

# MINUTES OF THE SIXTH MEETING OF THE RTN NETWORK

ON

## "REACTIVE INTERMEDIATES"

(held in Bremen, Germany, from 26 - 30 March 2003)

This meeting was organized by Bruker and was held at Bruker Daltonics, in Bremen, from 26 -30 March 2003. The list of representatives from each research group participating in the Network, and attending the Business and Scientific meetings, was as follows:

John Dyke (Co-ordinator) from Southampton, Kees de Lange (Network manager) from Amsterdam, Dolores Gauyacq from Orsay, Maria Lourdes Costa from Lisbon, Vladimir Bondybey and Martin Beyer from Garching, Theofanis Kitsopoulos from Crete, and Goekhan Baykut from Bruker-Daltonics.

The following Young Researchers (YRs) and guests were also present at this Meeting: **Giacomo Levita** and Mariana Ghosh from Southampton, David Mitchell from Porton, **Ewa Witkowicz** and **Josselin Philip** from Amsterdam, N. Shafizadeh from Orsay, **Marcin Frankowski, Iulia Balteanu, and Petru Balaj** from Garching, and **Rachel Toomes** from Crete (YRs supported by the Network are shown in bold). The speakers invited to this meeting to give keynote lectures were as follows:- Jochen Franzen from Bruker Daltonics, Karl Peter Wanczek and John Burrows from the University of Bremen, Wim van der Zande from Nijmegen, Chris Mayhew from Birmingham, Laura Gagliardi from Palermo, Ulrich Boesl from Garching, and S. Willitsch from the ETH, Zürich. They also attended all the Scientific sessions held during the meeting and participated in the discussions.

After arrival on Wednesday, March 26, the participants met for an informal dinner, at the Hotel Munte, where the participants stayed for the meeting.

According to the schedule, on Thursday, March 26, the meeting started at 9.00 am, at the Bruker Conference Room, in the main Building "Attika" floor. John Dyke welcomed all participants and outlined the objectives of the Network Meeting, following the conclusions drawn at the 5th Network Meeting, in Southampton.

He stated that two Yrs, **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. Also, unfortunately Dr Andrew Bell (Group Leader of the Porton node) had had to withdraw at the last minute

John Dyke then presented the organisation of the business meetings (BM) that were undertaken during the meeting following the schedule: BM1: Thursday (11.30-12.00) - "The Mid-Term Review" (YRs attending); BM2: Friday (15.00- 16.00) - "Organisation of the Network and Financial Management" (YRs in a separate meeting); BM3: Saturday (14.30-15.30) - Discussion plans on FP6 (YRs in a separate meeting).

After this introduction Gokhan Baykut (Bruker) chaired the first scientific session, which started with the following programme:

9.15 Keynote lecture: Dr Franzen (Bruker)

*Strange phenomena in Paul ion traps*

10.00 **Marcin Frankowski** (Garching)

Spectroscopy of rare gas molecules: XeC<sub>2</sub> and HXeCCH in solid xenon and argon.

10.30 **Rachel Toomes** (Crete)

Imaging of reaction products with rotational state resolution using crossed molecular beams.

11.00 Coffee Break

After the coffee break, at 11.30 h, John Dyke started Business Meeting 1, by re-examining the following points.

#### 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	X
3.	Orsay	√	X	√	X
4.	Forth	√	X	√	X
5.	Porton	√	X	X	√
6.	Lisbon	√	√	√	√
7.	Munich	√	X	√	√
8.	Bruker	N/A	N/A	N/A	N/A

➤ **Objectives of the 6th Network Meeting in Bremen 2003**

1. To assess existing joint projects and activate new ones.
2. To continue mobility of YRs and start industrial placement(s).
3. To try to increase joint publication list (20 by Mid-Term Review?)  
(current number of joint publications is 5 - Soton-Porton, Soton-Garching, Soton-Lisbon(3)).
4. To plan for Mid-Term Review (Sept. 3-7, Orsay) and the 3rd Annual Report (deadline for financial and research reports to Co-ordinator is September 30<sup>th</sup>)
5. To make a major effort to fill existing YR vacancies in the Network (in Orsay, Lisbon and Southampton).
6. To ensure the Web-page is up-to-date.
7. To encourage YRs to participate in the discussion/ask questions after each scientific talk.

