential energy curves, invited lecture, Final EPIC Conference, Roma, 2005
18. P.Scheier, S.Ptasinska, S.Denifl, S.Feil, M.Winkler, B.Mroz, M.Probst, S.Matejcik, E.Illenberger, T.Märk, Destruction of uracil and thymine at subexcitation energies,Invited lecture, AMOP 05, USA, 2005.
19. S.Ptasinska, S.Denifl, V.Grill, F.Rondino, F.Zappa, E.Illenberger, T.D.Märk, P.Scheier, Isotope and site labelling for the identification of resonances in dissociative electron attachment to biomolecules, invited lecture, 52nd Annual Meeting of the Radiation Research Society, Denver, 2005.
20. S.Ptasinska, S.Denifl, V.Grill, F.Zappa, M.Probst, P.Scheier, T.D.Märk, Low energy interactions with complex molecules, Invited plenary lecture, 4th LEEMI on Negative Ions: Experiment and Theory, Smolenice 2005.
21. S.Ptasinska, P.Sulzer, F.Rondino, V.Grill, P.Scheier, D.P.A.Kilgour, T.D.Märk, Explosives detection by low energy electrons, Invited lecture, 4th LEEMI on Negative Ions: Experiment and Theory, Smolenice 2005.
22. S.Feil, L.Feketeova, V.Grill, S.Matt-Leubner, H.Deutsch, K.Becker, M.Probst, P.Scheier, T.D.Märk, Fundamental plasma processes revisited: electron/molecule- and ion/surface-reactions, Invited lecture at Symposium on Plasma Physics and Technology, Praha, 2006.
23. T.D.Märk, Biomolecules, ESF , Obergurgl, 2006.

24. T.D.Märk, Invited lecture, Molecular processes, IAEA Atomic and Molecular Data for Fusion Energy Research, Int.Center Theoretical Physics Trieste, 2006.
25. T.D.Märk, Invited lecture, Electron Impact Ionization, IAEA Atomic and Molecular Data for Fusion Energy Research, Int.Center Theoretical Physics Trieste, 2006.

Conference participations – lectures and/or posters

1. J.Fedor, R.Parajuli, K.Gluch, S.Matt-Leubner, A.Stamatovic, M.Probst, P.Scheier, T.D.Märk, Metastable decay of Rg²⁺ (Rg= Ne, Ar, Kr, Xe): mechanisms, dynamics and energetics, XIV Symp. Applied Plasma Physics (SAPP), Jasna, 2003
2. S.Denifl, S.Matejcik, S.Ptasinska, G.Hanel, B.Gstir, A.Stamatovic, P.Scheier, T.D.Märk, Electron attachment and electron impact ionisation of biomolecules, Jahres-Tagung der deutschen Massenspektrometrie-gesellschaft DGMS, Münster, 2003.
3. K.Gluch, J.Fedor, R.Parajuli, S.Matt-Leubner, A.Stamatovic, O.Echt, P.Scheier, T.D.Märk, Decay of ions studied by three sector field mass spectrometry, Jahres-Tagung der deutschen Massenspektrometrie-gesellschaft DGMS, Münster, 2003.
4. S.Denifl, G.Hanel, S.Ptasinska, B.Gstir, S.Matejcik, A.Stamatovic, P.Scheier, T.D.Märk, Electron impact and attachment studies of biomolecules, 15th Int. Symp. Electron Molecule Collisions and Swarms, Prag, 2003
5. S.Ptasinska, S.Denifl, A.Abedi, P.Scheier and T.D.Märk, Dissociative electron attachment to glycine by low energy electron impact, 15th Int. Symp. Electron Molecule Collisions and Swarms, Prag, 2003
6. S.Ptasinska, S.Denifl, A.Abedi, P.Scheier and T.D.Märk,, Electron attachment to biological relevant molecules, ÖPG Jahrestagung, Salzburg, 2003
7. S.Feil, K.Gluch, S.Matt-Leubner, M.Probst, H.Deutsch, K.Becker, A.Stamatovic, T.D.Märk, Positive and negative ion formation following electron impact on uracil, DAMOP, Tucson, 2004.
8. S.Denifl, S.Ptasinska, P.Scheier, T.D.Märk, Electron impact and attachment studies of DNA and RNA bases, ESF Conference on Molecules of Biological Interest in the Gas Phase, Exeter, 2004
9. S.Ptasinska, S.Denifl, P.Scheier, T.D.Märk, Inelastic electron interaction (attachment/ionization) with sugar molecules and amino acids, ESF Conference on Molecules of Biological Interest in the Gas Phase, Exeter, 2004
10. S.Ptasinska, S.Denifl, P.Limao-Vieira, P.Scheier, T.D.Märk, Damage of sugar molecules by electron impact, 8th European Conference on Atomic and Molecular Physics (ECAMP), Rennes, 2004
11. S.Eden, J.Tabet, F.Gobet, B.Farizon, M.Farizon, M.J.Gaillard, M.Carre, S.Ouaskit, T.D.Märk, Electron-loss and target ionisation cross sections for water vapour by 20-150 keV neutral atomic hydrogen impact, 8th European Conference on Atomic and Molecular Physics (ECAMP), Rennes, 2004
12. J.Tabet, S.Eden, B.Couplier, F.Gobet, B.Farizon, M.Farizon, M.J.Gaillard, M.Carre, S.Ouaskit, P.Scheier, T.D.Märk, Ionisation of water by 20-150 keV protons: separation of direct ionisation and electron capture processes, 8th European Conference on Atomic and Molecular Physics (ECAMP), Rennes, 2004
13. S.Ptasinska, S.Denifl, P.Candori, P.Limao-Vieira, P.Scheier and T.D.Märk, Inelastic electron interaction (attachment/ionization) with sugar molecules and amino acids, ION 2004, Kasimirz Dolny, 2004.
14. S.Feil, K.Gluch, S.Matt-Leubner, P.Scheier, J.Limatrakul, M.Probst, H.Deutsch, K.Becker, A.Stamatovic, T.D.Märk, Absolute partial cross sections for positive and negative ion formation following electron impact on uracil, 332.WE Heräaus Seminar on Processes Driven by low energy electron molecule interactions, Bad Honnef, 2004.
15. S.Ptasinska, S.Denifl, P.Candori, S.Yoon, P.Scheier, E.Illenberger, T.D.Märk, Radiation damage of nucleosides by low energy electrons, 332.WE Heräaus Seminar on Processes Driven by low energy electron molecule interactions, Bad Honnef, 2004.
16. S.Feil, K.Gluch, S.Matt-Leubner, A.Stamatovic, H.Deutsch, M.Probst, P.Scheier, T.D.Märk, Absolute partial and differential electron impact ionization cross sections for hydrocarbons and uracil, 14th Symp. Atomic, Cluster and Surface Physics (SASP 2004), La Thuile, 2004.

