

Report on ESF Exploratory workshop on 'Ultracold Chemistry'

Held at European Physical Society, Mulhouse France February February 7 to 10, 2005

Summary: This Exploratory meeting was attended by 24 researchers from 7 European Countries who 23 presented talks. This was the first meeting to discuss the opportunities for studying chemistry using cold atoms and molecules as reactive species. The meeting concluded that this is a novel and exciting new area of research that is suitable for rapid exploitation. The meeting further concluded that Europe was well prepared to develop this research, and that such a research programme, once established, would allow Europe to take the lead in a novel and exciting new area of science. The participants agreed that it was important to develop such a research programme and would seek support at both National and EU level with a collaborations being strongly supported as they were beneficial to the community, the first part of which was formed at this ESF Workshop.

Summary of the scientific programme and discussion

To date most chemistry has been performed under terrestrial conditions of standard temperature and pressure or under conditions pertaining to industry (e.g. high temperature combustion). In contrast chemistry at low temperatures for example the chemistry leading to an understanding of the chemical reactions leading to ozone depletion in the stratosphere ($200\text{K} < T < 270\text{K}$) or the reaction dynamics at temperatures below 50K necessary to understand molecular formation processes in interstellar space have only been developed in the last two decades. At such low temperatures many room temperature reaction channels are closed and reactions are often governed by tunneling with the mechanisms being more akin to those encountered in collision physics- for example the product formation being similar to resonance formation in quantum scattering. Of primary interest are the effects of rotational and vibrational excitation and their manifestation in reaction properties. In addition the ability of external stimuli (e.g. photons and electrons) to trigger chemistry ensures that low temperature chemistry is a new and as yet little understood (and poorly modelled) process albeit one that is prevalent in the upper atmosphere and is the basics of astrochemistry.

Such research requires an interdisciplinary research incorporating both experimental and theoretical expertise in (i) physical and ionic chemistry (ii) atomic and molecular physics (iii) quantum chemistry/molecular structure and (iv) cold atom optics. This workshop was the first opportunity for researchers investigating cold atoms and molecules to formally link with groups conducting research in chemical reactions. It was also be a unique opportunity for researchers in these themes to meet researchers in the applied fields of atmospheric chemistry and astrochemistry where low temperature reactions play a key role. The style of an ESF workshop was an ideal forum or such a meeting since it engendered an informative and open discussion amongst the delegates, most of whom had never met before and who were unfamiliar with the concepts of the other participants research. Recent experimental advances have made it possible to cool gas-phase molecules to temperatures *below 1 K and trap them in well-defined states*. Even lower temperatures have been achieved for molecules in cold atom traps. These novel capabilities open the way to new technologies based on quantum control of molecular processes and provide us with new ways to explore the fundamental principles that govern low-temperature chemistry.

The meeting concluded that ultracold chemistry might be conveniently (though still rather artificially) divided into several temperature regimes;

1. The very coldest molecules have been produced in atomic traps at temperatures between 1 nK and 1 μ K by photoassociation, 3-body collisions and magnetic tuning through Feshbach resonances. Molecular Bose-Einstein condensates (BECs) have been produced for molecules such as ${}^6\text{Li}_2$ and ${}^{40}\text{K}_2$, formed from pairs of fermionic alkali metal atoms in highly excited states. Efforts are under way to extend these techniques to heteronuclear (dipolar) molecules and to transfer the condensate population to low-lying states. The condensates already produced offer new possibilities for complete quantum control of macroscopic molecular assemblies. Dipolar quantum gases, once produced, will offer novel physical properties based on long-range interactions and offer new opportunities for quantum computing and quantum information theory.

2. The temperature regime between 1 mK and ≥ 1 K is being accessed by a quite different set of methods based on cooling molecules from room temperature by methods such as molecular beam deceleration, buffer gas cooling and slow molecule guiding. Molecules such as OH and NH_3 have already been decelerated and trapped, and many others are under investigation. These studies both offer a new route to condensation for chemically stable species and create a new laboratory in which low-energy beams of state-selected molecules can be collided either with themselves or with molecules in traps.

