

Molecular Dynamics News

number 87, February 1997

MDN is an informal newsletter of coming attractions and current events in the world of reaction dynamics and associated phenomena. It is produced without profit through the support of its subscribers* and patrons. Please renew your subscription by using the form at the bottom of this page.

The format for **MDN** is

- a Announcements of *open positions* (faculty and postdoctoral).
- b Information about *papers*, whether accepted or not, which are available for distribution. Please state in separate lines: *Title. Journal* (If ms. has been accepted - otherwise state *unpublished*). *Author(s). Address.* (Star author to whom correspondence should be addressed and whose mailing address is given.) In a separate final line provide a *one-sentence punch line*. Please follow this format.
- c Announcements of *conferences, topical meetings, etc.* Availability of *special materials* (e.g., annual reports, computer programs, experimental designs and tips, etc.). *Progress* (or activity) *reports* about work which is not yet published but which may be of interest to our community.
- d Electronic mail addresses and FAX numbers.

MDN is edited by Prof. Vincenzo Aquilanti, Dipartimento di Chimica dell'Università, 06123 Perugia, Italy (electronic mail: AQUILA@HERMES.CHM.UNIPG.IT)
and **Prof. Roger W. Anderson, Dept. of Chemistry, University of California, Santa Cruz, CA 95064, U.S.A. (electronic mail: ANDERSO@CATS.UCSC.EDU).**

Send all material for issue 88 to Prof. Roger W. Anderson (**You are encouraged to use electronic mail: ANDERSO@CATS.UCSC.EDU**). (Please keep line length less than 75 characters.) Editing time will be saved if submissions correspond to the formats found in this issue (#87). The closing date for issue number 88 is April 1, 1997.

*1997 Calendar-Year subscription for **MDN**, (six issues).

North America: (\$20/year US currency) : Your check for one or more years should be paid out to The Regents of the University of California. Send it to Roger W. Anderson, and include your name, address, and optional information like email addresses and FAX numbers.

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Now anyone can access the newsletter as a LaTeX, dvi, HTML or Postscript file. A Web browser such as Mosaic with suitable viewers allows people to read the files on their computer screens. Alternatively the files can be downloaded for local viewing or printing. Subscribers choosing this delivery option will receive an email announcement when a new issue is posted. For information you are welcome to visit the Molecular Dynamics News World Wide Web site:

<http://www.ucsc.edu/mdn>

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We appreciate electronic mail with your reactions to this proposal and with updated email addresses. Please send your email messages to MDN@CHEMISTRY.UCSC.EDU

We continue to send hardcopy newsletters by mail to subscribers who request this form of delivery.

The MDN e-mail list will of course continue, as detailed below

MOLECULAR DYNAMICS NEWS EMAIL LIST

All members of the chemical physics community are invited to join the (free) "molecular-dynamics-news" email list. The "molecular dynamics" in the title is to be interpreted as meaning "dynamical processes in molecules" rather than "classical simulations of molecular motion". The list can be used to distribute details of conferences, vacant academic and postdoctoral positions, changes of address and other news in the Molecular Dynamics field. It also serves as an archive of up-to-date email addresses for people in the field. The list was created by Jeremy Hutson in June 1993 and now (January 1997) has about 1300 members. Instead of being maintained manually, the list is operated by a system called "mailbase". People can join or leave the list simply by sending messages to the mailbase program, without the list owner needing to do anything. To join the email list, send a message to the Internet address mailbase@mailbase.ac.uk containing a line of the form:

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join molecular-dynamics-news John F Kennedy
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You do not need to tell the program your email address, as it picks it up from the message header. It does need to be told your real name, so that it can maintain a useful list of email addresses.

When you join, you will receive some introductory information on how to circulate information to the molecular-dynamics-news list, and on the mailbase system itself.

If you would like a list of the current members, send a message containing the line
review molecular-dynamics-news

to the address mailbase@mailbase.ac.uk

Note that messages distributed via the e-mail list are not normally printed in the newsletter, unless the Editors receive an explicit request to do so.