➤ **Decisions Taken at the Soton Meeting**

1. The 6th Network Meeting will be held in Bremen, March 26-30, 2003.
2. The Network Co-ordinator will notify Brussels that we would like a six-month no-cost extension, to allow the Workplan to be achieved, given the slow starts of projects in Amsterdam and Crete.
3. The Mid-Term Review will be held in Orsay, Sept. 2003.
4. The last Network meeting will be held in Porton, Sept. 2004.
5. We will aim to implement joint projects and mobility of YRs before the next meeting.
6. We should aim to make industrial placement(s) before the Mid-Term Review.
7. The YRs need to put forward a training and interaction plan, and be more involved in discussions/questions at scientific sessions.
8. The Group Leaders need to check that the material on the Web-page is up-to-date. If not, please send new material to the Network Manager.

➤ **Milestones of the Training Programme**

1. By the Mid-Term Review at least 40% of the training deliverables —(in terms of man-months) must be achieved.
2. The YRs must have given two presentations on their projects and results to the Steering Committee *and will have attended a Team Building and Presentation Skills course.*
3. The Mid-Term Report is the basis of discussion at the Mid-Term Review; it must be ready two months before the meeting and sent to the EU—**i.e. by the end of JUNE.**
4. Principal Contractor needs to agree Agenda and date with the Commission at least two months prior to the meeting (i.e. by end of JUNE).
5. YRs need to agree and put forward a Training Plan.
6. Criteria
  - a. Man-Months (> 40%)
  - b. Duration of the Work-Programme (> 66%)
  - c. Training Elements, Joint Research Programmes and Industrial Visits-----  
underway?

**MID-Term Review—in Orsay Sept. 3-7 2003**

**Local Organiser Prof.Dolores Gauyacq**

**PURPOSE**

It is principally an opportunity for the partners, the YRs and the Representative(s) of the Commission to discuss questions or issues which may not be clear from the official documentation or the Contract.

**It is not a scientific evaluation of the Network nor should it be the first point in the course of the Contract at which problems are brought to the attention of the Commission.**

**Particular attention is paid to the Training and Networking Aspects.**

The structure of the Network and the Contract's Work Programme will also be reviewed and, if necessary, contract modifications defined.

The Mid-Term Review is a valuable source of feedback to the Network Management.

➤ **Structure of the MTR Report**

A1. Scientific Highlights

A2. Joint Publications and Patents

B1. Project Objectives

B2. Research Method and Work Plan

B3. Schedule and Milestones

B4. Research effort of the Participants

B5. Network Organisation and Management

B6. Cohesion with Less Favoured Regions and associated states.

B7. Connections to Industry

➤ **Main Steps in Organising the Mid-Term Review (MDT)**

**1. Setting a date and Venue**

It is recommended that the MTR is held in conjunction with a regular Network meeting.

**2. Agenda and Participants**

The Agenda and the full list of participants have to be agreed between the Co-ordinator, the Manager and the Project Officer at least 2 months before the meeting.

The participants will include the Co-ordinator, the Manager, all Group Leaders, task leaders and YRs whose appointments are currently financed by the Network.

Each of these participants will be expected to make a presentation of their work and experience within the Network.

A Network Administrator may also attend.

An Expert Reviewer will accompany the Project Officer.

In general, other participants should only be present if they have a role to play in the meeting.

YRs who have been in the Network but have completed their contracts at the time of the MTR may also be invited to share their experiences, at the discretion of the Co-ordinator and Manager, and at the Network's expense.

### **3. The Co-ordinator Report**

The Co-ordinator and Manager are expected to prepare the Mid-Term Report. **The Report and the Agenda must be distributed to all participants at least 1 month before the meeting.**

### **4. The MTR Meeting**

The meeting will normally require one whole day. It may be chaired by the Commission's Project Officer or by the Co-ordinator (by prior arrangement).

The Agenda will include a report by the Co-ordinator and a *tour de table* of each of the Group Leaders and Task Leaders.

Each YR will also be required to make a report of their experiences and fill in a confidential (anonymous) questionnaire for statistical follow-up by the Commission.

If participants agree, separate sessions will also be held between the Project Officer/Expert Reviewer and

(i) the Senior Scientists and

(ii) the YRs to give each group a chance to air concerns which they may not want to discuss in front of the group as a whole.