3. The intermediate range of temperatures between 1 μ K to 1 mK has come to be called the 'ultracold regime'. Collisions between ultracold molecules will be crucial in achieving condensation for molecules cooled from room temperature and the regime can also be accessed by photoassociation in laser-cooled gases.

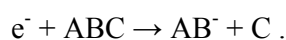
4. Chemistry at higher temperatures (though still low by normal standards !) 1 to 30K are better understood and may be used to predict effects that might occur at lower temperatures. Chemical reactions occurring between 10 and 15 K are crucial to molecular astrophysics, but are poorly understood in both experimental and theoretical terms. Extrapolating high-temperature rate measurements to astrophysical temperatures is notoriously unreliable. However, here too there have been experimental advances that allow rate coefficients for selected reactions to be measured at temperatures down to 15 K. Extensions of these techniques to the region between 1 K and 10 K are now envisaged, and will complete the link between ultralow-energy collisions and low-temperature chemistry.

In all these areas, theory provides a unifying structure that links different regimes of energy and temperature. At the very lowest temperatures (below 1 μ K), atomic and molecular interactions occur in the Wigner regime, with the energy-dependence of cross sections governed by simple power laws that depend on long-range forces. Even here, however, full quantum dynamics calculations are needed to understand complex processes such as reactivity and energy transfer. New theory will also be needed to understand photoassociation and the effects of applied electric and magnetic fields, which will be used to tune interactions and control collisions.

At slightly higher temperatures, collisions become more complex. Different partial waves start to interfere. Collisions acquire directionality and scattering resonances become important. Reactive scattering resonances are widely believed to dominate chemical reaction rates at low temperatures, and an improved theoretical understanding of them is badly needed. The new techniques that are now emerging will allow experiments and theory to confront one another at temperatures below 1 K, and this will produce new understanding of resonant collisions.

Low-temperature chemical processes can usefully be divided into those with and without barriers. Reactions without barriers quickly become statistical and are conventionally described by capture theories. Reactions with barriers might be expected to become very slow at low temperatures, but in several cases substantial tunnelling rates persist even in the low-temperature limit. This is likely to be a general phenomenon, but requires full investigation. In particular, long-range potential wells exist in the entrance and exit channels of many reactions; such wells dramatically decrease tunnelling path lengths and increase tunnelling rates, as well as creating the conditions needed for scattering resonances and long-lived collision complexes. However, there are very few reactions for which the long-range wells are properly characterized and their effects understood.

There are also many interesting phenomena involving low-temperature ions and electrons. Ion traps provide a different entrance to the ultracold regime, and low-temperature ion-molecule reactions are important in astrophysical environments. Low-energy electron-molecule collisions are also of great importance. In this case, however, the energy scales are somewhat different. In quantum-mechanical terms, collisions enter the “ultracold” regime when the de Broglie wavelength is large compared to molecular dimensions. For heavy-particle collisions this occurs below 1 mK, but for electrons it occurs below about 10 meV. Such low temperature collisions may form resonance states in turn forming anions that may open new chemical pathways. For example dissociative electron attachment (DEA).



results in a product anion whose chemical reactivity is completely different from the parent species. Furthermore such DEA processes are often ‘open’ even at incident electron energies of a few meV well below the bond dissociation energies. Hence low energy electrons may be used to initiate chemistry at low collisional temperatures.

The meeting also reviewed several areas in which the application of low temperature chemistry was likely to be important. These include both atmospheric and astrophysical processes. The latter are perhaps most relevant to the meeting since in the interstellar medium temperatures as low as 4 K are common, yet in these regions active chemistry must occur to explain the formation of the many complex chemical species observed there. Ion-Molecule chemistry and surface chemistry are believed to be prevalent.

Full details of the talks presented at the meeting are in programme handbook. Also see <http://www.isa.au.dk/eps-uc/>

Conclusions:

The study of ultracold chemistry, or the reactions between ultracold targets is a new discipline that is being made possible by the development of next experimental techniques. It is an exciting and innovative area of research whose potential has yet to be exploited. It is also a field in which quantum mechanical phenomena are expected to dominate. The exploratory meeting was the first opportunity to bring together researchers who, in Europe can develop this field.. Accordingly plans to develop this field and the formation of an integrated research community are to be pursued, with the applications to ESF for a Programme grant and to the EU Framework programme.