There is a new spectroscopy email list. To join this email list, send a message to the Internet address mailbase@mailbase.ac.uk containing a line of the form:

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join spectroscopy-group John Kennedy
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a. Open Positions

POST DOCTORAL AND VISITING

UNIVERSITY OF MASSACHUSETTS, THEORETICAL MOLECULAR DYNAMICS

A postdoctoral position is currently open in my group, starting immediately. Over the past decade we have used a number of quantum and classical techniques to study the dynamics of several fundamental reactions on surfaces. Funding is available for several projects. One project involves the modeling of Eley-Rideal reactions, in which a gas phase atom or molecule reacts with a surface-adsorbed species. Studies of recombinative desorption are also planned. Another project investigates the dissociative adsorption of molecules on metal surfaces. Methods are being developed to include the effects of finite surface temperature in these reactions. Quantum methods are usually used to couple the reactants to the lattice phonons. The position is available for up to three years, starting at \$27,500 per year for the first year, plus full benefits (medical/dental).

Please send inquiries and three letters of recommendation to: Bret E. Jackson, Department of Chemistry, University of Massachusetts, Amherst, Massachusetts 01003 USA, 413-545-2583 office, 413-545-4490 FAX, jackson@tyrone.chem.umass.edu

UNIVERSITE DE MONTREAL, Departement de chimie

We (Benoit Roux and Tucker Carrington Jr) are looking for a postdoctoral fellow to work on the development and application of mixed quantum-classical methods. We are combining state of the art quantum mechanical tools (discrete variable representations and time dependent and time independent iterative methods) and classical trajectories to study molecules and reacting systems for which quantum effects are important but which are too big to study with a purely quantum mechanical approach. We have applied adiabatic and TDSCF mixed quantum-classical methods to calculate a proton transfer rate for acetylacetone. Experience with quantum and/or classical dynamical methods is important. The starting date is flexible.

The Universite de Montreal has a strong theory group and is located in an attractive, interesting city. Interested candidates should contact either Tucker Carrington or Benoit Roux. Tucker Carrington Jr., Departement de chimie, Universite de Montreal, Case postale 6128, succursale Centre-ville, Montreal (Quebec) H3C 3J7, Canada, tel: (514) 343-2123, fax: (514) 343-7586, e-mail: tucker@ere.umontreal.ca

UNIVERSITY OF UTAH, DEPARTMENT OF CHEMISTRY

I anticipate a postdoctoral position being available starting anytime within the next several months. The research involves studying vibrational mode effects and energy disposal in reactions of small polyatomic ions. The goals are to develop a more complete picture for the mechanisms of vibrational effects in polyatomic reactions, to examine the possibilities for vibrational control of reactions, and generally to understand the unique mechanistic features observed in these reactions. The reactant ions are created by MPI/PFI and sophisticated guided-ion beam techniques are used to measure product recoil energy and angular distributions.

References are given below for several papers in this area. More complete descriptions of this project, and others going on in the group, can be found on the web at

<http://www.chem.utah.edu/heb/faculty/anderson.htm>. Information on the University of Utah and the state of Utah can be found starting at <http://www.chem.utah.edu/> and <http://www.state.ut.us/>.

Two types of positions are possible. One is the usual postdoctoral research associate position, involving only research. In addition, the University of Utah runs a Faculty Intern program. In these positions, approximately 7/8 effort goes into research, averaged over the calendar year, and the other 1/8 time is spent in mentored teaching at the undergraduate level. This teaching experience can be quite valuable for those considering college teaching careers. Previous Faculty Interns have been successful at obtaining teaching positions at good colleges.

