

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

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

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**Network home page: [www.isa.au.dk/epic](http://www.isa.au.dk/epic)**

## Part A: Research Results

### A1 Scientific Highlights;

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 positron interactions with molecules. Its research is broadly divided into two sub-topics based upon the type of molecular targets involved.

1. Studies of interactions with halogenated targets are relevant to industrial plasmas, in particular those used in the semiconductor industry.
2. 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;*

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  
Dept of Physics, Nuovo University of Lisbon

The Network officially started in September 2002 although funds were only received in December 2002 and most network staff were appointed in 2003. With the appointment of Younger researchers the volume and pace of research has greatly accelerated in 2004 with over 300 publications being generated by members of the Network since the commencement of the Network. The Network has shown itself to be a dynamic, rapidly evolving an innovative and unique research programme that has gained international recognition amongst leading scientists in Europe, the USA and Japan.

The study of electron impact with biomolecules has received particular attention with several partners (UIBK, FUB, ULRS, OU) producing 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. Several papers have been published in internationally leading journals (PRL, J Chem. Phys.). Indeed such is the rapid development of this research topic that a new EU Network to investigate interactions with DNA and its

constituent molecules has been submitted under Framework VI 'Interdisciplinary and Inter sectorial Call for Proposals'. This network has widened the participation to ion and photon interactions with biomolecules and establishes partnerships with the clinical community.

The second highlight concerns the potential of slow electrons to act as a soft tool to control a chemical reaction 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. For example the FUB team have shown that the surface of a thin film of 1,2-C<sub>2</sub>F<sub>4</sub>Cl<sub>2</sub> molecules can be completely transformed into molecular chlorine (and byproducts, possibly perfluorinated polymers). The effect of complete transformation is based on both the *selectivity* and particular *energy dependence* of the *initial* step of the reaction which is dissociative electron attachment (DEA) to C<sub>2</sub>F<sub>4</sub>Cl<sub>2</sub> [1-3] and the fact that the initial molecule is efficiently decomposed by subexcitation electrons while the product Cl<sub>2</sub> is virtually unaffected. 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 Microscopes).

### **Developing the Network New EU programmes affiliated to the Network;**

As a result of the establishment of collaborations between Partners and recognition of the success in developing a research strategy in those areas of research covered by EPIC the Network has been able to deepen contacts with other members of the academic community and with several applied/industrial partners. For example the OU team in particular has provided results on several fluorocarbon replacements for the semiconductor industry that have 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 and the third in Slovakia in January 2005. The formation of an International Network of Centres of Excellence in Plasma Technology (COE Plasma) in April 2004 in Nagoya Japan included representation from the EPIC Community and in 2005 the second COE Forum will be held in Germany with EPIC participation. 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 programme evolving from the EPIC Network has led to EPIC members seeking further funding to build upon EPIC, These applications have met with success and. 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](http://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 a joint EPIC/COST Training Workshop will be held at Potsdam Berlin and EPIC and COST RADAM will participate both in the international Miller conference on Radiation chemistry to be held in Nice in September and the microdosimetry conference in Venice in November. The COST RADAM has to date allowed over 50 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 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) 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 it is planned to combine the EIPAM and EPIC annual Meetings at Castel Gondolfo in Italy June 25 to 30.

Another aspect of the research conducted 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 2004 a special ESF 'Exploratory Workshop' on ultracold collisions is to be held in Mulhouse, France that will bring younger EPIC members together with younger researchers in cold atom/molecules

**Conclusions on Status of the EPIC Network;** The EPIC Network has fulfilled 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 year 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.

Thus the network continues to develop its activities not least due to the superb set of younger researchers we have been able to recruit, we are confident that the third (and final) year of the Network will see even greater success and for the latest news request you view the Network webpage and those of the partners (<http://www.isa.au.dk/epic>)

### **Difficulties encountered to date**

No major difficulties have been encountered to date. 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 request a formal extension to December 2005 (the date on which funds for the Network were actually received) – this will allow all partners to complete their training and ensure no younger researcher's appointment is curtailed.*

In October 2002 the Network co-ordinator 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 requires 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 are in weekly contact. Some rearrangement of funds between OU and UCL is also necessary to meet these arrangements.