Final Workshop Programme

Sunday February 6th 2005

Up to 18.00 Participants arrive

18.00 Dinner

Monday February 7th 2005

09.00	Registration and Introduction to ESF Activities	
<u>Session 1:</u>	<u>Ultracold Chemistry – Overview</u>	
09.30 to 10.15	Chemistry in the Cold - Novel Approaches and New Applications of Low Temperature Chemistry	Professor N J Mason
<i>10.15 to 10.45</i>	<i>Coffee</i>	
10.45 to 11.30	Cold Virtual States	Professor D Field
11.30 to 12.15	The Big Chill: The behaviour of chemical processes at ultra-low collision energies	Professor F Gianturco
12.15 to 12.45	Discussion and summary	
<i>12.45 to 13.45</i>	<i>Lunch</i>	
<u>Session 2:</u>	<u>Making Cold Molecules</u>	
13.45 to 14.30	Manipulation of polar molecules with electric fields	Professor G Meijer
14.30 to 15.15	Molecular deceleration for studies of ultra-cold collisions	Professor T Softley
15.15 to 16.00	Cold molecular ion studies in traps	Dr M Drewsen
<i>16.00 to 16.30</i>	<i>Tea</i>	
16.30 to 17.15	Making cold molecules with cold atoms and chirped laser pulses	Professor F Masnou
17.15 to 18.00	Atom-Diatom Collisions in Bose and Fermi Gases	Professor J Hutson
18.00 to 18.45	Cold and ultra-cold collisions involving alkali atoms and diatoms	Professor J M Launay
<i>19.30</i>	<i>Reception</i>	

Tuesday February 8th 2005

<u>Session 3:</u>	<u>Cold Chemistry with Cold Atoms/Molecules</u>	
09.30 to 10.15	Quantum-state controlled ion chemistry at low temperatures	Dr R Wester
<i>10.15 to 10.45</i>	<i>Coffee</i>	
10.45 to 11.30	Metastable complexes formation and photochemistry in superfluid helium. Spectroscopy of Rb ₂ and KRb on the surface of He nanodroplets	Dr C Callegari
11.30 to 12.15	Towards Stark deceleration of SO ₂ to investigate it's cold photofragmentation	Dr C Lisdat
12.15 to 12.45	Discussion and summary	
<i>12.45 to 13.45</i>	<i>Lunch</i>	
<u>Session 4:</u>	<u>Low Temperature Chemistry</u>	
13.45 to 14.30	Coherent Control and Cold Chemistry	Professor R Kosloff
14.30 to 15.15	The CRESU apparatus: a unique tool to study reaction kinetics and energy transfer processes at ultra low temperatures	Dr A Canosa
15.15 to 16.00	The Low Temperature Frontier in Molecular Ion Collision Experiments	Dr H Kreckel
<i>16.00 to 16.30</i>	<i>Tea</i>	
16.30 to 17.15	Discussion of simple models of ultra cold chemical reactivity	Dr T Stoecklin
17.15 to 18.00	The Thermochemical Kinetics of Pure and Doped Ices in the Range 140-240k: a multidagnostic experimental Study	Dr M Rossi
18.00 to 18.30	Discussion and summary	
<i>19.00</i>	<i>Dinner</i>	

Wednesday February 9th 2005

<u>Session 5:</u>	<u>Astrochemistry</u>	
09.30 to 10.15	Experimental studies of gas phase reaction kinetics and energy transfer at very low temperatures	Professor I Sims
<i>10.15 to 10.45</i>	<i>Coffee</i>	
10.45 to 11.30	The chemistry and morphology of astrophysical ices	Dr M Collings
11.30 to 12.15	Laboratory physico-chemical processing of astrophysical ice analogues	Dr A Dawes
12.15 to 12.45	Discussion and summary	
<i>12.45 to 13.45</i>	<i>Lunch</i>	