If interested, please send a curriculum vitae and arrange to have three letters of recommendation sent to:
Prof. Scott Anderson, Chemistry, University of Utah, Salt Lake City, UT 84112. Email is fine. The position pays a competitive salary with full benefits. The University of Utah is an equal opportunity employer.
Prof. Scott L. Anderson, Chemistry Department, University of Utah, Salt Lake City, UT 84112,
anderson@chemistry.utah.edu, Ph:(801)585-7289, FAX:(801)581-8433

UNIVERSITY OF ILLINOIS AT CHICAGO, DEPARTMENT OF CHEMISTRY

A post-doctoral position is open in the group of Prof. Robert Gordon at the University of Illinois at Chicago in the area of coherent control of chemical reactions. We have recently demonstrated control over the branching between ionization and dissociation of HI and DI (Science, 270, 77 (1995)), and we are starting more ambitious experiments involving bond-selective photodissociation. Other research involves controlling the photofragment state distribution by selecting the electronic "gateway" state which determines the subsequent interference in the asymptotic region (JCP, 103, 6811, (1995)).

Candidates for this position should have experience with YAG- and excimer-pumped dye lasers, pulsed molecular beams, and ion optics. The position is to start in the Spring of 1997, and funding is available for more than one year. Please send resumes and arrange for letters of recommendation to be sent to Robert Gordon, Department of Chemistry (m/c 111), University of Illinois at Chicago, 845 W Taylor Street, Chicago, IL 60076.

UNIVERSITY OF FREIBURG, GERMANY, DEPARTMENT OF PHYSICS

The Collaborative Research Center 276 "Correlated Dynamics of Highly-excited Atomic and Molecular Systems" is seeking a young, highly-qualified physicist as Theory Group Leader.

The group will work in the field of theoretical atomic, molecular or cluster physics with special emphasis on resonant and multi-fragmentation processes. Preference will be given to candidates interested in the interaction of strong laser fields with atoms, molecules or clusters.

The position (BAT IIa/Ib) is for a period of five years, starting on 1.1.1998, and subject to acceptance of a research proposal by the Deutsche Forschungsgemeinschaft. The University is seeking to increase the number of women faculty members, and encourages suitably-qualified women to apply.

Applicants should send a brief outline of a research proposal (1-3 pages) along with curriculum vitae and list of publications to: Prof. Dr. Ch. Schlier, Speaker SFB 276 Fakultät für Physik, Universität Freiburg Hermann-Herder-Str. 3, D-79104 Freiburg, Germany e-mail: schlier@uni-freiburg.de phone: +49-761-203-5818, FAX: +49-761-203-5873

UNIVERSITY OF ROME, DEPARTMENT OF CHEMISTRY, THEORETICAL CHEMICAL PHYSICS GROUP

Applications are invited for a postdoctoral position, funded by the Max-Planck-Research Society, to work in the area of quantum and classical dynamics applied to elementary processes in neutral and ionized rare gas clusters. The position would be available from early 1997 for a period of 12 months and could be extended for a second year or more. For further details please contact Prof. Franco A. Gianturco, Department of Chemistry, The University of Rome, Citta Universitaria, 00185 Rome, Italy. Fax: +39-6-49913305; e.mail: FAGIANT@CASPUR.IT.

UNIVERSITY OF TRENTO - ITALY, Department of Physics

A postdoctoral research position for 2 years is available in the research group of Davide Bassi and Paolo Tosi at Trento University, Italy, starting summer-fall 1997. The candidate will participate to the experimental activity of the group on molecular reaction dynamics by measuring cross-sections as a function of the collision energy in a guided-ion tandem mass spectrometer. Experience in one or more of the following fields is preferred: mass spectrometry and ion guides, electronics, vacuum and cryogenics techniques.

Applicants should contact as soon as possible Dr. Paolo Tosi (tosi@science.unitn.it).

For more info on the research activity <http://www-physics.science.unitn.it/booklet95/pag27-Bas.html>

NEW YORK UNIVERSITY - POSTDOCTORAL POSITION IN THEORETICAL CHEMISTRY

A postdoctoral position in theoretical chemistry is available in the research groups of Professors Zlatko Bacic and Jules W. Moskowitz. Projects include multidimensional quantum treatment of the bound states, spectra and photofragmentation dynamics of van der Waals and hydrogen bonded complexes and clusters, as well as spectroscopy and diffusion of atoms and molecules adsorbed on surfaces. Experience in quantum time-independent or time-dependent bound state or scattering calculations is required. The position is available from April 1997, but a later starting date is negotiable. Salary is competitive, commensurate with experience. Please send curriculum vitae and two letters of recommendation to Prof. Zlatko Bacic, Department of Chemistry, New York University, New York, New York 10003, USA (Telephone: 212-998-8435, Fax: 212-260-7905, E-mail: bacic@zlatko.chem.nyu.edu).