The largest 'difficulty' of the network to date has been its success ! Many other European groups as well as UC, 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 a collaboration partnership with Japanese government/industry ASET consortia 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. It is an environment in which the young researchers can and do thrive ! We 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 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 coming years will provide much of the momentum and creativity of the EU research programme. Training of these younger researchers has and will require a set of 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 will be repeated in December 2004. A theoretical methods workshop will be held in Prague February 14 to 18 2005 This meeting is 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 precludes more senior staff since they may have preconceptions as to which methodology to follow. Younger researchers from India and Brazil will 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 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. The standard of the presentations was uniformly high.

The first of the EPIC Yrs to complete their training have all proceeded to new posts with Dr N Jones (UAR) being given a senior post at the Aarhus Storage Ring Facility commencing October 2004, testimony of the impact she has made during her time there as an EPIC Younger Researcher. Dr Abdoul Carime (FUB) has applied for a 5 year research position at the Open University which if successful will become a permanent academic post. Ms Sylwia Ptasinska (UIBK) has submitted her thesis (within the three year period) and is expected to graduate in November 2004.

## **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.

### **Partner 1; Open University**

- 1 *Electron and photon induced processes in SF<sub>5</sub>CF<sub>3</sub>*  
*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 CH<sub>3</sub>CN*  
*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<sub>x</sub>, CF<sub>x</sub> SiH<sub>x</sub> SiF<sub>x</sub> (x =1 – 4) and CCl<sub>4</sub> 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) 519-32
- 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*  
J D 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, VUVphotoabsorption 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 O<sub>2</sub> and O<sub>3</sub> 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 CF<sub>3</sub>I*  
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 SF<sub>5</sub>CF<sub>3</sub>: Negative ion formation  
from single molecules, clusters and nanofilms*  
R Balog, M Stano, P. Limão-Vieira, C König, I Bald, N J Mason and E Ilenberger *J. Chem  
Phys* (2003) **119** 10396 (1,4)

- 25 *Electronic State spectroscopy of acetaldehyde, CH<sub>3</sub>CHO 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, C<sub>2</sub>H<sub>3</sub>CN and acetonitrile, CH<sub>3</sub>CN*  
*Electronic State spectroscopy of acetaldehyde, CH<sub>3</sub>CHO 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 CF<sub>3</sub> 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, C<sub>2</sub>F<sub>4</sub>*  
S. Eden, P. Limão-Vieira<sup>1</sup>, 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 N<sub>2</sub>O and O<sub>2</sub>*  
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 SF<sub>5</sub>CF<sub>3</sub> 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 *Electronic State spectroscopy of c-C<sub>4</sub>F<sub>8</sub> and c- C<sub>5</sub>F<sub>8</sub> studied by high resolution VUV photo-absorption*  
E Vasekova, N J Mason, P Limao-Vieira and S V Hoffmann  
*Chem Phys Letters* ( submitted) (1,6)
- 39 *Electron interaction cross sections for CF<sub>3</sub>I, C<sub>2</sub>F<sub>4</sub> and CF<sub>x</sub> (x=1-3) radicals*



*I. Rozum, P. Limão-Vieira, S. Eden, N. J. Mason and J. Tennyson*

*J Chem Phys RefData (1,2,6)*

- 40 Mechanistic studies on the formation of the amino acid glycine in extraterrestrial ices P D Holtom, C J Bennett, Y Osamura, N J Mason and R I Kaiser  
Submitted to Nature(2004)
41. Formation of carbon monoxide and carbon dioxide during 2- 4eV carbon ion irradiation of water ice  
A Dawes, M P Davis, P D Holtom, N J Mason, R W McCullough, I D Williams, R Trassl and R I Kaiser  
Submitted to Icarus (2004)
- 42 . *Dissociative Electron Attachment to dinitrogen pentoxide N<sub>2</sub>O<sub>5</sub>*  
*P Cicman, G A Buchanan, B Gulejova, J D Skalny, N J Mason, P Scheier and T D Maerk*  
*J Chem Phys (2004) Submitted (1,3)*
- 43 Electron Scattering cross Section for SF<sub>6</sub> and SF<sub>5</sub>CF<sub>3</sub> at intermediate and high energies (100 to 1000eV)  
P Limao-Vieira, F Blanco, J C Oller, A Munoz, J M Perez, G Garcia and N J Mason (2004) submitted
- 44 *Electron stimulated desorption of Cl from absorbed and condensed Cl<sub>2</sub>; Effects of environment and orientation.*  
*P Tegeder, R Balog, N J Mason and E Illenberger*  
*PCCP (2004) submitted (1,4)*