### **5. Follow up**

Following the MTR meeting, the Project Officer will send the Expert Reviewer's Report to the Co-ordinator and will write a letter detailing any recommendations/actions to be taken to implement best practice, any adjustments to the Work Programme, Training Programme etc.

A time-scale for the implementation of any changes will also be agreed. If no actions are necessary, the Project Officer may conclude the MTR process.

## ➤ **Summary of Tasks of the Principal Participants**

### **The Network Co-ordinator**

--to propose a date and venue for the MTR Meeting as soon as possible and not less than 2 months in advance.

--not less than 2 months before the agreed date, to propose an Agenda and list of participants to the Commission's Project Officer.

--not less than 1 month before the meeting, to prepare the MTR report and send it to all participants.

--to organize the logistics of the meeting.

--to present an overview of the Network's progress to the meeting.

--to circulate the Commission's assessment to all Network Partners and to arrange for any necessary follow-up.

### **Network Manager**

Tasks not defined by the Commission, but must be defined by the Network.

### **Suggest the following**

--assist the Co-ordinator with preparation of his agreed tasks.

--report on progress of joint Network projects and publications.

--report on YR placements at other centres.

--report on industrial placement(s) and involvement of industry in the Network's activities.

--be prepared to deal with questions concerning the web-page

### **The Expert Reviewer**

--to agree the Date of the MTR meeting.

--to prepare for the meeting by examining the MTR report and the contract as well as any other material provided in advance of the meeting and seek supplementary information if required.

- to attend the meeting and be prepared to structure the discussion, involving all participants.
- to discuss together with the participants areas of possible actions to be taken.
- to prepare the Review Report and transmit it to the Project Officer within one month following the meeting. Confidential information should be contained in a cover letter.

### **The Project Officer**

- to provide the Co-ordinator with the MRT Manual.
- to agree the Agenda and list of Participants.
- to propose and agree with the Co-ordinator and Manager the choice of expert Reviewer.
- to prepare for the meeting by examining the MTR report, the contract and relevant background information, notably the original proposal and the Network's Home Page. In particular, the progress with the appointment of YRs, Networking aspects and the financial performance to date will be examined.
- to chair the MTR meeting (or agree to allow the Co-ordinator to chair it).
- to arrange for the YRs present to complete the Network Fellow questionnaire.
- within one month of the meeting, to send the Expert Reviewer's Report and the Commission's opinion on the MTR to the Co-ordinator.
- to follow up any actions that may be required in co-operation with the Co-ordinator.

➤ **Agenda of MTR Meeting**

1. Introduction—by Project Officer and Expert Reviewer (10 mins)

2. Co-ordinator's and Manager's Report (1 hour)

(a) Scientific (20 minutes)

--the scientific, technological or socio-economic reasons for carrying out research in the field covered in the research

--research objectives of the **joint** work/projects

--scientific highlights of the work so far

(b) Networking (20 minutes)

--methodological approach and Workplan

--how the Network functions and how the partners collaborate in practice

--connections to industry

(c) Training (20 minutes)

--training programme (distinguishing between that for pre-and postdocs)—

--summary table of use of budget to date and projection until the end of the contract

--any proposed revision to the contract.

**Tour de Table (by Team)**

--each scientist in charge should present the role and contribution of their research team to the Network, the benefits of the Network to their own work and any criticisms.

--each task leader (e.g. A.Bell and D.Gauyacq) should similarly present the role and contributions of their task to the overall project.

**--the YRS----**

--each YR should present themselves, their background, their work and their experience as a Network fellow.

Each presentation should go beyond the scientific project and should include their impressions of how they have been welcomed in the host institute, integrated in the team, helped with practical matters in settling into their new environment.

Any comments (positive or negative) on the Network are also welcomed.

If there are several YRs in one team, they should combine their comments on the non-scientific points above.

**Sufficient time should be built into the Agenda to allow for questions and discussion.**

### **YR Reports**

This will be a report by each YR on his/her project.  
Again sufficient time should be built into the Agenda to allow for questions and discussion.

### **Meeting between the YRs and the Project Officer/Technical Expert**

This is intended to allow the Young Researchers to speak freely with the Project Officer/Technical Expert about their experiences in the Network.