NATIONAL CHUNG-CHENG UNIVERSITY, DEPARTMENT OF CHEMISTRY, THEORETICAL CHEMISTRY GROUP

Applicants are invited for postdoctoral positions to work in the area of (1) cluster formation, stability and dynamics and (2) molecular optical nonlinearities. The position would be available from August 1997 for a period of 12 months and could be extended for a second year or more.

Please send resumes and arrange for letters of recommendation to be sent to: Prof. Shyi-Long Lee, Department of Chemistry, National Chung-Cheng University, Chiayi, Taiwan. FAX: 886-5-2721040; e-mail: sllee@nas01.ccu.edu.tw.

POSTDOCTORAL POSITION IN HELSINKI

A postdoctoral position is available in the Laboratory of Physical Chemistry, University of Helsinki for about two years. The monthly grant is about 2000 ECU (approx. 3760 DM) tax free. The successful candidate who must be of EU nationality (but not from Finland) is expected to perform theoretical research in the field of overtone spectroscopy: local modes, Fermi resonances, internal coordinate Hamiltonians, potential energy surfaces.

More information can be obtained from Prof. Lauri Halonen tel. +358-9-19140280, fax +358-9-19140279, email: lauri.halonen@csc.fi.

b. Preprints

A coupled-cluster ab initio study of triplet C₃H₂ and the neutral-neutral reaction to interstellar C₃H

J. Chem. Phys

Christian Ochsenfeld, Ralf I. Kaiser, Yuan T. Lee, Arthur G. Suits, Martin Head-Gordon
Department of Chemistry, University of California at Berkeley Berkeley, CA 94720, USA

For the initially formed C₃H₂ collision complexes of molecular beam experiments ab initio calculations are presented. Resolving energetics and properties of these intermediates is essential for the understanding of the reaction of C(³P) with C₂H₂ to form interstellar cyclic and linear isomers of C₃H. Computed reaction energies agree with results from molecular beam experiments. The combination of crossed molecular beam experiments and ab initio calculations allows to identify two reaction channels for the carbon-hydrogen exchange and to explain astronomical observations of a higher c-C₃H to l-C₃H ratio in dark clouds as compared to hotter envelopes of carbon stars.

Diffusion in one-dimensional disordered systems: analytical study verified by Monte Carlo simulations

Unpublished

L.D.A. Siebbeles and Yu.A. Berlin

Interfaculty Reactor Institute, Mekelweg 15, 2629 JB Delft, The Netherlands

Analytical expressions for the time-dependent diffusion coefficient describing the thermally activated hopping motion in a disordered energy landscape were obtained by use of the effective medium approximation. The results were shown to be accurate by comparison with computer simulations.

The zero-point energy problem in classical trajectory simulations at dissociation threshold

Journal of Chemical Physics

Drew A. McCormack and Kieran F. Lim*

School of Biological and Chemical Sciences, Deakin University, Geelong, Victoria 3217, Australia
lim@deakin.edu.au

ZPE constraints in classical trajectories are applied to the H₂He system and water at energies just below the (quantum) dissociation threshold.

Zero-point energy correction for trajectory rate data

J. Chem. Soc., Faraday Trans.

Kieran F. Lim.

School of Biological and Chemical Sciences, Deakin University, Geelong, Victoria 3217, Australia
lim@deakin.edu.au

The relationship between various ZPE preservation schemes is discussed.

Zero-point energy constraints in RRKM and non-RRKM molecules

Unpublished.

Drew A. McCormack and Kieran F. Lim*

School of Biological and Chemical Sciences, Deakin University, Geelong, Victoria 3217, Australia
lim@deakin.edu.au

ZPE constraints in classical trajectories preserve the RRKM behaviour of dissociating Al₃ clusters but not the non-RRKM behaviour of HNC isomerisation.

