

**MINUTES OF THE 7th MEETING OF THE RTN NETWORK  
ON "REACTIVE INTERMEDIATES"**

**(held in Saint Lambert des Bois, France, from 3 - 7  
September 2003)**

This meeting was organized by the Orsay group and was held at Centre Port Royal, in Saint Lambert des Bois near Orsay, from 3 -7 September 2003. The list of representatives from each research group participating in the Network, and attending the Business and Scientific meetings, was as follows (YRs supported by the Network are shown in bold):

John Dyke (Co-ordinator) from Southampton, Kees de Lange (Network Manager) and Wim Ubachs from Amsterdam, Dolores Gauyacq from Orsay, Maria Lourdes Costa from Lisbon, Vladimir Bondybey and Martin Beyer from Garching, Theofanis Kitsopoulos from Crete, Peter Watts and Andrew Bell from Porton Down and Gökhan Baykut from Bruker-Daltonics.

The following Young Researchers (YRs) and guests were also present at this Meeting:

**Giacomo Levita** from Southampton (the other two YRs from Southampton, **Lucia Zuin** and **Fabrizio Innocenti**, were unfortunately unable to attend as they had synchrotron time at Trieste and were doing experiments there during the time of the meeting), **Urs Hollenstein** and **Josselin Phillip** from Amsterdam, **Vassilios Dracopoulos**, K. Alnama and C. Crepin-Gilbert from Orsay, **Romeo-Olariu** from Lisbon, David Mitchell from Porton Down, **Marcin Frankowski**, **Iulia Balteanu**, and **Petru Balaj** from Garching, and **Rachel Toomes** from Crete.

The speakers invited to this meeting to give keynote lectures were the following:- Jean-Michel Launay from the University of Rennes, Anne Zehnacker and Christian Alcaraz from CNRS, Orsay, and Séverine Boyé from the University of Orsay. They also attended all the Scientific sessions held during the meeting and participated in the discussions.

After arrival on Wednesday, September 3rd, the participants met for an informal dinner, at Centre Port Royal, where the participants stayed for the meeting. According to the schedule, Thursday, September 4th, was dedicated to the Mid-Term Review Meeting.

The "Reactive Intermediates" meeting started on Friday, Sept. 5th at 9.00 am. After the welcome by John Dyke, Dolores Gauyacq chaired the first scientific session, which started with the following programme:

- |            |   |
|------------|---|
| 9:00-9:45  | Jean-Michel LAUNAY (University of Rennes)<br>"Quantum dynamics of insertion reactions involving metastable atoms and H <sub>2</sub> " |
| 9:45-10:15 | <b>Urs HOLLENSTEIN</b> (Vrije Universiteit Amsterdam)<br>"Rotational resolved spectra of xenon"                                       |

After the coffee break, at 10.45 h, John Dyke started Business Meeting 1, by making the following announcements concerning the two next Network Meetings:

- The next meeting will be held at Porton Down, in 2004, from 29<sup>th</sup> March to 2<sup>nd</sup> April.
- The last meeting will be held in Amsterdam, in 2004, in September-October.

The Co-ordinator then discussed the following points:-

• **Decisions Taken at the 6<sup>th</sup> Network Meeting in Bremen**

1. The 7<sup>th</sup> Network Meeting will be held in Orsay , September 3-7<sup>th</sup>, 2003.
2. The last Network meeting will be held in Porton Down, September, 2004.
3. Joint Publications which can be guaranteed for submission before September 2003 are:  
Crete-Amsterdam (1) Prof Kitsopoulos will check on whether three other publications have been submitted already and will inform the Network manager about this for the web page.  
Garching-Lisbon (2)  
Southampton-Lisbon (2)  
Orsay-Southampton (1)
4. We should aim to make one industrial placement, between Garching and Bruker, before the Mid-Term Review (MTR).
5. The deadline for submitting the MTR report to Brussels is July 1<sup>st</sup>.
6. We should continue to implement joint projects and mobility of YRs before the next meeting.
7. YRs need to agree and implement a Training and Interaction Plan.
8. YRs need to continue to be involved in discussion/questions at scientific sessions of Network meetings using the approach suggested at the Bremen meeting (YRs ask questions first at each talk).