### **Meeting between the Co-ordinator, the Scientists in charge and the Project Officer/Technical Expert**

This meeting is intended to give the senior scientists an opportunity to talk to the Project Officer/Technical Experts about their own experience in the Network, of the Network Fellows and to raise any matters which they wish to discuss in a smaller group.

### **Open Discussion**

This discussion will round off the meeting by identifying strengths and weaknesses of the Network, particularly in relation to the Training Programme and the joint research. Identification of best practice in the Network and recommendations will be made by the Project Officer/Technical Expert.  
Comments on the report and the Network's web pages will also be made.

12.00 – Introduction to YR Meeting and Organisation of Workshops to Discuss Joint Projects.  
Chaired session by Kees de Lange

### **➤ YR Meeting**

The following points were discussed:

- Participation in discussion after lectures
- Training plan
- Update web site
- Joint publications
- Industrial placements

➤ **Organisation of the Workshops**

The workshops were organised as follows:

*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**

**Informal Discussions**

**Orsay – Amsterdam**

**Southampton – Lisbon**

**Southampton – Garching**

12.15 – 13.15 Workshop 1 took place while the YRs had a separate meeting.

Lunch, at 13.15 was served at Bruker.

The second scientific session, chaired by Dolores Gauyacq, then started with the following programme:

14.30 Keynote lecture: Karl Peter Wanczek (University of Bremen)  
Ion-molecule reactions with emphasis on magnetic ion traps.

15.15 **P. Balaj** (Garching)  
Wet electrons and their reactions.

15.45 P. Brechignac (Orsay)  
Spectroscopy and photostability of PAH cations.

16.15 Coffee

## 16.45 Report on Workshop 1

### **Southampton – Orsay**

The collaboration between Southampton and Orsay is going well.

It involves

1) “Photodissociation of hydrocarbons, studied by Synchrotron Radiation”

**Lucia Zuin** visited Orsay twice and **Fabrizio Innocenti** visited Orsay three times.

They plan to come back in July for four weeks.

2) Preliminary analysis of CIS spectra autoionizing Rydberg state of OH.

### **Crete – Garching**

Collaboration possibilities:

1) A student from Crete comes for six months to work on the existing Cavity Ringdown (CRDS) set-up in Garching. What is needed is a choice of suitable metal clusters to study as well as discussions of the project with the possible candidates.

2) Experiment on spectroscopy of mass selected clusters. One co-worker from Garching will go to Crete with the metal cluster source, which will be mounted on the molecular beam set-up. In these experiments, metal clusters solvated by Ar atoms,  $Mn^+Ar_m$ , will be generated, and their fragmentation studied using lasers available in the Laboratory.

3) Two possible ZEKE experiments

a) Person from Garching comes to Crete for one month to do an experiment on the Photoelectron imaging apparatus.

b) A student from Crete comes to Garching to collaborate on experiments using the existing ZEKE apparatus.

### **Amsterdam – Lisbon**

Collaboration postponed until a YR is appointed in Lisbon

### **Porton Down - Bruker**

It was not possible to discuss this, as the group leader from Porton (A. Bell) unfortunately could not attend the meeting.

17.00 Workshop 2 Chaired by Kees de Lange  
YRs had separate meeting.

18.00 End of the Meeting

20.0 Dinner at Globus Restaurant.

**Friday March 28<sup>th</sup>** (at Bruker Conference Room Main Building “Attika” Floor)

On Friday the first scientific session, Chaired by Theofanis Kitsopoulos was arranged as follows:

- 8.45 Keynote Lecture: Wim van der Zande (Nijmegen)  
Diatomic and triatomic anions and cations: dynamics under collisions with electrons and their role in the middle atmosphere.
- 9.30 Keynote Lecture: Harold Linnartz ( Vrije Universitate, Amsterdam)  
High Resolution Spectroscopy of molecules of atmospheric interest.  
Cluster ions.
- 10.00 Keynote Lecture: Laura Gagliardi (Palermo)  
Electronic spectroscopy of small molecules in the gas-phase:  
a quantum-chemical perspective.

10.45 Coffee Break

After coffee, at 11.00, a tour to Bruker Daltonics took place followed by lunch at 12.45 (at Bruker).

The second scientific session of the day was chaired by Chris Mayhew and followed the programme.