Adsorption of Organic Molecules on Large Water Clusters

J. Phys. Chem., **101** (1997) March.

M. Ahmed, C.J. Apps, C. Hughes, N.E. Watt and J.C. Whitehead
Chemistry Department, Manchester University, Manchester, M13 9PL.
j.c.whitehead@man.ac.uk

A study of the sticking efficiencies for a range of organic species on large water clusters.

Adsorption of N_xO_y -based molecules on large water clusters: An experimental and theoretical study

J. Phys. Chem., **101** (1997) March

M. Ahmed, C.J. Apps, R. Buesnel, C. Hughes, I.H. Hillier, N.E. Watt and J.C. Whitehead

Chemistry Department, Manchester University, Manchester, M13 9PL.

j.c.whitehead@man.ac.uk

A study of the sticking and reactivity of N_xO_y species on large water clusters interpreted by ab initio calculations for prototype systems.

The photodissociation dynamics of OCIO between 300 and 370 nm: Fragment translational energy release and recoil anisotropy

Journal of Chemical Physics

A. Furlan, H.A. Scheld and J.R. Huber

Physikalisch-Chemisches Institut, Winterthurerstrasse 190 CH-8057 Zuerich

jrhuber@pci.unizh.ch

The decay $OCIO(^2A_2) \rightarrow ClO(X) + O(P)$ is shown to create ClO fragments in highly inverted vibrational state distributions which become extremely broad ($n \sim 1 - 16$) with increasing excitation energy and thus could enhance various thermodynamically unfavorable atmospheric reactions in connection with ozone depletion.

Endohedral fullerene production

Nature **382** (1996) p. 407-408R.

Tellgmann, N. Krawez, S.-H. Lin, I.V. Hertel and E.E.B. Campbell

Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, Postfach 1107, Rudower Chaussee 6, 12474 Berlin, Germany

The production of thin films containing ca. 30% endohedral $Li@C_{60}$ as determined by LDMS is reported. The rovib. movement of the Li inside the C_{60} cage is observed by IR spectroscopy.

Ultrafast Laser Pump and Control in Small Sodium-Ammonia Clusters

Femtochemistry, Ultrafast Chemical and Physical Processes in Molecular Systems, ed. Majed Chergui, Lausanne, Schweiz, World Scientific (1996) p. 250-254

C.P. Schulz, J. Hoehndorf, P. Brockhaus, F. Noack, I.V. Hertel

Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, Postfach 1107, Rudower Chaussee 6, 12474 Berlin, Germany

Ultrafast dynamics of $Na(NH_3)_n$ ($n = 1, 2$) is studied using amplified 150 fs Ti:Sapphire laser radiation. Femtosecond pump probe experiments using the red photon (820 nm) to excite and the second harmonics (410 nm) to ionise the clusters show that the first electronically excited state of $NaNH_3$ (A^2E) is stable for at least time $t \sim 1$ ns.

Ultrafast Fragmentation and Ionisation Dynamics in Ammonia Clusters

Femtochemistry, Ultrafast Chemical and Physical Processes in Molecular Systems, ed. Majed Chergui, Lausanne, Schweiz, World Scientific (1996) p. 255-258

Th. Freudenberg, W. Radloff, H.-H. Ritze V. Stert, F. Noack and I.V. Hertel

Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, Postfach 1107, Rudower Chaussee 6, 12474 Berlin, Germany

The formation of protonated and unprotonated ammonia cluster ions is studied by femtosecond two colour two photon pump-probe techniques. $(NH_3)_n$ and $(ND_3)_n$ clusters with n up to 8 are investigated. Several distinct intermediate steps in the time evolution ranging from 40 fs to over 100 ps can be distinguished and are discussed in a consistent scheme for the excitation, ionisation and protonation dynamics.