17. B.Concina, K.Gluch, S.Matt-Leubner, O.Echt, P.Scheier, T.D.Märk, Fullerene binding energies deduced from evaporation experiments: a more comprehensive study based on both kinetic energy release and metastable fractions, 14th Symp. Atomic, Cluster and Surface Physics (SASP 2004).
18. K.Gluch, S.Matt-Leubner, O.Echt, R.Deng, A.Stamatovic, P.Scheier, T.D.Märk, Kinetic energy release distributions and binding energies deduced from C₂ evaporation for fullerene ions C_n⁺ (with 42<n<90), 14th Symp. Atomic, Cluster and Surface Physics (SASP 2004).
19. S.Ptasinska, P.Candori, S.Denifl, S.Yoon, P.Scheier, T.D.Märk, Electron interactions with nucleosides of DNA and RNA: thymidine and uridine, 1st International COST Conference on Radiation damage in biomolecular systems, Lyon 2004.
20. S.Denifl, J.Fedor, K.Gluch, S.Feil, S.Matt-Leubner, A.Stamatovic, F.Hagelberg, M.Probst, O.Echt, P.Scheier, T.D.Märk, The metastable decays of rare gas cluster ions: Experimental realization and theoretical treatment, Meeting EPIC, Obergurgl 2004.
21. S.Ptasinska, S.Denifl, P.Candori, P.Limao-Vieira, P.Scheier, T.D.Märk, Damage of sugar molecules by electron impact, CMBI Meeting, Vill, 2004.
22. S.Denifl, S.Ptasinska, P.Candori, S.Yoon, P.Scheier, T.D.Märk, Electron interactions with nucleosides: thymidine and uridine, CMBI Meeting, Vill, 2004.
23. J.Fedor, P.Cicman, B.Couplier, S.Pfeil, K.Gluch, P.Scheier, T.D.Märk, Dissociative electron attachment to water, CMBI Meeting, Vill, 2004.
24. S.Feil, K.Gluch, K.Becker, S.Matt-Leubner, P.Scheier, T.D.Märk, Absolute cross sections for positive and negative ion formation following electron impact on uracil, CMBI meeting, Vill, 2004.
25. J.Fedor, K.Gluch, S.Matt-Leubner, O.Echt, F.Hagelberg, A.Wisthaler, T.D.Märk, Dissociation processes in metastable rare gas dimer ions, ICPEAC, 2005.
26. K.Gluch, S.Matt-Leubner, S.Feil, O.Echt, C.Lifshitz, S.Denifl, S.Ptasinska, B.Concina, P.Scheier, T.D.Märk, High resolution measurements of fullerenes and endohedrals, Symposium on Size Selected Clusters, Brand, 2005.
27. J.Fedor, K.Gluch, S.Matt-Leubner, O.Echt, P.Scheier, F.Hagelberg, K.Hansen, J.U.Anderson, T.D.Märk, Decay behaviour of dimer ions: kinetic energy distributions and 1/t law, Symposium on Size Selected Clusters, Brand, 2005.
28. S.Denifl, S.Ptasinska, F.Martinez, K.Gluch, S.Feil, P.Scheier, T.D.Märk, High resolution electron ionization study of helium clusters, Symposium on Size Selected Clusters, Brand, 2005.
29. S.Ptasinska, S.Denifl, V.Grill, E.Illenberger, P.Scheier, T.D.Märk, Radiation damage in biomolecular systems by low energy electrons, EYIC 2005, Gniezno, 2005.
30. P.Sulzer, M.Stano, S.Feil, M.Winkler, S.Ptasinska, V.Grill, F.Zappa, T.D.Märk, P.Scheier, Inelastic interaction of free electrons with gas phase porphyrins, EPIC meeting, Viterbo, 2005.
31. A.Ptasinska, S.Denifl, M.Stano, P.Sulzer, F.Zappa, A.Stamatovic, O.Echt, P.Scheier, T.D.Märk, Free electron attachment to higher order and endohedral fullerenes, EPIC meeting, Viterbo, 2005.
32. F.Zappa, P.Sulzer, B.Mielewska, A.Milosavljevic, S.Ptasinska, S.Denifl, P.Scheier, T.D.Märk, Inelastic electron interaction with sugar molecules, EPIC meeting, Viterbo, 2005.
33. M.Stano, S.Denifl, S.Ptasinska, K.Gluch, S.Feil, P.Scheier, T.D.Märk, Appearance energies for electron impact ionization of helium clusters, EPIC meeting, Viterbo, 2005.
34. A.R.Milosavljevic, P.Sulzer, B.Mielewska, F.Rondino, F.Zappa, B.P.Marinkovic, T.D.Märk, P.Scheier, Inelastic electron interaction (attachment/ionization) with furan and tetrahydrofuran, 4th LEEMI on Negative Ions: Experiment and Theory, Smolenice 2005.