- 14.00 Keynote Lecture: Ulrich Boesl (Garching)  
Laser excitation and time-of-flight mass spectrometry:  
molecular spectroscopy, photodissociation, and chemical analysis.

14.45 Framework 6 John Dyke

The situation of a future FP6 research application was summarised by the Co-ordinator:

- **Our Application for a Network of Excellence**

This was discussed at some length. The conclusion is as follows:-

**CONCLUSION - Better to wait for next Call in November 2003 and see if overlap with our EoI with areas identified in the Call is higher (i.e. are more fundamental areas of research favoured in this 2<sup>nd</sup> call?)— before deciding to prepare a full NOE bid.**

- **ALTERNATIVE — apply for a Marie-Curie Training Network**

--this would be seen as an extension of our existing Network

--a Network of ca. 8 groups is favoured

--deadline for applications is November 2<sup>nd</sup>, 2003

--in Marie-Curie Training Networks  
pre-docs favoured over post-docs

--if a postdoc appointed, there must be a good reason for making the appointment  
e.g. bringing a particular expertise to the Network

--involvement of SMEs (Medium Enterprises) encouraged.

### **Possible Participating Groups in the FP6 Marie-Curie Network**

1. Soton
2. Amsterdam ( Vrije Univ.)
3. Orsay
4. Forth
5. Lisbon
6. Munich

### **Possible New Groups**

- |               |              |   |
|---------------|--------------|---|
| 7. Birmingham | C. Mayhew    | Ion-Molecule Chemistry                                      |
| 8. Rome       | S. Stranges  | Studies of Radicals with<br>Synchrotron Radiation           |
| 9. Palermo    | L. Gagliardi | Computational Chemistry                                     |
| 10. Zurich    | F. Merkt     | High Resolution PES of Radicals                             |
| 11. Würzburg  | I. Fischer   | Time Resolved PES of Radicals<br>and Excited State Dynamics |

### **What to do if one wants to participate:**

**by June 1<sup>st</sup> the following should be sent to the Co-ordinator**

-- a description of what one can offer—expertise , techniques (2 pages of A4).

-- identification of three other groups that one can definitely collaborate with and send a description of these possible collaborations

**Each existing Network member should look for AT LEAST ONE new collaboration with new Network members ( 2 sides of A4 max.)**

---helpful if one can identify ONE SME who can participate in this network.

At 15.15 the **YRs short presentations** started:

**E. Witkowicz** (Amsterdam): Reactive species produced by planar plasma discharge investigated with TOF-MS and CRD spectroscopy.

- G. Levita** (Southampton): Recent advances in the study of pyrolysis of azides.  
**I. Balteanu** (Garching): Very low rate constants of bimolecular CO adsorption on anionic gold clusters.  
 D. Mitchell (Porton): Fragmentation and reactions of organophosphate compounds in an ion trap mass spectrometer.

At 17.00 the Poster Session was held; posters presented were as follows:-

- G. Levita** (Southampton): Recent advances in the study of pyrolysis of azides.  
**I. Balteanu** (Garching): Very low rate constants of bimolecular CO adsorption on anionic gold clusters.  
 D. Mitchell (Porton Down): Fragmentation and reactions of organophosphate compounds in an ion trap mass spectrometer.  
**E. Witkowitz** (Amsterdam): Reactive species in a planar plasma expansion studied by CRD spectroscopy and TOF mass spectrometry.  
**M. Frankowski** (Garching): Spectroscopy of rare gas molecules: XeC<sub>2</sub> and HXeCCH in solid xenon and argon.  
**R. Toomes**(Crete): Imaging of reaction products with rotational state resolution using crossed molecular beams.  
**P. Balaj**(Garching): Wet electrons and their reactions.  
**J. Philip**(Amsterdam): Narrowband XUV laser source for the study of predissociation in N<sub>2</sub>.  
 N. Shafizadeh (Orsay) VUV photodissociation of allene.  
 M. Lourdes Costa (Lisbon) Adsorption of azidoacetone and azidoacetonitrile on Ni.  
 S. Willitsch (Zürich): ZEKE-PFI photoionization of radicals.  
 C. Mayhew (Birmingham): SIFT studies of ion-molecule reactions.

The meeting was over at 18.00.