Thermionic emission and fragmentation of C_{60}

Phys. Rev. Lett, submitted

K. Hansen* and O. Echt†

* Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, Postfach 1107, Rudower Chaussee 6, 12474 Berlin, Germany

† Physics Department, University of New Hampshire, Durham, NH 03824, USA

We analyze the rate of delayed (thermionic) ionization of photo-excited C_{60} molecules. The rate has a power law dependence, indicating the presence of a continuum of rate constants. The value of the exponent provides information about the competition between delayed ionization and unimolecular fragmentation; it is equal to the ratio of the ionization energy and the activation energy for fragmentation. This result provides a novel method to measure the controversial bond dissociation energy of neutral C_{60} . We obtain a value of 11.9 ± 1.9 eV.

Extraction and HPLC Isolation of $Li@C_{60}$ with CS_2

Journal of the American Chemical Society, submitted

A. Gromov, W. Kraetschmer, N. Krawez, R. Tellgmann and E.E.B. Campbell*

Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, Postfach 1107, Rudower Chaussee 6, 12474 Berlin, Germany

Films containing ca. 30% of the endohedral material can be separated from the rest by means of HPLC.

Ultra Short Pulse Laser Ablation of Silicon: A MD-Simulation Study

Phys. Rev. B, submitted

R.F.W. Herrmann*, J. Gerlach† and E.E.B. Campbell*

* Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, Postfach 1107, Rudower Chaussee 6, 12474 Berlin, Germany

† GMD-FIRST, Rudower Chaussee 5, 12489 Berlin, Germany

Laser ablation of silicon surfaces has been investigated by Molecular Dynamics (MD) simulations. The laser pulse lengths investigated covered the range of 10 fs to 5 ps. Structures of approximately $100 \text{ \AA} \times 100 \text{ \AA} \times 50 \text{ \AA}$ were simulated. The ablation shows a strong dependence on pulse length, on pulse energy and on the number of laser shots.

Micromachining of Quartz with Ultrashort Laser pulses

Appl. Phys. A, submitted

H. Varel, D. Ashkenasi, A. Rosenfeld, M. Waehmer, E.E.B. Campbell

Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, Postfach 1107, Rudower Chaussee 6, 12474 Berlin, Germany

Well-defined and highly reproducible channels of a few micrometres diameter and lengths of over 1 nm have been produced in quartz with laser pulses of 790 nm wavelength (Ti:Sapphire) and pulse lengths of 100-200 fs. The channel depth can be controlled by the laser fluence and number of laser shots. Comparisons were made with laser pulse lengths of 2.8 ps, 30 ps and 5 ns.

Stability of Carbon Clusters C_N for $44 < N < 104$

Int. J. Mass. Spectr. & Ion Processes

P.E. Barran#, S. Firth#, A.J. Stace#, H.W. Kroto#, K. Hansen* and E.E.B. Campbell*

*Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, Postfach 1107, Rudower Chaussee 6, 12474 Berlin, Germany

School of Chemistry and Molecular Sciences, University of Sussex, Brighton BN1 9QJ, U.K.

Relative binding energies for $C_{N-2} - C_2$ have been determined for fullerene ions in the range $46 < N < 104$. The values were derived from metastable fractions observed in a time-of-flight reflectron mass spectrometer. The timescale of the experiments was such that radiative cooling of the fullerene ions did not play an important role thus simplifying the data analysis. The results are compared with previous values of relative dissociation energies for C_2 loss.

Dissociation energies for large fullerenes ($N > 60$) are significantly higher than previously estimated.

Ultrafast dynamics in ammonia clusters: Analysis of protonated and unprotonated cluster ion signals

Z. Phys. D, submitted

Th. Freudenberg, W. Radloff, H.-H. Ritze and V. Stert, F. Noack and I.V. Hertel
Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, Postfach 1107, Rudower Chaussee 6,
12474 Berlin, Germany

The dynamics of ammonia clusters excited to the A state with 160 fs laser pulses of 6.2 eV was studied by pump-probe experiments with a low probe photon energy of 3.1 eV. Protonated as well as unprotonated cluster ion signals have been observed. The time evolution of both species is characteristic of the intermediate rearrangement and fragmentation processes.