## **Partner 2; University College London**

1. *I Rozum, NJ Mason and J Tennyson*  
*Electron collisions with the CF<sub>2</sub> radical using the R-matrix method*  
*J. Phys. B: At. Mol. Opt. Phys., 35, 1583-1591 (2002).(1,2)*
2. 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)*
3. 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)*
4. A Faure and J Tennyson.  
R-matrix calculations for polyatomic molecular ions: electron scattering by H<sub>3</sub><sup>+</sup> and H<sub>3</sub>O<sup>+</sup>  
*J. Phys. B: At. Mol. Opt. Phys., 35, 1865-1873 (2002).*
5. 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).*
6. 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).*
7. 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).*

8. A Faure and J Tennyson.  
Rate coefficients for electron-impact rotational excitation of H<sub>3</sub><sup>+</sup> and H<sub>3</sub>O<sup>+</sup>  
Mon. Not. Roy. astr. Soc., 340, 468-472 (2003).
9. I Rozum, NJ Mason and J Tennyson.  
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10. J Tennyson, JD Gorfinkiel, I Rozum, CS Trevisan and N Vinci.  
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11. A Faure, J Gorfinkiel and J Tennyson.  
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12. Laricchia, S Armitage, DE Leslie and P Van Reeth.  
Positron and positronium interactions with atoms and molecules  
Radiation Physics and Chemistry (2003) in press
13. DE Leslie, S Armitage and G Laricchia.  
Positronium Beam Production and Scattering  
contributed paper, Positron03 Workshop, Denmark
14. C Arcidiacono, A Kover and G Laricchia.  
Electron ejection from collisions of positrons with helium  
contributed paper, Positron03 Workshop, Denmark
15. M Szluinska and G Laricchia  
Ionization processes induced by positrons  
contributed paper, Positron03 Workshop, Denmark
16. M Szluinska, P Van Reeth and G Laricchia.  
Empirical scaling of positron- and electron- impact ionization cross-sections  
contributed paper, Positron03 Workshop, Denmark
17. G Laricchia, S Armitage and DE Leslie  
Positronium induced collisions  
invited paper, Positron03 Workshop, Denmark
18. A Kover, C Arcidiacono and G Laricchia.  
Experiment on positron-atom scattering  
invited paper, Positron03 Workshop, Denmark
19. DE Leslie, S Armitage and G Laricchia.  
Production of collimated positronium from molecular nitrogen  
J Phys B 35 (2002) 4819-4827
20. S Armitage, DE Leslie, AJ Garner and G Laricchia.  
Fragmentation of positronium in collision with He atoms  
Physical Review Letters 89 (2002) 173402-1
21. M Szluinska, P Van Reeth and G Laricchia.  
Empirical scaling of positron- and electron-impact ionization cross sections  
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Total positron-impact ionization and positronium formation from the noble gases  
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Scattering of positrons and positronium by atoms and molecules in  
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1. Evidence for Mode Selectivity in DEA to SF<sub>6</sub> (Bunsentagung Kiel, May)  
Chemistry with Low Energy Electrons, Tag der Chemie, Berlin-Adlershof, June
2. Probing Biomolecules by Low Energy Electrons, Tag der Chemie, Berlin-Adlershof, June
3. Electron Attachment Processes: from Unimolecular Decomposition in Single Molecules to Polymerization Processes in Clusters, Tag der Chemie, Berlin-Adlershof, June
4. Electron Attachment to Selectively Excited Molecules, ICPEAC Stockholm, July
5. Dissociative Electron Attachment to H<sub>2</sub>O<sub>2</sub>, ICPEAC Stockholm, July  
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2. G.P. Karwasz, R.S. Brusa, A. Zecca - Positron Spectroscopy in Atomic and Solid State Physics, 4th FAMO Workshop on Atomic & Molecular Physics and Optics, Jurata, 19-21 September 2002, The International Society for Optical Engineering Conference Proceedings, Volume 5258, p. 96
3. G.P. Karwasz, Z.Lj. Petrović and J. Mechlińska-Drewko, Electron diffusion coefficients in triatomic gases – measurements and models  
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### **Partner 7: IPC Heyrovsky Institute of Physical Chemistry, Academy of Sciences of the Czech Republic**

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4. R Curik.  
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**Partner 8 UPSO Laboratoire des Collisions Atomiques et Moléculaires Université Paris-Sud, Orsay, France**