<u>Session 6:</u>	<u>New Directions</u>	
13.45 to 14.30	Decelerating heavy polar molecules	Dr R Darnley
14.30 to 15.15	Production of three-body Efimov molecules in tight atom traps	Dr T Kölher
<i>15.15 to 15.45</i>	<i>Tea</i>	
15.45 to 16.15	Summary	Professor N Mason
16.15 to 18.00	Discussion and summary of meeting.	
<i>19.30</i>	<i>Conference Dinner</i>	

Thursday February 9th 2005

<u>Session 7:</u>		
09.30 to 10.15	Forward look and discussion of report of the workshop	
<i>10.15 to 10.45</i>	<i>Coffee</i>	
10.45 to 12.00	Writing report of workshop	
<i>12.00 to 13.00</i>	<i>Lunch</i>	
13.00	Departure	

Participants Contact Details and Countries of Origin

Dr. C. Callegari
Institut für Experimentalphysik
Technische Universität Graz
Petersgasse 16
8010 Graz
Austria
Tel: +43 316 873 8161
Fax: +43 316 873 8655
Mobile: +43 650 754 7072
Email: carlo.callegari@tugraz.at

Dr. A. Canosa
Laboratoire PALMS - Equipe Astrochimie
Experimentale
Campus de Beaulieu - Bât 11C
Universite de Rennes 1
35042 RENNES Cedex
France
Tel: 33 (0)2 23 23 69 96
Fax: 33 (0)2 23 23 67 86
Email: andre.canosa@univ-rennes1.fr

Dr. M. Collings
University of Nottingham
School of Chemistry
Floor A - Physical Chemistry
University Park,
Nottingham
NG7 2RD UK
Tel: 0115 95 13472
Fax: 0115 95 13562
Email: pczmpc@unix.ccc.nottingham.ac.uk

Mr. R. Darnley,
Room 606 Blackett Laboratory
Prince Consort Road
London
SW7 2AZ
UK
Tel: +44 (0) 207 594 7588
Fax: +44 (0) 207 594 7714
Email: richard.darnley@imperial.ac.uk

Dr. A. Dawes
(Room N0081a)
Department of Physics and Astronomy
The Open University
Walton Hall
Milton Keynes
MK7 6AA UK
Tel: +44 (0)1908 858255
Fax: +44 (0)1908 654192
Email: a.dawes@open.ac.uk

Dr. M. Drewsen
Department of Physics and Astronomy
University of Aarhus
Bygning 520
Ny Munkegade
DK-8000 Aarhus C
Denmark
Tel.: +45 8942 3752
Fax: +45 8612 0740
Email: drewsen@phys.au.dk

Prof. D. Field
University of Aarhus
Institute for Storage Ring Facilities
Ny Munkegade
8000 Aarhus C
Denmark
Tel: +45 8942 3650
Fax: +45 8612 0740

Prof. F. A. Gianturco
The Theoretical Chemical Physics Group
Department of Chemistry
University of Rome "La Sapienza"
P.le A. Moro,5 - 00185 Rome
Italy
Tel: +39-06-49913305
Fax:

Email: dfield@ifa.au.dk

Email: fa.gianturco@caspur.it

Prof. J. M. Hutson
Dept. of Chemistry
University of Durham
Durham
DH1 3LE
UK
Tel. (0191) 334 2147 (UK)
+44 191 334 2147 (International)
Fax: +44 191 384 4737
Email: j.m.hutson@durham.ac.uk

Dr. T. Kohler
Department of Physics
University of Oxford
Clarendon Laboratory
Parks Road
Oxford, OX1 3PU
UK
Tel: +44 (0) 1865 272276
Fax: +44 (0) 1865 272400
Email: t.koehler1@physics.ox.ac.uk

Prof. R. Kosloff
Department of Physical Chemistry,
Hebrew University,
Jerusalem 91904,
Israel
Tel: 972-2-6585485
home: 972-2-6529946
Fax: 972-2-6513742
E-mail: ronnie@fh.huji.ac.il

Dr. H. Kreckel
Max-Planck-Institut fuer Kernphysik
Saupfercheckweg 1
69117 Heidelberg
Germany
Fon: +49 06221 516452
Fax: +49 06221 516602
Email: holger.kreckel@mpi-hd.mpg.de