• **Objectives of the 7<sup>th</sup> Network Meeting**

1. To plan for the 3rd Annual Report. The deadline for submission of the Financial and Research Reports to the Co-ordinator is September 30<sup>th</sup>.
2. To assess existing projects and activate new ones.
3. To continue mobility of YRs and continue industrial training.
4. To make a major effort to fill existing vacancies in the Network (in Southampton, Crete, and Lisbon—1 person-year in each centre?)
5. To try to increase joint publication list (current number of joint publications is 12)

- **Self-assessment of activity**

Node	Name	Research Active	YR sent to another node (ideally for 2 months)	YR received from another node (ideally for 2 months)	Joint Publications
1.	Soton	√	√	√	√
2.	Amsterdam	√	√	√	X
3.	Orsay	√	√	√	X
4.	Forth	√	√	√	X
5.	Porton	√	√	X	√
6.	Lisbon	√	√	√	√
7.	Munich	√	X	√	√
8.	Bruker	N/A	N/A	N/A	N/A

Various ways of removing crosses in this Self-Assessment Table were discussed. Joint publications should be forthcoming to remove the crosses in column 6.

- **Financial Statement**

A Financial Statement for each node was presented. Financial plans were reviewed and plans were made for next year.

- **Other Important Points**

1. Deadline for the next Network application is Nov 2<sup>nd</sup> --- we shall go ahead with a "Reactive Intermediates" Network application with 12 Nodes.
2. Time sheets for YRs need to be kept up-to-date---and are needed with every Annual Report—the Lisbon one is a good example. YRs should keep these up-to-date.
3. If a YR leaves the Network, an Annex A Questionnaire needs to be completed by the YR before he/she leaves the Network; it is the responsibility of group leaders to see that they are completed.

- **Financial Planning**

1. In the next Cost Statement, Group Leaders must provide information on their expected YR appointments for the next reporting period in order that the most suitable periodic payment can be made.
2. In the last and next Cost Statement, the cost of travel of the YR to the “home scientific community” must be included---one such charge can be claimed each year.
3. In the last Cost Statement, this charge was not claimed in Centre 1, 2, 3 and 6 (Southampton, Adam, Orsay, and Lisbon). For the last year, if not already claimed, these costs can be included in next years Cost Statement.
4. For the next Periodic Payment, the Beyer formula will be applied consistent with the agreed budget limits for each node, i.e. we give each partner a percentage of the periodic payment in proportion to what they have spent, relative to the total expenditure of the Network that year.

At 11.30h Discussion of Joint Projects took place according to the following plan:

**Workshop 1**

Southampton - Orsay  
Crete - Garching  
Amsterdam - Lisbon  
Porton Down - Bruker

**Workshop 2**

Crete - Amsterdam  
Orsay - Lisbon  
Garching - Porton Down - Bruker

**Workshop 3**

Crete - Orsay  
Southampton - Amsterdam  
Lisbon - Garching - Porton Down - Bruker

**Workshop 4**

Orsay - Amsterdam  
Southampton - Lisbon  
Southampton - Garching

The YRs had a separate meeting.

Lunch, was served at 13.00h.

The second scientific session, chaired by Theo Kitsopoulos, started with the following programme:

- 17:00-17:45 Anne ZEHNACKER (CNRS, Orsay)  
“Chiral discrimination in jet-cooled van der Waals complexes: a spectroscopic study.”
- 17:45- 18:30 Wim UBACHS (Vrije Universiteit, Amsterdam)  
“Exotic excited states in the H<sub>2</sub> molecule ”

19:00

Dinner

At 21:00 the poster session took place. The following posters were presented:

**Josselin PHILIP** (Vrije Universiteit Amsterdam, The Netherlands)

“Frequency mixing scheme for the production of tunable narrowband XUV radiation (91-95 nm)”

**Giacomo LEVITA** (University of Southampton UK)

“Thermal Decomposition of organic azides - a PES and IR matrix spectroscopy study - Review of recent advances”

**Rachel TOOMES** (FORTH Heraklion-Crete)

“Slice-imaging detection of photofragments”

**Lucia ZUIN and Fabrizio INNOCENTI** (University of Southampton UK)

“Angular distributions of photoelectrons from oxygen atoms using synchrotron radiation”