Partner 4: FUB Institut fuer Physikalische und Theoretische Chemie, Freie Universitaet

1. *Dissociative Electron Attachment to Formic Acid (HCOOH)*
Andrzej Pelc, Wolfgang Sailer, Paul Scheier, Michael Probst, Nigel J. Mason, Eugen Illenberger and Tilmann D. Märk *Chem. Phys. Letters* **361** (2002) 277-284.(1,3,4)
2. *Dissociative Electron Attachment Study to Nitromethane*
Wolfgang Sailer, Andrzej Pelc, Stefan Matejcik, Paul Scheier, Eugen Illenberger and

- Tilman D. Märk, J. Chem. Phys.* **117** (2002) 7989-7994.(1,3,4)
3. *Electron Attachment to Simple Organic Acids*
Andrzej Pelc, Wolfgang Sailer, Paul Scheier, Nigel J. Mason, Eugen Illenberger and Tilman D. Märk *Vacuum* **20** (2003) 429-433.(1,3,4)
 4. *Electron Attachment to C₂Cl₄ and Trojan Horse Ionisation* Herwig Drexel, Wolfgang Sailer, Verena Grill, Paul Scheier, Eugen Illenberger and Tilman D. Märk, *J. Chem. Phys.* **118** (2003) 7394-7400.(3,4)
 5. *Electron Attachment to Uracil: Effective Destruction at Subexcitation Energies*
G. Hanel, B. Gstir, P. S. Denifl, P. Scheier, B. Farizon, M. Farizon, E. Illenberger and T. D. Märk *Phys. Rev. Letters* **90** (2003) 188104-1 – 188104-4.(3,4)
 6. *Dissociative energy electron attachment to acetic acid* Wolfgang Sailer, Andrzej Pelc, Michael Probst, Jumras Limtrakul, Paul Scheier, Eugen Illenberger and Tilman D. Märk *Chem. Phys. Letters* **378** (2003) 250-256. (3,4)
 7. Complete chemical transformation of a molecular film by subexcitation electrons
Richard Balog and Eugen Illenberger *Phys. Rev. Letters* **91** (2003) 213201/1 – 213201/4.
 8. Dehydrogenation of Adenine Induced by Slow (< 3 eV) Electrons
Hassan Abdoul-Carime, Sascha Gohlke, and Eugen Illenberger
Chem. Phys. Letters **380** (2003) 595-599.
 9. *Electron attachment to chlorouracil: A comparison between 6-ClU and 5-ClU*
Stephan Denifl, Stefan Matejcik, Sylwia Ptasinska, Bettina Gstir, Michael Probst, Paul Scheier, Eugen Illenberger and Tilman D. Märk *J. Chem. Phys.* **120** (2004) 704-709. (3,4)
 10. Thymine Excision from DNA by Subexcitation Energies
Hassan Abdoul-Carime, Sascha Gohlke, Esther Fischbach, Jessica Scheike and Eugen Illenberger *Chem. Phys. Letters* **387** (2004) 267.
 11. Conversion of Amino Acids by Electrons at Subexcitation Energies
Hassan Abdoul-Carime, Sascha Gohlke and Eugen Illenberger
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Part B

Comparison with the Joint programme of work (ANNEX 1 of the Contract)

B1: Project Objectives

The major objectives of the proposed Network were to:

- (i) Train young researchers in the latest experimental and theoretical techniques for studying electron/positron induced chemistry by providing them with the opportunity to undertake research within internationally renowned research centres.
- (ii) Provide the most co-coordinated study ever undertaken, either experimental or theoretical, of the fundamental chemistry initiated by the irradiation by electrons and positrons of molecules (from diatomic to macromolecules) and
- (iii) To develop a new understanding of the basic processes by which such chemical reactions are induced and how such reactions are modified by their local environment.

In particular the Network aimed;

1. Study fundamental electron and positron energy transfer processes.
2. Study electron and positron impact dissociation processes yielding reactive neutral, anionic and cationic species.
3. Study how such processes are modified in the different phases of matter (gases, clusters and on surfaces).
4. Probe new reaction processes initiated in denser phases of matter (e.g. nucleophilic substitution).

Different molecular compounds have been selected to illustrate these processes in particular the halogenated hydrocarbons and fluorocarbons; simple biomolecules (e.g. the DNA and RNA bases and more recently simple sugars) and water. Excellent progress has been made towards achieving all these objectives

B2 Research method and Work plan

Experimental techniques

Authoritative investigations of electron/positron-molecule interactions requires the adoption of several different experimental methods within this Network all the current state-of-the-art experimental techniques for probing electron/positron induced reactions with molecules were adopted by the researchers in their ongoing studies and were made available to the younger researcher. Furthermore these techniques have been developed making the participants amongst the leading pioneers of techniques for producing sources of biomolecules for example recently UIBK has developed a technique for incorporating biomolecules into cold helium droplets while FUB and UBIK have produced clusters of biomolecules and FUB and OU are studying DNA itself. The UAR group has pioneered the development of the first synchrotron based photo-ionisation electron source, a source that is capable of producing electron beams with resolutions of 2 meV at incident energies as low as 1 meV. With such a source it is possible to study electron impact induced rotational excitation and makes it possible to probe threshold phenomena at the onset of each mode of molecular excitation and has led to the investigation of a new class of scattering processes, named cold collisions with the electrons at temperature comparable to those of cold atoms. Their instrument has now been developed to study such low energy interactions in the condensed phase such that electron induced chemical reactions may be probed.

The UCL team has developed corresponding methods for the investigation of single and multiply charged ionization (with and without positronium formation) including the first near-threshold measurements and the first complete (e,2e) type experiments with positrons.

Techniques for generating positronium beams have also been developed and applied to the study of the interaction of simple atomic and molecular targets. Methods for extending these to more complex targets and probing those interactions that transfer energy directly into the target molecule are currently under development with the appointment of younger members of the research network. This work has been complemented by the development of a new apparatus in Trento Italy (Sub node of URLS) to study high resolution positron-molecule scattering, including measurement of molecular electronic and vibrational excitation.

Experimental teams in Berlin (FUB) and Paris (UPSO) have pioneered the transfer of gaseous phase experimental and theoretical techniques into the study of electron molecule collisions upon surfaces and are recognized as international leaders in this field. Research performed this year through a collaboration of network members has led to a new understanding of state selective dissociation on surfaces with subsequent consequences for site selective chemistry using STM technology. Their collaborative work demonstrating that electron reactions can also bind *specific functional groups* to a surface in a controlled way has received international acclaim. In particular their demonstration that DEA of acetonitrile $\text{CH}_3\text{CN} + e^- \rightarrow \text{CH}_2\text{CN}^- + \text{H}$ can be used in the functionalization of hydrogenated diamond to attach organic groups to surfaces has great significance in the nanotechnology area where 'nanoscale lithography' may be induced by electron patterning.