Prof. J.M. Launay
PALMS/SIMPA - UMR 6627 du CNRS,
Universite de Rennes I - Bat. 11B
35042 Rennes Cedex
France
Phone: +33 2 23 23 56 63
Fax: +33 2 23 23 56 62

Dr. C. Lisdat,
Institute for Quantum Optics,
University Hannover, Welfengarten 1,
30167 Hannover.
Germany
Tel. +49 511 762 4265
Fax +49 511 762 2211

Email: Jean-Michel.Launay@univ-rennes1.fr

Email: lisdatt@iqo.uni-hannover.de

Prof. N. Mason
The Open University
Walton Hall
Milton Keynes
MK7 6AA
UK
Tel: +44 1908 655132
Fax: +44 1908 654192
Email: n.j.mason@open.ac.uk

Prof. F. Masnou-Seeuws,
Laboratoire Aimé Cotton,
Bât. 505, Campus d'Orsay,
91405 ORSAY Cedex
France
Tel: 33(0)1 69 35 20 52(bureau); 20
00(standard);
33(0)6 24 06 93 11(portable).
Fax: 33(0)1 69 35 21 00.
Email: francoise.masnou@lac.u-psud.fr

Prof. dr. G. Meijer, director
Fritz-Haber-Institut der Max-Planck-
Gesellschaft
Faradayweg 4-6
D-14195 Berlin
Germany
Tel.: (+49) 30 8413 5602 (direct) / 5600
(secr.)
Fax: (+49) 30 8413 5603
Email: meijer@fhi-berlin.mpg.de

Dr. M. J. Rossi
Laboratory of Atmospheric Pollution
Studies (LPAS)
Ecole Polytechnique Fédérale de Lausanne
(EPFL) EPFL/ENAC/ISTE/LPASCH
H5 (Bâtiment CH) Station 6 CH-1015
LAUSANNE Switzerland
Tel.: +41 (0)21 693 53 21
Fax: +41 (0)21 693 36 26
Email: michel.rossi@epfl.ch

Prof. T. P. Softley
Chemistry Research Laboratory,
University of Oxford,
Mansfield Rd,
Oxford, OX1 3TA
UK
Tel: +44 (0) 1865 275428
Fax: + 44 (0) 1865 275410
Email: tim.softley@chem.ox.ac.uk

Dr. M. Weidemüller, Professor of Physics
Chair for Atomic & Molecular Quantum
Dynamics
Faculty for Mathematics and Physics
Albert-Ludwigs-Universität Freiburg
Hermann-Herder-Str. 3
D - 79104 Freiburg
Germany
Phone: +49-(0)761-2035740
Fax: +49-(0)761-2035707
Email: m.weidemueller@physik.uni-freiburg.de

Dr R. Mukerji
Department of Physics and Astronomy
The Open University
Walton Hall
Milton Keynes
MK7 6AA UK
Tel: +44 (0)1908 858255
Fax: +44 (0)1908 654192
Email: r.mukerji@open.ac.uk

Prof. I. Sims
PALMS - UMR 6627 du CNRS
Equipe: "Astrochimie Expérimentale"
Bat. 11c, Campus de Beaulieu,
Université de RENNES 1,
35042 RENNES Cedex,
France
Tel.: +33 2 23 23 69 18
fax.: +33 2 23 23 67 86
Email: ian.sims@univ-rennes1.fr

Dr. T. Stoecklin
Laboratoire de Physico-Chimie Moléculaire
351 Cours de la Libération
F- 33405 Talence
France
Tel : 33 (0)5 40 00 25 98
Fax : 33 (0)5 40 00 66 45
Email: t.stoecklin@lpcm.u-bordeaux1.fr

Dr. R. Wester, Professor of Physics
Chair for Atomic and Molecular Quantum
Dynamics
Faculty for Mathematics and Physics
Albert-Ludwigs-Universität Freiburg
Hermann-Herder-Str. 3
D - 79104 Freiburg
Germany
Tel: +49-(0)761-2035740
Fax: +49-(0)761-2035707
Email: roland.wester@physik.uni-freiburg.de