20.0 Dinner (at Globus)

### **Saturday March 29<sup>th</sup> (in Hotel Munte Conference Room)**

The first scientific session of the day was chaired by Martin Beyer

- 9.00 Keynote Lecture S. Willitsch (ETH, Zurich)  
 Threshold ionisation spectroscopy: high resolution investigation of radicals and ions
- 9.45 **Josselin Philip**(Amsterdam)  
 Narrowband XUV Laser Source for the study of predissociation of N<sub>2</sub>.
- 10.45 Kees de Lange  
 Charged-particle imaging studies with femtosecond lasers: the NO dimer.
- 11.15 Coffee / Tea

#### 11.40 Workshop 3

12.0 The Co-ordinator examined some important points during the Business Meeting, as follows:

##### ➤ **Miscellaneous Points—from Brussels**

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 next Cost statement, Group Leaders must include the cost of travel of the YR to “the home scientific community”----- one such charge can be claimed each year. In the last Cost statement, this charge was not claimed in Centres 1, 2, 3 and 6 (Soton, Amsterdam, Orsay, Lisbon). (For the last year, if not already claimed, the cost of this can be included in next years Cost statement).
3. On Feb 1<sup>st</sup>, 2003 Ms Getsiou responded to our request for a six-month no cost extension.

Ms Getsiou was not sympathetic to our request for a no-cost extension—instead she recommended we should

- transfer Money to another Node
- employ people from other nodes
- employ a Second Postdoc at a node
- note that we can transfer up to 20% of Money of one Node to another Node, without Contract Amendment.

##### ➤ **Other Important Points**

--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.

--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.

##### ➤ **Overview of the Budget**

The Co-ordinator presented an up-to-date summary of income and expenditure, and the suggested division of payments for the 2<sup>nd</sup> Periodic Payment, received from Brussels.

## 12.15 Report on Workshops 2 and 3

### **Workshop 2**

#### **Crete – Amsterdam**

**Ewa Witkowicz** (Amsterdam) had a successful visit to Crete where the plasma source from Amsterdam was tested.

**Rachel Toomes** (Crete) will visit Amsterdam to perform imaging experiments with Maurice Jansen/ Kees de Lange. A student of Maurice Jansen is already working in Crete and another is arriving in May.

#### **Orsay – Lisbon**

Collaboration will continue with Antonio Paiva (Lisbon) visiting Orsay. It has been agreed that, once the experimental set-up is operational to allow the azide work to start, samples will be sent there. A. Paiva will then visit (Orsay) to perform the REMPI experiments with the Orsay group.

#### **Garching – (Porton Down) - Bruker**

There is a considerable overlap in interests, as well as complementary expertise between the two participants of the Network, and collaboration in at least two different areas is in progress.

1. A Temperature-Controlled ICR Cell is currently being developed in Garching, which will be used to study the stability and fragmentation of ions and ion clusters by infrared blackbody radiation. With this cell, whose construction is currently nearing completion, it will be possible to investigate the fragmentation processes not only at ambient temperature, but also over the range of about 100-500 K. While the testing of the cell will be carried out in Garching, consultations regarding the technical details of the design with the engineers and experts at Bruker are highly desirable. For this purpose, a 1–2 week stay at Bruker in Bremen for one of the Garching YRs working on this project is planned. The expertise available there will help to accelerate the process. It is planned that the first results obtained in the course of implementation and testing of the new cell will be published jointly by the Munich group and Gokhan Baykut at Bruker.
2. A second area of crucial interest for the Munich research group where extensive expertise is already available at Bruker in Bremen involves the electrospray, ESI source. In Munich, the electrospray source, which was provided by Bruker, should be used in, at least, two different experiments. In the first place, the source should be used to deposit mass selected molecular ions in low temperature matrices. While this has, thus far not been accomplished either in the Munich laboratory, or anywhere else, it appears quite feasible, and should provide the best hope of introducing large organic or bioorganic molecules into a solid matrix environment. In the second place, the source should be used to generate multiply charged hydrated, or in general solvated ions for FT-ICR mass spectrometric studies. While the studies of reaction in singly charged ions and hydrated ion clusters yielded a wealth of new results about aqueous chemistry, the current laser vaporization source in Garching is not capable of generating doubly charged ions. The electrospray source should fill this gap. Again, while the Munich group has relatively little experience with electrospray sources, an extensive expertise in this area is available at Bruker in Bremen. A visit by a Garching YR working on these experiments to Bremen, to learn to run the ESI source, and possibly to do some

preliminary experiments with hydrated ions there should accelerate and advance these studies.