UPSO and OU have also extended the researcher into a new area – that of astrochemistry, their research exploring pathways by which molecules may form in ices within the Interstellar medium. UPSO have demonstrated electrons induced CO_2 formation in condensed formic and acetic acids in a very wide range of energies (.7 to 20 eV). They have also shown that glycine is readily formed by electron irradiation of condensed mixtures of NH_3 and acetic acid while the OU team has demonstrated glycine formation in co deposited films of methylamine and CO_2 in both cases the glycine was found to be formed in the zwitterionic form.

Theoretical Methods

The UCL team has led the modern development of the R-Matrix method for treating electron interactions with molecules. For diatomic molecules the R-matrix method has been extended to the nuclear coordinate which has allowed for the first time full, *ab initio* non-adiabatic treatments of vibrational excitation and dissociative electron attachment. UCL have recently developed a novel procedure for treating near-threshold electron impact dissociation. In addition the UCL group has recently extended their code to treat polyatomic molecules with the first results for a complex biomolecule (Tetrahydrofuran) being obtained in 2005. This work is complemented by the team in Bonn (sub-node of FUB) who use a similar formalism and who from 2006 will share the code and development with the team in Prague. One of the younger members of the UCL theory group Dr J Gorfinkiel who has been a member of the EPIC network has recently been awarded a lectureship at the Open University and will establish a new research theoretical research group dedicated to electron/molecule scattering, an essential part of this will be collaborations with two other Network partners URLS and ICP. Finally in 2006 the UCL team will commence a new research programme using the R-matrix method to study theoretical interactions of low energy positrons with molecular targets. This work will be aided by employment of a former EPIC YR Dr K Franz.

The group at URLS has provided considerable theoretical support of the experimental programme of the RTN and during the project:

- Successfully established a robust computational model which can treat several vibrational modes for nonlinear polyatomic molecules which become excited by either electron or by positron impact. This approach has been successful in reproducing

partial, state-to-state cross sections that could be compared with the experimental findings.

- Studied the efficiency of attaching slow positrons to molecular targets in the gas phase and to relate the efficiency of such a process with the vibrational energy content of the molecular species in order to explain the enhanced annihilation rates found for polyatomic molecules in terms of their initial vibrational content.
- Set up a general physical and computational model for the study of the patterns for Dissociative Electron Attachment (DEA) observed experimentally for biological systems (e.g. the purine bases appearing along the DNA double helix structures) and which are held responsible for the detachment of several fragments depending on the electron energy and on the specific resonant states being formed.
- Analysed in some detail the efficiency of the rotational/vibrational excitation processes by both electrons and positrons on diatomic molecular gases at collision energies very close to the excitation thresholds or at ultralow collision energies in case of “hot” molecular targets undergoing collisional de-excitation

Thus the network has developed the research methods outlined in the original proposal pioneering several new methodologies such that internationally many of the Network participants have been recognized as international leaders in the field.

B3 Schedule and Milestones

The work plan was set out in terms of three inter-linked scientific strands namely the study of:

- Electron and positron induced reactions in the gaseous phase.
- Reactions in molecular clusters and aggregates and
- Reactions in the condensed phase.

For each of these strands four specific molecular targets have been chosen since these provide the opportunity to determine the reactivity as a function of particular site and/or chemical bond. The targets selected are:

- Halogenated hydrocarbons (CH_xR_y where R is any halogen species F, Cl, Br and I and $x + y = 4$ and the fluorocarbons (CF_xR_y where R is Br, Cl (or H) and $x + y = 4$).
- Simple bio-molecules that form the bases of DNA and RNA (adenine, cytosine, guanine, thymine and uracil) often called the *building blocks of life*.
- WATER, the universal solvent.

By the end of the RTN most of the research aims had been met, indeed in several cases exceeded.

In the original Annex 1 the following milestones were declared

- Year 1:** Advertising/ recruitment of Younger Researchers. Establishment of Network WWW site.
- (Month 1 -6) First Network meeting to determine specific project schedule and identify molecular targets to be studied by each partner laboratory.

(Month 7-12) Experimental research programme on halogenated hydrocarbons and fluorocarbons commenced.

Master class in 'Theory of Molecular dynamics and symmetry' organised by UCL

Master Class in Theoretical Modelling organised by ULRS.

Master class in surface preparation and UHV techniques organised by FUB and UPSO.

Year 2: Master class in preparation and synthesis of bio-molecules organised by UIBK. Workshop on New Chemical synthesis using positrons (arranged in collaboration with International Positron workshop).

Second Network meeting to review progress on research programme (Mid - Term review).

Year 3. Third and concluding Network meeting. Publication of Network results through compilation of a series of review articles

The First Network meeting to determine specific project schedule and identify molecular targets to be studied by each partner laboratory was held at the coordinator's new institution in February 2002. The second Network meeting and mid term review was held at Obergurgl in Austria in June 2004 and the third Network meeting was held (jointly with the ESF EIPAM meeting) in Viterbo Rome in June 2005. A post EPIC meeting is planned at EIPAM 2 in Malta in September 2006.

The Master class in preparation and synthesis of bio-molecules was held in the UK arranged by OU in September 2003. The Master class in 'Theory of Molecular dynamics and symmetry' organised by and Master Class in Theoretical Modelling was delayed due to late appointments of Younger researchers and was held in Prague in February 2005. A master class in surface preparation and UHV techniques has been held twice in December 2003 and December 2004 at the University of Liege with support from Alcatel vacuum Ltd. It is to be repeated in December 2006 since the format and training has been recognized as having a wider generic use for experimental scientists.

1. Electron and positron induced reactions in the gaseous phase

Teams involved: OU, UCL, UIBK, FUB, ULRS, UAR, and ICP

Experimental Programme: The different fragmentation patterns induced by low energy electrons and positrons have been explored many halogenated hydrocarbons and fluorocarbons. The electronic state spectroscopy has been extensively investigated by OU and differential cross sections measured. Yields of both anionic and cationic fragments have been measured together with their kinetic energy by UIBK and FUB. Total electron scattering cross sections have likewise been measured at low energy ($< 1\text{eV}$) by UAR and such cross sections provide a complementary means of determining the probability of a specified molecule to undergo dissociative attachment. This work has attracted the interest of many groups worldwide involved in plasma etching. This has led to the development of strong links with the Japanese semiconductor plasma industry (see above).