“Photoelectron spectroscopy of atomic nitrogen with synchrotron radiation”

“An initial investigation of S and SH with angle resolved photoelectron using synchrotron radiation”

David MITCHELL (Porton Down)

“Fragmentation of di-alkyl alkyl phosphonates in an ion trap mass spectrometer”

**Iulia BALTEANU** (Garching)

“Reactions of large ionic platinum clusters  $Pt_n^{+/-}$ ,  $n = 1-26$ , with small molecules”

**O. Petru BALAJ** (Garching)

“H/D exchange at methyl groups in anionic water clusters”

**Marcin FRANKOWSKI** (Garching)

“Spectroscopy of the  $XeC_2$  molecule in xenon, argon and krypton matrices”

**Vassilios DRACOPOULOS** (Orsay)

“Comparison of photodissociation fragments from allene and propyne in the 12-27 eV energy range”

K. ALNAMA (Orsay)

“Photodynamics of ethylene in the VUV region, using synchrotron radiation”

On Saturday, September 6<sup>th</sup>, the first and second scientific sessions, chaired by Andrew Bell were arranged as follows:

- 9:00-9:45 Maria de Lourdes COSTA (New University of Lisbon)  
“Overview of the working progress on the azides, in the network collaboration”
- 9:45- 10:15 **Iulia BALTEANU** (Garching)  
“Reactions of large ionic platinum clusters  $Pt_n^{+/-}$ , n = 1-26, with small molecules”
- 10:15-11:00 Coffee Break
- 11:00-11:45 Christian ALCARAZ (CNRS, Orsay)  
“Importance of radicals in the chemistry of planetary ionospheres”
- 11:45-12:15 **Romeo-Iulian OLARIU** (University of Lisbon)  
“Atmospheric degradation of the phenols compounds: gas-phase products and aerosol formation from the OH radical reaction.”

A continuation of the poster session took place afterwards until 13.00h. Lunch was then served.

The afternoon scientific session, chaired by Martin Beyer, started according to the programme:

- 14:30-15:15 Dr. Gökhan BAYKUT (Bruker-Daltonic, Bremen)  
“Electron capture dissociation of protonated polypeptides and proteins”
- 15:15-15:45 David Mitchell (Porton Down)  
“Studies of cycloalkanone fragmentation using electrospray ion trap mass spectrometry”
- 15:45-16:45 Dr. Séverine BOYÉ (Orsay University)  
“Gas-phase absorption studies of fluorescent protein chromophores at the ELISA storage ring”

At 16:45 a Discussion of Joint Projects took place following the previously mentioned plan:

### **Workshop 1**

#### **Southampton - Orsay**

Interaction is going well. One joint paper is ready for submission with a Southampton YR as co-author. One thing that has not been achieved since last time is that no progress has been made on the analysis of OH data from Southampton. A visit is proposed of both F. Innocenti (for one week) and John Dyke (for a few days) to Orsay before Christmas to:

1. Discuss and do OH rotational simulations
2. For F. Innocenti to analyse fluorescence data taken in an earlier run at Orsay on allene and propyne.

### **Crete - Garching**

At the Bremen meeting, we proposed that spectroscopy of transition metal complexes will be carried out at FORTH with the Garching cluster source. A new source was built for that purpose and is available for experiments at other nodes.

Placement of a YR for 2-3 weeks is planned. The Garching postdoc Dr. Zheng Sun, who is on an Alexander von Humboldt-Fellowship, will go to FORTH to work on the ZEKE apparatus there. A placement of 3 weeks is planned for the end of October.

### **Lisbon - Amsterdam**

We agreed that the main focus of collaboration would lie in the field of training. Staff members (De Lange, Ubachs) from Amsterdam could be invited to a summer school (or other training course) on Molecular Spectroscopy to be held in Lisbon in 2004.

Moreover, a postdoc (**Romeo Olariu**) could be trained in the operation of lasers and applications in spectroscopy, preferably also including the detection of excited states of radicals.

### **Porton Down - Bruker**

Porton will send staff to Bruker to discuss the deposition of energy into trapped ions in order to produce ion fragmentation. Hopefully this will be before Christmas 2003, depending on staff availability at Bruker.