### **Workshop 3**

#### **Crete – Orsay**

This is progressing mainly through the research of Prof S.Couris who is interacting with the Orsay group

#### **Southampton – Amsterdam**

John Dyke will visit Amsterdam after June 1<sup>st</sup>, to discuss

- a) Possible XUV projects on radicals in Amsterdam (also involving Orsay) (with W. Ubachs).
- b) Possible CRDS experiments on ions/radicals.
- c) Possible electron imaging experiments (with M. Jannsen).

A number of molecules and ions were discussed, including ClO<sub>2</sub>.

#### **Lisbon – Garching – Porton Down – Bruker**

One joint publication on the reaction of azidoacetonitrile with ionic rhodium clusters, both anionic and cationic, is ready to be submitted to JACS (probably).

A second one, on matrix spectra of azides is currently in preparation.

A considerable amount of data was taken also on the reactions of Rh<sub>n</sub> clusters with azidoacetone. Some problems were encountered with sample degradation and decomposition.

The data need to be analysed. It must be decided if:

- a) there are results worthy of publication
- b) the experiments have to be repeated, and/or
- c) the project is not worth pursuing.

A Portuguese master student will join Martin Beyer and Iulia Balteanu, for two weeks, depending on Garching availability, to use FTICR to look for clusters of azidoacetic acid with rhodium, in order to compare with results obtained on an existing Ion-Trap Mass spectrometer in Lisbon.

Lisbon will send another graduate student, next April to carry out studies, with Martin Beyer(Garching), employing FTICR for the study of fragmentation of some organic azides.

Peter Watts from Porton will then come to Garching to join the experiments. He will come to Lisbon to discuss the results.

### **Informal Discussions**

#### **Orsay – Amsterdam**

Prof Dolores Gauyacq (Orsay) will visit Amsterdam with Prof. John Dyke (Soton) before September 2003 to discuss possible VUV experiments on radicals.

### **Southampton – Lisbon**

Collaboration on organic azides is going well. **Giacomo Levita** visited Lisbon for two months. António Dias (Ph. D. student) will visit Southampton, for 2-3 months.

Collaboration on the synchrotron project is continuing with António Dias, and António Paiva collaborating on projects, which use the Southampton spectrometer at the Elettra synchrotron source.

### **Southampton – Garching**

A student from Munich will go to Southampton before December 2003 to do theoretical work.

13.00 Lunch (in Hotel Munte)

The last scientific session was chaired by John Dyke

14.0 John Burrows ( University of Bremen )  
Remote sensing of atmospheric constituents

15.0 Mariana Ghosh (Southampton)  
Spectroscopic studies of the atmospherically important reaction  $\text{Cl}_2 + \text{DMS}$  with spectroscopic methods.

15.45 Coffee/Tea

16.00 Final Summary Session

#### ➤ **Plans made in Workshops**

Kees de Lange presented a "Summary of Plans for Joint Projects"

#### ➤ **Summary of YR Meetings**

**Marcin Frankowski** summarised the results of the YRs meetings. A summary of his presentation is as follows:-

#### **YR Training Plan**

1. Scientific training "Learning by doing"
  - a) literature study
  - b) knowledge exchange / sharing ideas / collaboration

- c) experiment
    - understanding and planning experiments / development of time management skills
    - data acquisition / processing
    - analysis of experimental results
  - d) obtaining experience with theoretical calculations
2. Collaboration among the groups – exchange of YRs
  3. Presentation skills development
    - a) writing publications
    - b) oral and poster presentations at 6 monthly meetings
    - c) web page
  4. Contribution to planning of research and network meetings – team work
  5. Development of team building skills
  6. Web page of Young Researchers
  7. Foreign language courses

**Closing remarks-** John Dyke 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 Bruker for their warm hospitality in hosting the meeting, and for providing an excellent venue for the meeting.

In particular, Dr Gokhan Baykut (Bruker) was thanked for all his hard work and attention to detail in organising an excellent meeting.

The Conference Dinner, at 20.00 h, ended this meeting.

## **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 , Sept. 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)—3 already submitted? (Prof Kitsopoulos will check on this) (info. to the Network Manager for the Web-page please)  
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).