1. Electron H/Si(100) interaction : H- desorption and surface vibrations  
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12. A.Laikhtman, A. Lafosse, Y. Le Coat, R. Azria, A. Hoffman Low energy electron scattering from H-Si(100)-2x1 : reflectivity and vibrational excitation To be submitted to *Surf. Sci.*
13. C.D. Marinica, J.P. Gauyacq, D. Teillet-Billy Inelastic electron scattering on a molecule embedded in a host medium: role of the electronic structure of the medium To be published
14. C.D. Marinica, C. Ramseyer, D. Teillet-Billy, J.P. Gauyacq Adsorbed molecule on a metal surface covered with a rare gas Ar monolayer : adsorption site effect on the  $N_2^- 2\Pi_g$  resonance To be published

For further details please see the Network webpage and those of the partners  
(<http://www.isa.au.dk/epic>)

## Part B

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

#### B1: Project Objectives

The major objectives of the proposed Network are 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-ordinated 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 will;

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; halogenated hydrocarbons and fluorocarbons; simple biomolecules (e.g. DNA and RNA bases) and water.

These objectives remain unchanged after the first year and excellent progress has been made towards achieving 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 are available to the researchers. In the first year of the Network these techniques have been developed still further making the participants amongst the leading pioneers of techniques or producing sources of biomolecules and ongoing work (led by younger researchers employed by the Network) is leading to the study of DNA itself with high resolution electron scattering apparatus (OU, FUB and UIBK) and the development of new techniques for probing DNA including use of Atomic Force Microscopy - AFM (OU and UAR). 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 .

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.

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 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. In contrast the study of positron interactions in the condensed phase under single collision conditions has yet to be explored and this network is providing the first opportunity for developing techniques (both experimental and theoretical) to initiate such studies.

### **Theoretical Methods**

The UCL team have 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. This work is complemented by the team in Bonn (sub-node of FUB) who use a similar formalism. URLS have long employed methods based on single centre expansions to study electron interactions with polyatomic molecules. Such calculations may be used to study larger molecules still beyond the scope of the R-matrix method (e.g. biomolecules). Furthermore URLS have considerable experience of performing vibrational and rotational excitation calculations on polyatomics. UCL and URLS are collaborating in studies to provide cross sections for those targets for which experiments remain too difficult (eg radicals). The transfer of electron scattering methodologies from the gaseous phase to the treatment of inelastic electron scattering on molecules physisorbed on metal surfaces has been pioneered by the UPSO team.

The group at URLS have developed several dedicated scattering codes for treating the quantum dynamics of low-energy positron beams in a molecular gas, specifically one containing polyatomic molecules. These codes are now shared and have developed jointly with younger network members employed by ICP. This Network therefore contains the only research teams currently able to evaluate annihilation rates in polyatomic gases and who are able to evaluate total and differential elastic cross sections below the Ps formation threshold.

*Thus the network has developed the research methods outlined in the original proposal with significant progress being made in the first year, progress that is expected to be accelerated still further in year 2 as younger members complete their initial training.*

### B3 Schedule and Milestones

The work plan is 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.

#### 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).

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.

At this meeting it was agreed to continue to organise the research of this Network in this manner. 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 ( $\text{CH}_x\text{R}_y$  where R is any halogen species F, Cl, Br and I and  $x + y = 4$  and the fluorocarbons ( $\text{CF}_x\text{R}_y$  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.

In the course of 2003 and 2004 most if not all of the research aims have been met. The Master class in preparation and synthesis of bio-molecules was held in the UK arranged by OU in September 2003. 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 is to be held in Prague in February 2005. Master class in surface preparation and UHV techniques has been held twice in December 2003 and December 2004.

## **1. Electron and positron induced reactions in the gaseous phase**

**Teams involved :OU, UCL, UIBK, FUB, ULRS, UAR, 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 be 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 Japanese industry ,

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. This work has dramatic consequences for our understanding of radiation damage and has attracted worldwide attention in international media.

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.

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  $\text{CF}_x$  radicals with CF supporting electron attachment but CF not, the consequences of which are dramatic for design of future industrial semiconductor plasmas. The UCL group have also reported the first results for electron induced dissociation of the water molecule. ULRS have performed the first calculations on complex biological molecules (glycerine) 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 to be 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. The 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 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. 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 is also planned.

### **Network training:**

A Master class in preparation and synthesis of bio-molecules planned for year 2 was organized by the co-ordinator 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 will be repeated in December 2004. A theoretical methods workshop will be held in Prague February 14 to 18 2005 This meeting is 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 precludes more senior staff since they may have preconceptions as to which methodology to follow. Younger researchers from India and Brazil will also attend 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. Annual presentations by younger researchers are an essential requirement for their training in communication and presentation skills and they will be expected to give update talks at the next Annual meeting in Castelgondolfo June 25 to 30 2005.