The most dramatic progress in the network has been in the study of electron scattering from bio-molecules in particular the DNA bases adenine, cytosine, guanine, thymine and RNA base uracil and most recently the larger biomolecules including glycine, simple sugars and acids. UIBK and FUN have shown that dissociative electron attachment is a dominant process at low electron energies and is both bond (C-H versus C-N) and site selective (N1-H versus N3-

H) in the DNA bases. These pioneering results suggest that may be possible to explore DNA damage at a basic molecular level. Indeed recent work by FUB, OU and UIBK has demonstrated a correlation between electron attachment rates to biomolecules and their carcinogenicity and may be used to suggest new compounds to be adopted in radiation therapy as treatment enhancing sensitizers, e.g. 5-bromouracil. Such pioneering research has led to an active and growing international research community, *one in which the EU is recognised as amongst the most active and leading members.*

We have also started an extensive study of water with completion of a comprehensive review of current state of knowledge of electron interactions with water. This work is seen to be pivotal to future research radiation damage. Recent advances comprise of the assembling an authoritative data review of electron interactions with water(OU) and the conduct of detailed gas phase dissociative electron attachment experiments to water (UIBK/OU). These experiments have been complemented by detailed theoretical calculations (UCL and ULRS) see below.

The research with positrons has developed rapidly in the last year. Detailed measurements of the total ionization cross-section by positron-impact on He have been performed from threshold up to 850eV by the UCL team. The positronium formation cross-section (QPs) for this target has thus been extracted. New results have also been obtained for QPs from CO₂ and H₂O. In the case of CO₂, the present QPs agrees well at high energies with previous determinations but the accord is poor on the position and magnitude of the peak. In the case of H₂O, the UCL have recorded the first QPs and shown that Ps formation in e⁺- H₂O collisions is non-negligible. In particular, at ~2eV above threshold, QPs has been found to be 6 times larger than a previous indirect estimate. However, it is noted that the Ps formation contribution to the total cross-section is significantly lower than in the case of the inert atoms.

The total cross-sections for positron and positronium scattering from H₂O molecules have also been measured for incident energies between 7-417eV and 10-100eV, respectively. The new data for both positrons and positronium display little energy dependence over the energy range investigated. The system has been characterized with respect to its angular acceptance both for positrons and positronium in order to correct the data for forward scattering effects once differential cross-sections become available.

First results have also been obtained for direct ionization cross-sections (both integrated and differential) of H₂O by positron impact. Fragmentation paths have also been identified. These studies have significance for the use of positrons in radiotherapy.

Theoretical Programme: Methodology and general purpose codes, built upon existing codes constructed by teams in the network, have been developed to study fundamental electron interactions with halogenated hydrocarbons and fluorocarbons leading to excitation and dissociation. These have highlighted the different electron attachment processes to the CF_x radicals with CF supporting electron attachment but CF not, the consequences of which are dramatic for design of future industrial semiconductor plasmas. Recently the UCL group has developed their computational code to study larger molecular systems with first results on tetrahydrofuran being presented at the EPIC Network meeting. The UCL group has also reported the first results for electron induced dissociation of the water molecule. ULRS have performed the first calculations on complex biological molecules (glycine) pioneering new methods for probing radiation damage studies at the molecular level. In collaboration with

ICP they have likewise developed methodology to study positron interactions with simple molecular targets, results that are now being tested by experiments performed at UCL.

Task 2. Reactions in clusters and aggregates

Teams: UCLE, ULCP, FUB, UIBK, UPSO

The goals of this research programme are to compare the electron induced reactions in the gas phase with those observed in simple cluster or aggregates and to determine the importance of intra-cluster scattering phenomena (electron transfer between the cluster components) in both primary and secondary chemical reactions. Some initial work in preparing clusters of halogenated hydrocarbons and fluorocarbons to study the role of such reactions as a function of cluster size and chemical composition have been performed by FUB some of which is in collaboration with OU. These studies have shown the dramatic changes to be found when electrons interact with even simplest dimmers. This work is now being extended to pioneering studies of electron attachment to bio-molecules and to targets consisting of a bio-molecule clustered either with water or simple organic molecules (acetic and formic acid dimmers). The ability to trap biomolecular clusters in He droplets has been demonstrated by UIBK and the possibility of forming Watson Crick pairs in mixed nucleoside base clusters is being explored. This experimental research has been complemented by theoretical calculations at ULRS.

Task 3. Reactions in the condensed phase

Teams: OU, UIBK, FUB, UPSO. Electron induced reactions from molecules absorbed upon surfaces have been studied both theoretically and experimentally. In this Network we have undertaken experimental studies on the formation and evolution of negative ion resonances in electron scattering from halogenated hydrocarbons and fluorocarbons absorbed on either metallic or ice surfaces. Dramatic changes in the dissociation pathways have been seen for molecules frozen on a surface compared to the gas phase. Such results suggest that with sufficient understanding it may be possible to perform selective bond breaking chemistry of surfaces using emerging STM technology, hence allowing truly nanoscale chemistry to be undertaken. A collaborative project between FUB and UPSO has demonstrated that electron reactions can also bind *specific functional groups* to a surface in a controlled way. In particular their demonstration that DEA of acetonitrile $\text{CH}_3\text{CN} + e^- \rightarrow \text{CH}_2\text{CN}^- + \text{H}$ can be used in the functionalization of hydrogenated diamond to attach organic groups to surfaces has great significance in the nanotechnology area where 'nanoscale lithography' may be induced by electron patterning.

This exciting prospect has led to the formation of an ESF 5 year Programme starting in 2004 in which.

- Theoretical modelling of these systems will be developed using a new R-matrix method to investigate how the environment influences the molecular inelastic scattering properties i.e. vibrational excitation, electronic excitation and dissociative attachment processes.
- Investigations for extending techniques developed for electron studies to using positrons to probe surfaces are also planned.
- The ability to utilize DEA in STM technology for single molecule engineering on a surface will be investigated.

Network training: A Master class in preparation and synthesis of bio-molecules planned for year 2 was organized by the co-coordinator as part of the new UK National Quantum, Atomic and molecular physics meeting in September 2003 and Master class in UHV techniques was held in December 2003 and was repeated in December 2004. A theoretical methods workshop was held in Prague February 14 to 18 2005. This meeting was organized by the YRs themselves and will provide them with a unique opportunity to discuss the future development of theoretical modeling of electron/positron interactions with molecules. The

meeting specifically precluded more senior staff since they may have preconceptions as to which methodology to follow. Two younger researchers from India and Brazil also attended the meeting (funded by non EPIC Funds).