### **Workshop 2**

#### **Crete - Amsterdam**

There are two issues of interest between the two laboratories.

- a) Ion imaging photo-dissociation experiments as performed with the sliced imaging technique in Crete and the combination of ion imaging techniques with orientated molecules and using femtosecond pump-probe techniques by Janssen at the Laser Centre VU in Amsterdam. A project will be defined between Janssen and Kitsopoulos for experiments in Amsterdam that will be carried out by Rachel Toomes, currently a Network post-doc at Crete.
- b) As a follow-up on previous measurements on the ARIADNE experimental set-up by Ewa Witkowicz, employed as a Network postdoc in Amsterdam, there is an interest in the Amsterdam group to extend those measurements using other gaseous mixtures and perhaps also using a dissociation laser in the ARIADNE time-of-flight mass spectrometric setup at Crete. Visits of Amsterdam scientists to Crete will depend on the appointment of a PhD-student on the project of cavity-ring-down spectroscopy on plasma discharge jets, which is supervised by Linnartz and Ubachs.

### **Orsay - Lisbon**

Collaboration will continue with Antonio Paiva (Lisbon) visiting Orsay. It has been agreed that, once the

experimental set-up is operational, the azide work will start and samples will be sent there. A. Paiva will then visit (Orsay) to perform REMPI experiments with the Orsay group.

#### **Garching - Porton Down - Bruker**

YR placement (**Petru Balaj**) to Bremen is planned for 1 week in October, exact dates to be fixed, to work on ESI/Ion trap or ESI/FT-ICR mass spectrometers. The ESI source loaned to Garching by Bruker is going to be installed on the FT-ICR instrument, which makes it possible to compare FT-ICR data in Garching with Ion-Trap data from Porton. The project of mass-selected deposition of ions coming from the electrospray is continuing. A mass selected protonated dye like a coumarin dye will be deposited, and its laser induced fluorescence recorded as a function of excitation wavelength. In parallel, a high-current electrospray ion source will be built to ensure a sufficient ion density for the detection of infrared absorption.

#### **Southampton-Porton Down**

This interaction is active and on-going. Regular visits between Porton Down and Southampton involve running *ab initio* calculations to underpin ion-molecule reaction studies undertaken at Porton Down.

#### **Workshop 3**

##### **Crete - Orsay**

The collaboration between Stelios Couris and the Orsay group will continue on the photolysis of hydrocarbon and radical production. The group of Stelios Couris is planning to visit Orsay in order to perform laser based experiments (REMPI, LIF and later on CRDS) on small hydrocarbons ( $C_2H_4$ ,  $C_2H_6$ ,  $C_3H_4$ ,...).

##### **Southampton - Amsterdam**

There is a common interest in studying highly excited states of radicals. The Amsterdam group looks forward to combining their knowledge of narrow-band VUV radiation sources with the Southampton expertise in radical sources. The primary interest is in studying ClO, ClO<sub>2</sub>, and ozone, aiming at photodissociation properties of these species. The Southampton group will perform a literature study on the problems and will put forward ideas for experiments in which the requirement where high resolution is an ingredient. These ideas will be sent by Southampton to Amsterdam by December 1<sup>st</sup>, 2003.

Experimental work on MPI at Amsterdam with the Southampton group will take place after Christmas, when an application will be made to European Infrastructure Fund for time at the Laser Centre.

##### **Lisbon - Garching - Porton Down - Bruker**

YR from Garching (**Iulia Balteanu**) will work on the multitechnique apparatus for two weeks in Lisbon. A Lisbon student with Peter Watts (Porton) and possibly David Mitchell (Porton) will come to Garching to work on ion-molecule reactions of organic azides with  $Ar^+$  and  $ArH^+$  generated in the laser vaporization source. A joint publication

on  $\text{Ar}^+$  + azidonitriles is in preparation.