*In summary we have met and exceeded the scientific milestones set for the second year of 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 chairs the committee. Professor E Illenberger acts 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 nominates 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 will be interviewed by a mentor (from a different partner) and questioned as to their progress and upon the training received, these comments will be examined by the management committee and where appropriate action taken. In order to have an unbiased review of the research and training of the Network the Management Committee invited Professor Loucas Christophorou to act as external assessor of the Network. Professor Christophorou is an internationally acclaimed researcher who having spent many years in the USA as a leader of the electron scattering community has recently returned to Europe to the National Academy in Athens. His reports on the Initial Network meeting and first annual meeting are available in the meeting minutes.

**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 (UPS0)

Research teams working on each strand meet 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 will be 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 is 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 were impressive. External speakers at the meeting commented upon the success of the Network both as a research and co-ordination forum.

Other network meetings were held in collaboration with the COST P9 'Radiation damage' meeting in Lyons in June 24-27 2004, 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.

**Network Newsletter and Communications.** Communications between the Network is enhanced through a Newsletter. This is circulated electronically and will include updated reports by each of the partners (and their sub nodes), abstracts of papers submitted for publication, meeting information and reports, adverts for postdoctoral positions, news of visits between nodes and a monthly review of latest international research papers in the electron/positron induced chemistry scattering (drawn from Web of science database). An abbreviated version of the Newsletter will be available for to all international researchers upon registration with the Network. The Newsletter is placed on the Network's WWW site which will also include full details of the partners their research interests, ongoing research, personal profiles etc. Interim reports and pre-prints of publications will be available electronically from the Network web pages. [www.isa.au.dk/epic](http://www.isa.au.dk/epic)

#### **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 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

Recruitment: Research positions available under the Network were 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). However by January 2003 all the partners had filled their posts. Some candidates were still completing their PhD and therefore did not join their partners until later in the year or at the beginning of year 2. No Postdoctoral candidate was allowed to take up the post until they had definitively completed their PhD thesis. We therefore have a complete cohort of young researchers in post in year 2. However due to the late start of some posts we have postponed some of the training courses planned in year 1 year 2.

The following table compares the current status of young researchers (Pre-Doc and Post-Doc) as of June 2002 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 2004 (person-months)</i>		
	<i>Pre-doc (a)</i>	<i>Post-doc (b)</i>	<i>Total (a+b)</i>	<i>Pre-doc (c)</i>	<i>Post-doc (d)</i>	<i>Total (c+d)</i>
OU (UCLE)	0	36	36	0	28	28
UCL (UCLP)	0	24	24	15	8	23
UIBK	36	8	44	24	0	24
FUB	12	18	30	12	18	18
ULRS	0	36	36	0	11	11
UAR	0	24	24	0	24	24
IPC	38	6	44	26	0	26
UPSO	0	30	30	0	14	14
<b>TOTAL</b>	86	182	268	67	84	151

Notes on recruitment:

1. OU A Postdoc has been appointed (D Mayr from Austria) from 1/7/2003 to work on experimental programme at the OU. A theoretical postdoc (Dr Simone Taioli) has been appointed from 1/1/2004. This post will be shared with UCL as computational facilities are at UCL. The movement of the Co-ordinator from UCL to the OU in October 2002 has necessitated some organisational changes in training between UCL and OU not foreseen when Annex was drawn up since the Co-ordinator was at UCL. All months now allocated
2. UCL. Ms Cristiana Arcidiacono pre-doc 1/9/03 24 months (appointed after node experienced difficulties finding an eligible post-doc). Dr Zoran Pesic post-doc 12/1/2004 16 months.