Those young researchers in post by July 2003 presented their work at formal session of the Network meeting held in Prague on July 30, 2003. All Younger researchers employed by the Network presented their work at the mid-term review in at Obergurgl in June 2004 and at the EPIC/EIPAM meeting in Viterbo Italy, June 25 to 30 2005

In summary we have met and indeed exceeded the scientific and training milestones set for the network.

B4 Organisation and Management

Management Committee. A Management Committee was established at the initial Network Meeting held in the UK in February 2003. The management team is comprised of the leaders of each of the 8 partners and two co-opted members elected by the Network participants (Professor Tennyson from UCL and Professor A Zecca, ULRS). Professor N J Mason chaired the committee. Professor E Illenberger acted as Secretary with special responsibility for ensuring training of the younger members is reviewed. Minutes of the Committee meetings are recorded and are available for scrutiny by the Commission. Each partner nominated a member of their research group as *mentor* for the Young Researchers employed by them in the Network. At the annual meeting all younger researchers were interviewed by a mentor (from a different partner) and questioned as to their progress and upon the training received, these comments were examined by the management committee and where appropriate action taken. We take this opportunity to thank Ms J Welsh and Ms B Harker (Open Univeristy,UK) who provided Secretarial support for the Network.

Research strand leaders. To maintain focus the research programme has been divided into three inter-linked scientific strands each reviewed by task leaders.

Task 1; Electron and positron induced reactions in the gaseous phase

Strand Leader: Experimental Professor D A Field (UAR)

Task 2. Reactions in clusters and aggregates

Strand leader; Professor T Märk, (UIBK)

Task 3. Reactions in the condensed phase

Strand Leader: Dr R Azria (UPSO)

Research teams working on each strand met at least once annually to discuss progress and plan future work. The meetings are chaired by the strand leader. As some strands obviously overlap, joint task meetings were organised as appropriate at the annual meeting. Between meetings informal contacts are maintained by email and through the Network electronic Newsletter (See below).

Annual Scientific Meetings. An annual scientific meeting was held. In July 2003 the first network meeting was held in Prague July 30 to August 1. The first day of the meeting was a closed meeting of the network at which the younger members of the network presented their work. The remainder of the Network meeting reviewed scientific progress in the three strands and held a general discussion allowing new results to be reviewed and new research avenues to be debated. Part of this meeting was held jointly with the Electron molecule and Swarms meeting allowing international colleagues to learn of the Network research programme. This was particularly useful as it has enabled the network to establish research links with US, Australian, Japanese, Indian and Brazilian research groups, making it a catalyst for

international research in electron and positron induced chemistry. The second annual meeting which included the Mid-term review was held at Obergurgl, Austria from June 19th to 22nd June 2004. As well as receiving comments from the Commission representative (which were very supportive) the meeting reviewed the progress of the Network both in research and training. As indicated above progress in both areas had been impressive. External speakers at the meeting commented upon the success of the Network both as a research and co-ordination forum.

The third annual meeting was held jointly with the first ESF EIPAM (Electron Induced Processing At the Molecular level) Programme. All EPIC YRS then employed by the Network presented their research orally and in posters, the wider interests of the audience ensured a lively discussion! The standard of the presentations was uniformly high. Management team meetings were held at the conference.

Other network meetings were held in collaboration with the COST P9 'Radiation damage' meeting in Lyons in June 24-27 2004 and Berlin 16-20 March 2005 (www.isa.au.dk/cost). EPIC members also participated in the International Miller conference on Radiation chemistry held in Nice in September <http://web.cnrs-orleans.fr/~webcbm/miller/index.htm> and the microdosimetry conference held in Venice in November <http://micros05.lnl.infn.it/>. The ESF Network Collisions in Atom Traps (CATS) – Durham UK March 2 - 30 2004 and the ESF Programme Electron Induced Processing of Atoms and Molecules (EIPAM) held as part of the 332th Wilhelm and Else Heraeus Seminar, "Processes Driven by Low Energy Electron-Molecule Interactions" 1st-4th September, 2004 at Bad Honnef, Germany. The network also had a major presence at the Eighth European Conference of Atomic and Molecular Physics (ECAMP) to be held in Rennes, France July 6-10, 2004 and for which N J Mason was the Chairman. EPIC members also participated in the 3rd Conference on the Elementary Processes in Atomic Systems (CEPAS 2005) 31st August-2nd September 2005, Miskolc, Hungary and LEEMI IV - Negative Ions: Experiment and Theory 6th-9th October 2005, Castle Smolenice Slovakia.

Subsequent to the end of the Network the EPIC community was able to meet once more at the EIPAM Meeting held in Valetta, Malta September 16 to 20, 2006 where RTN YRS were able to present results of their work performed in the latter part of the Network. <http://www.isa.au.dk/meetings/eipam06/>.

It should also be noted that the success and rapid development of the research in biomolecules led by this RTN led to the grant from the ESF to host a special meeting in 2006 entitled Biomolecules from Gas Phase Properties to the Actions Relevant to Living Cells Obergurgl, Austria, 24th-29th June. http://www.esf.org/esf_genericpage.php?section=10&language=0&genericpage=2434 This was chaired by two RTN partners (N J Mason (OU) and E Illenberger (FUB)) and attracted over 100 participants including Nobel Laureate Robert Huber.

Cohesion with Less Favoured Regions and Associate members

The Network has sought to make major interaction with the newly joined EU countries with the majority of the young researchers coming from new accession countries. This is to be expected since it is the students from those countries that would require the most training in the new techniques and skills. In addition one node (Prague) is based in Eastern Europe and sub node of Austria is based in Comenius University in Bratislava. We have in addition sought to acquire additional resources to allow members of these communities to attend Network meetings (e.g EPS and ESF funds) in the new Networks discussed above there are representations and partners from most of the Eastern European newly joined EU states.

Active collaborations have been established with groups in Gdansk and Siedlce in Poland and Belgrade in Serbia. One former member of the OU group (Dr P Vieira) has recently been appointed Associate Professor in New university, Lisbon, Portugal and continues to collaborate with several partners (OU,FUB,UAR and UIBK) as well as Professor G Garcia, CSIC, Madrid who has become an affiliate of the OU group.