#### **Workshop 4**

##### **Orsay - Amsterdam**

Both groups have an interest in studying photo-predissociation processes in small molecules, in particular in the highly excited Rydberg states of the  $\text{CO}_2$  molecule, which is of atmospheric interest. Moreover, there is a fundamental molecular physics interest in the problem of a Rydberg molecule in which the ionic core experiences a Renner-Teller effect and in which the unpaired core-electron interacts with the orbiting Rydberg electron. After the Amsterdam group has prepared the XUV-laser set-up for pump-probe experiments, and has tested the set-up on predissociation in nitrogen the planned experiments on  $\text{CO}_2$  could start with involvement of YRs and senior scientists from Orsay. The Orsay team will first make a bibliographical study of the problem and will put forward ideas for possible experimental investigations on the Amsterdam set-up.

##### **Southampton - Lisbon**

Collaboration on organic azides is going well. **Giacomo Levita** visited Lisbon for two months. António Dias (Ph. D. student) visited Southampton for three months. Dr. Alan Morris from Southampton will visit Lisbon in September for two weeks. One joint paper on thermal decomposition of azidoacetamide was submitted and two others are nearing completion.

Collaboration on the synchrotron project is continuing with António Dias, and António Paiva collaborating on this project, which uses the Southampton spectrometer at the Elettra synchrotron source (Trieste). One joint paper on O atoms was published and another on SH has just been submitted.

##### **Southampton - Garching**

There are two possible areas of collaboration

1. *Ab initio* calculations in Southampton in support of experimental work in Garching; there is an open offer for a YR to visit Southampton to achieve this.
2. ZEKE spectroscopy on  $\text{Me}_2\text{S}$  complexes. These are being studied by PES in Southampton. Subject to availability on the Garching ZEKE spectrometer, an open offer exists for a YR from Southampton to visit Garching to carry out ZEKE measurements on these complexes.

**The YRs had a separate meeting at the time of these joint project discussions**

**17.00 Final Summary Session**

### **Summary of YR Meetings**

**Marcin Frankowski** , spokesperson for the YRs, summarized the results of the YRs meetings.

A summary of his presentation is as follows:-

1. YR's Web Page will be kept in the current form and will be systematically updated.
2. It would be very useful if keynote lectures presented at the Network meetings would be oriented mostly towards general education on recent topics and research methods within the subject matter of the Network. This approach would fit better with the wide range of conducted research.
3. The current form of YRs' presentations including long and short talks given interchangeably at each second meeting should be kept, but the priority for giving full 30 minute talks should be given those YRs who want to present new results.

The Co-ordinator then presented the conclusions of this meeting as well as recommendations for the financial management:

#### **- CONCLUSIONS**

1. The 8<sup>th</sup> Network meeting will be held in Porton Down, 29<sup>th</sup> March-2<sup>nd</sup> April 2004.
2. The last Network meeting will be held in Amsterdam, September 2004.
3. Deadline of Financial and Research Report to Co-ordinator, is October 1<sup>st</sup> 2003.
4. Industrial placement of one YR from Garching to Bruker will be made before December 2003.
5. There is a need to continue to implement joint projects and mobility of YRs.
6. It is also necessary to continue to encourage joint publications.
7. Each group leader needs to regularly check the Network website and keep it up-to-date.

#### **- Financial Management**

1. Correct Expenditure Figures are needed from each node for the end of Year 3, by Oct 1<sup>st</sup> 2003 at the latest.
2. At the same time, accurate financial projections are needed for Year 4, to estimate expected underspending /overspending in each node.
3. For groups with a projected UNDERSPEND, a written case needs to be made on how to solve this problem: Orsay, Lisbon, Soton.
4. For groups with a projected OVERSPEND, a written case needs to be made for support from within the Network: Garching, Amsterdam.

5. The Co-ordinator and Manager will then propose a budget re-distribution and make a recommendation as to how this can be achieved.
6. The Co-ordinator and Manager need to make a written case to Brussels for a no-cost extension (e.g. six months).

**Closing remarks-**

The Co-ordinator thanked the invited speakers who all presented excellent contributions, and the YRs for their invaluable input, their oral contributions, their posters and their participation in the scientific discussions. He also thanked all members of the Network for contributing to the Mid-Term Review.

He then thanked Professor Dolores Gauyacq and her supporting team from Orsay for hosting the Mid-Term Review, organizing an excellent meeting, and for providing an excellent venue for the meeting.

The Conference Dinner, at 20.00 h, concluded the meeting.