3. UIBK. The Predoc (Ms **S Ptasinska** was appointed from September 2002) An eight month postdoc is being appointed.
4. FUB The Postdoc Dr Abdoul-Carime was appointed in January 2003 and has recently completed his post which was extened to 20.5 months and he is now applying to the OU for a Research fellowship which if successful will become a permanent appointment. . Mr Sedlack from Slovakia has been appointed a Predoc for 7 months
5. ULRS This node was the slowest to recruit its young researchers due to loss of candidate in 2002 following late transfer of funds form EU in fall of 2002. Dr S.Telega (from Poland) was in Rome for three months during 2003 and has returned in 2004. Dr Damian Pliszka (from Poland) has been in post since December 2003. Dr. Jan Franz (from Germany) will spend six months in Rome from Sept 2004 till April 2005. Dr Kai Willner (from France) will come in 2005 *All months now allocated*
6. UAR a Postdoc (Dr Nykola Jones) was in place from 1 September 2002 and was employed for the 24 months ending September, she has now been appointed to a senior post as one facility researcher responsible for the synchrotron facility..
7. ICP have appointed Peter Papp ( 4.11.2002 – 4.5.2003); Peter Hrušč (4.11.2002 – 4.5.2003) Vincent Brems (1.5.2004 -31.10. 2004) and Barbara Pezler (1.5.2004- 31.10. 2004) Barabara was subsequently found to be ineligible on grounds of age and a replacement is being dought.
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 will return for a 12 month second period

Integration of Young researchers: All the young researchers are 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 will present their work at the Midterm review. Exchange of younger members between the research teams is recommended and has been enacted by most partners in year 1 ( se joint publications arising from these actions) with the expectation of more intense exchanges in year 2 and 3 as the younger have become more active

**5.2 Training:** A Master class in preparation and synthesis of bio-molecules planned for year 2 was organized by the co-ordinator as part of the new UK National Quantum, atomic and molecular physics meeting in September 2003 and Master class in surface preparation and UHV techniques will be held in December 2003 while Master class in ‘Theory of Molecular dynamics and symmetry’ is now planned for later in 2004 (delayed until appointment of young theoretical researchers some of whom did not start until January 2004). 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 this was a essential requirement for their training in communication and presentation skills. In each partner laboratory the young researchers have been encouraged to make use of the institutes’s own training programmes 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: 4 of the younger researchers employed to date under the network are 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**

Host; Open University; United Kingdom

**Dr D Mayr** : Nationality Austrian; Age at appointment 27; Start date July 2003 End Date December 2004; Employment as Post-doc; Previous contact PhD University of Innsbruck

Host; Open University; United Kingdom and University College London

**Dr Simone Taoli** Nationality Italian; Age at appointment 30; Start date January 2004 End Date July 2005; Employment as Post-doc; NO Previous contact with nodes

Host; University College London

**Ms Cristiana Arcidiacono** Nationality Italian; Age at appointment 27; Start date September 2003 End Date December 2005; Employment as Pre-doc; NO Previous contact with nodes

**Dr Zoran Pesic** Nationality Serbian; Age at appointment 33; Start date January 2004 End Date May 2005; Employment as Post-doc; NO Previous contact with nodes

Host; Free University Berlin

**Dr Hassan Abdoul-Carime** Nationality French; Age at appointment 35; Start date November 2003 End Date August/September 2005; Employment as Post-doc; NO Previous contact with nodes.

Host; University of Innsbruck

**Ms Sylwia Ptasinska** Nationality Polish; Age at appointment 35; Start date January 2003 End Date August/September 2005; Employment as Pre-doc; NO Previous contact with nodes.

Host; University of Rome

**Dr S.Telega** Nationality Polish; Age at appointment 33; Start date August 2003 End Date October 2003; returning in 2004 Employment as Post-doc; NO Previous contact with nodes

**Dr Damian Pliszka** Nationality Polish; Age at appointment 31; Start date December 2003 End Date December 2004; Employment as Post-doc; NO Previous contact with nodes

Host; University of Aarhus

**Dr Nykola Jones** Nationality British; Age at appointment 25; Start date September 2002 End Date August 2004; Employment as Post-doc; Previous contact with nodes PhD student UCL.

Host; ICP Prague

**Peter Papp** Nationality ; Age at appointment ; Start date November 2002 End Date May 2003; Employment as Post-doc; NO Previous contact with nodes

**Peter Hrušč** Nationality Slovakian Age at appointment ; Start date November 2002 End Date May 2003; Employment as Post-doc; NO Previous contact with nodes

**Dr Vincent Brems** Nationality German Age at appointment ; Start date may 2004 End Date October 2004; Employment as Post-doc; NO Previous contact with nodes

**Barbara Pezler** Nationality Polish Age at appointment 39; Start date May 2004 End Date October 2004; Employment as Post-doc; NO Previous contact with other nodes

Host: University of Paris-Sud:

**Dr Daniel Caceres** Nationality Spanish Age at appointment 30; Start date March 2003 End Date March 2004; Employment as Post-doc; NO Previous contact with nodes.