Connections with industry A major result of the Network has been to develop contacts with the Semiconductor industry in Japan (see discussion above). As a result a series of EU Japan initiatives is in preparation to perform joint research on semiconductor plasmas and nanolithography.

B5 Training

5.1 Appointment of Younger researchers Research positions available under the Network were been widely advertised using electronic media, at conferences and by mail shots to major laboratories. The response was good but many of the applicants were not eligible for EU awards (being from non EU states such as the Former Soviet Union). Some candidates were still completing their PhD no Postdoctoral candidate was allowed to take up the post until they had definitively completed their PhD thesis. We therefore recruited a complete cohort of young researchers but due to the late receipt of the funds several posts were not filled until year 3. The grant was duly extended to December 31 2005 to allow completion of the training programmed.

The following table compares the current status of young researchers (Pre-Doc and Post-Doc) with the plan in the contract.

<i>Participant</i>	<i>Contract deliverable of Young Researchers to be financed by the contract (person- months)</i>			<i>Young Researchers financed by the contract Sept 2005 (person-months)</i>		
	<i>Pre-doc (a)</i>	<i>Post-doc (b)</i>	<i>Total (alb)</i>	<i>Pre-doc (c)</i>	<i>Post-doc (d)</i>	<i>Total (cod)</i>
OU (UCLE)	0	36	36	0	36	36
UCL (UCLP)	0	24	24	27	16.5	43.5
UIBK	36	8	44	42	8	50
FUB	12	18	30	18	24	42
ULRS	0	36	36	8	30	38
UAR	0	24	24	0	24	24
IPC	38	6	44	32	12	44
UPSO	0	30	30	0	30	30
TOTAL	86	182	268	127	180.5	307.5

Notes on recruitment:

1. OU D Mayr from Austria) was appointed from 1/7/2003 to 31/12/2004 to work on the experimental programmed at the OU. She married in 2004 changing her name to D Jaksch. Following completion of her EPIC post she was appointed a temporary lecturer and in December 2005 went on maternity leave. A theoretical postdoc (Dr Simone Taioli) was appointed from 1/1/2004. This post was be shared with UCL as computational facilities are at UCL. The movement of the Co-coordinator from UCL to the OU in October 2002 has necessitated some organizational changes in training between UCL and OU not foreseen when Annex was drawn up since the Co-coordinator was at UCL.
2. UCL. Ms Cristiana Arcidiacono was appointed as a pre-doc 1/9/03 for 24 months and is now completing her thesis. Dr Zoran Pesic appointed post-doc 12/1/2004 16 months is now working as a research fellow at Institut des Nano Sciences de Paris, Campus Boucicaut.

3. UIBK. The Predoc Ms S Ptasinska was appointed from September 2002 and gained her thesis in November 2004, she was subsequently appointed to fulfill the eight month EPIC post at UIBK. Two predocs were appointed on short contracts Michael Stano 21.02.2005 to 20.10.2005 and Michael Cingl 01.10.2005 to 31.12.2005
4. FUB The Postdoc Dr Abdoul-Carime was appointed in January 2003 until October 2004 Mr Tibor Sadlacko was appointed as a predoc from 1/1/2005 to 30/06/2005.
5. URLS. Dr. Jan Franz (Dec. 1st, 2004 to June 31, 2005) Dr. Franz is currently being employed by the University College Node of the same network to carry out similar research (low energy positron-molecule dynamics) Dr. Slawomir Telega visited in 2004 and from Jan 2005 – November 2005) after which he intends to continue his research in the group in Rome for another 9 months Dr. Kai Willner (May 2005 – November 2005)
Dr. Willne continued his research activities at the URLS Node supported by another research grant. Dr. L. Gonzalez-Sanchez (May 2005 – Dec 2005) Dr. Gonzalez intends to continue her present research in the same group in Rome for another year and is supported by another research grant.
6. UAR a Postdoc (Dr Nykola Jones) was in place from 1 September 2002 and was employed for the 24 months ending September 2004, she has now been appointed to a senior post as one facility researcher responsible for the synchrotron facility..
7. ICP appointed Peter Papp (4.11.2002 – 4.5.2003); Peter Hrušć (4.11.2002 – 4.5.2003) Vincent Brems (1.5.2004 -31.10. 2005) Michal Tarana (1.5.2004 -31.12. 2005)
8. UPSO 2 Predoctoral students were appointed in the first year each for 9 months, two new appointments were made in late 2003 and early 2004. The first postdoctoral post was filled in March 2003 for a 12 month period Dr D Caceres who returned for a second period in 2005. Dr D Pliska was then appointed as a postdoc for the remaining 12 months having worked in another node (URLS).

Integration of Young researchers; All the young researchers were provided with detailed description of aims and objectives of the EPIC network upon commencing their studies. Attendance at the network meetings is compulsory and all in post in July 2003 were required to give a presentation of their work by that date. All in post in June 2004 presented their work at the Midterm review and all in post in June 2005 presented their work at the EPIC/EIPAM Meeting Viterbo. Exchange of younger members between the research teams was strongly encouraged and has been enacted by most partners (see joint publications arising from these actions).

5.2 Training; A Master class in preparation and synthesis of bio-molecules planned for year 2 was organized by the coordinator as part of the new UK National Quantum, atomic and molecular physics meeting in September 2003 and Master classes in surface preparation and UHV techniques were held in December 2003 and 2004 while a workshop on ‘Electron scattering theory’ was held in Prague in February 2005. In each partner laboratory the young researchers have been encouraged to make use of the institute’s own training programmers for young researchers. These include career instruction, project management and timekeeping courses. In addition several have made use of specialized language courses to allow them to integrate with the country in which they are undertaking training.

Equal opportunities: 5 of the younger researchers employed under the network were women and have been advised of specialize training courses at their host institutions.

Interdisciplinary Aspects: The nature of the network makes the training necessarily interdisciplinary with aspects of physics, chemistry and biology being employed in the research studies as well as some aspects of technology and computer science and IT.

Factual information on the Young researchers employed on the Network

Host; Open University; United Kingdom

Dr D Mayr/Jaksch: Nationality Austrian; Start date July 2003 End Date December 2004; Employment as Post-doc; Previous contact PhD University of Innsbruck. In 2004 Dr Mayr married and thence became Dr D Jaksch. Maternity leave from November 2005 returning part-time to Open University November 2006

Host; Open University; United Kingdom and University College London

Dr Simone Taoli Nationality Italian; Start date January 2004 End Date July 2005; Employment as Post-doc; NO Previous contact with nodes. Now postdoc in Earth Sciences Department UCL

Host; University College London

Ms Cristiana Arcidiacono Nationality Italian; Start date September 2003 End Date December 2005; Employment as Pre-doc; NO Previous contact with nodes. In 2005 Ms Cristiana Arcidiacono gave the following presentations: "Triply differential ionization cross-sections by positron impact" at the National Workshop on Positron Physics in June 2005 in Belfast, UK; "Positron impact ionization of Water" at EPIC meeting in June 2005 in Viterbo, Italy; "Differential Ionization Studies by Positron Impact" at the international meeting on Low Energy Positron and Positronium Physics in July 2005 in Campinas, Brazil; "Differential Ionization Studies by Positron Impact" at CEPAS in 2005 in Miskolc, Hungary. Cristiana Arcidiacono's poster entitled "Positron impact ionization of Water" won the prize for best poster at LEPPP 2005 in Campinas, Brazil. She is currently writing a number of papers and her PhD thesis.

Dr Zoran Pesic Nationality Serbian; Start date January 2004 End Date May 2005; Employment as Post-doc; NO Previous contact with nodes. Dr Zoran Pesic is now a research fellow at Institut des Nano Sciences de Paris, Campus Boucicaut, 75015 Paris, France.

Host; Free University Berlin

Dr Hassan Abdoul-Carime Nationality French; Start date November 2003 End Date August/September 2005; Employment as Post-doc; NO Previous contact with nodes.

Mr Tibor Sedlacko Nationality Polish; Start January 2005 end June 2005 Employment as predoc. NO Previous contact with nodes Now returned Commenius University to complete PhD

Host; University of Innsbruck

Ms Sylwia Ptasinska Nationality Polish; Start date January 2003 End Date September 2005; Employment as Pre-doc; NO Previous contact with nodes. After being awarded her PhD employed as Postdoc in UIBk ten in Sherbrooke Univeristy Canada. Awarded prestigious UK Research fellowship to be held at Open Univeristy from April 2007

Mr M Stano Nationality Slovak; Start date February 2005 End Date October 2005; Employment as Pre-doc; NO Previous contact with nodes. Completed PhD in Slovakia postdoc in Univeristy of Iceland

Mr M Cingl Nationality Slovak; Start date October 2005 End Date December 2005; Employment as Pre-doc; NO Previous contact with nodes. Completing Phd Studies.

Host: University of Rome

Dr S. Telega Nationality Polish; Start date August 2003 End Date October 2003; returning in 2005 January to November Employment as Post-doc; NO Previous contact with nodes. Continuing as Postdoc in UARS in 2006

Dr Damian Pliszka Nationality Polish; Start date December 2003 End Date December 2004; Employment as Post-doc; NO Previous contact with nodes Then moved to UPSO for a further year. Now has a teaching lecturing post in Poland

Dr Jan Franz Nationality German; Start date December 2004 End Date June 2005; Employment as Post-doc; NO Previous contact with nodes. Now employed as postdoc in UCL

Dr Kai Willner Nationality German; Start date May 2005 End Date November 2005; Employment as Post-doc; NO Previous contact with nodes.

Ms L Gonzalez-Sanchez Nationality Spanish; Start date May 2005 End Date December 2005; Employment as Predoc; NO Previous contact with nodes. Continuing her studies in Rome

Host: University of Aarhus

Dr Nykola Jones Nationality British; Start date September 2002 End Date August 2004; Employment as Post-doc; Previous contact with nodes PhD student UCL. Appointed to University of Aarhus Staff as research officer.

Host: ICP Prague

Peter Papp Nationality Start date November 2002 End Date May 2003; Employment as Post-doc; NO Previous contact with nodes Peter Papp will defend his PhD dissertation shortly and will be postdocing at the Department of Plasma Physics, Comenius University, Bratislava

Peter Hrušč Nationality Slovakian Start date November 2002 End Date May 2003; Employment as Post-doc; NO Previous contact with nodes Peter Hrusc did not finish his PHD studies and left the faculty.

Dr Vincent Brems Nationality German Start date May 2004 End Date December 2005; Employment as Post-doc; NO Previous contact with nodes Now employed in Industry as computer modeller

Michal Tarana Nationality Slovak Start date May 2005 End Date December 2005 employed as predoc in 2005 NO Previous contact with nodes Michal Tarana is now a doctoral student in the Institute of Theoretical Physics, Charles University in Prague,

Host: University of Paris-Sud:

Dr Daniel Caceres Nationality Spanish; Start date March 2003 End Date March 2004; Returned for further six months in 2005 Employment as Post-doc; No Previous contact with nodes. In 2005 he was appointed a lecturer at University Carlos III in Madrid

Dr Damian Pliszka Nationality Polish; Appointed 1 February 2005 til December 31 2005.
He was previously at Trento Italy. Now has a teaching lecturing post in Poland.

Conclusion and thanks

We believe that this RTN on **Electron and Positron Induced Chemistry (EPIC)** has been a major influence in the international research community in electron and positron research. The innovative research developed in the Network has led to the rapid emergence of new field of research in the study of biomolecules and in plasma gases that are relevant to the study of radiation damage and development of the next generation of clean plasma technologies. Furthermore it has clearly established Europe as the leading research community in electron induced chemistry with applications for nanotechnology and surface processing.

However an even more important result of the Network has been the opportunity to develop a unique group of younger researchers who will act as the next generation of researchers in this field. We were fortunate to recruit an exceptional group of talented younger scientists who are already, through their award of permanent posts and fellowships advancing the field and demonstrating that they have the capability to ensure that EPIC based research will continue to be led by Europe in the next decade.

Finally we would like to thank the European Union for the award of this RTN and in particular thank Dr Sergio di Virgilio and Deborah Hall from the European Commission for their assistance in the organization and operation of the programme.

Professor N J Mason

Network co-ordinator