Fragmentation Analysis of Size Selected Sodium Clusters

J. Chem. Phys., submitted

I.V. Hertel and C.P. Schulz*, A. Goerke†, H. Palm and Gregor Leipelt†

* Max-Born-Institut for Nonlinear Optics and Short Pulse Spectroscopy, Postfach 1107, Rudower Chaussee 6, 12474 Berlin, Germany

† Info Process GmbH, D-79256 Buchenbach, Germany Physikalische Chemie, ETH Zuerich, Universitaetsstrasse 16, CH-8092 Zuerich, Switzerland

The fragmentation processes of small sodium clusters induced by photoionization are investigated for a size selected neutral cluster beam. We use the collision induced momentum transfer in a crossed beam experiment to achieve the separation of the masses. Photoions produced with photon energies up to 4.66 eV are mass analyzed in a time-of-flight mass spectrometer.

Vibrational predissociation of the ND₃-Ar van der Waals complex: Comparison with NH₃-Ar

Unpublished

J. Millan, N. Halberstadt,* G.C.M. van der Sanden, and A. van der Avoird*

LCAR-IRSAMC, Université Paul Sabatier, 118 route de Narbonne, 31062 Toulouse CEDEX, France

* Institute of Theoretical Chemistry, NSR Center, University of Nijmegen, Toernooiveld, 6525 ED Nijmegen, The Netherlands

Vibrational predissociation of ND₃-Ar through excitation to the ν_2 "umbrella" mode of ND₃ is investigated using the same ab initio potential and the same quantum mechanical method as used earlier for NH₃-Ar. The effect of exciting Van der Waals levels is examined. The results for ND₃-Ar are confronted with those for NH₃-Ar, where the quasibound states are more delocalized.

Experimental investigation of the rotational- and vibrational-state dependence of HF-Rg interactions

J. Chem. Phys. **105** (1996), 6375

E.J. van Duijn, R. Nokai and L.J.F. Hermans

The influences of the vibrational and the rotational quantum number upon the transport collision rate are found to be independent and have been determined for HF in a bath of He, Ar, Kr or Xe from experiments on light-induced drift.

The role of the rotational state in intermolecular interactions of H₂O with H₂ and CH₃Cl

International Journal of Thermophysics

E.J. van Duijn and L.J.F. Hermans

The transport collision rate (or cross section) of H₂O is found to decrease by 25% with increasing J in a bath of CH₃Cl, and by only 1% in H₂. This is attributed to the role of the dipole-dipole potential.

Variation of dipole-dipole interaction with rotational state: Experiment and theory

Unpublished

E.J. van Duijn, G. Nienhuis and L.J.F. Hermans, I. Kuscer

The transport collision rate (or cross section) of systems like HF-CH₃F can decrease by more than 40% with increasing J , due to increased averaging out of the dipole-dipole potential.

Level-crossing resonances in nuclear spin conversion of molecules

Phys. Rev. Lett. **77** (1996), 4732

B. Nagels, N. Calas, D.A. Roozmond, L.J.F. Hermans and P.L. Chapovsky

A sharp increase in conversion rate of gaseous CH₃F is observed when an electric field produces crossing of ortho and para energy levels, confirming mixing-of-states as the dominant conversion mechanism.

Laser-induced forces on small objects in a resonant background gas

Journal of Applied Physics

E.J. van Duijn, L.N. Cornelisse, P.L. Chapovsky and L.J.F. Hermans

Laser-induced forces resulting from internal-to-translational energy conversion in collisions of velocity-selectively excited molecules with surfaces are experimentally investigated. We use HF or CH₃F.

Multiscaling in Random Cluster-Cluster Aggregates

To appear in *Fractals in the Natural and Applied Sciences*, Edited by M.M. Novak (World Scientific, Singapore)

V.A. Markel, V.M. Shalaev, E.Y. Poliakov and Thomas F. George*

Office of the Chancellor / Departments of Chemistry and Physics & Astronomy - University of Wisconsin-Stevens Point

Stevens Point, Wisconsin 54481-3897

tgeorge@uwsp.edu

Two-point density correlation functions are studied numerically in computer-generated three-dimensional lattice cluster-cluster aggregates with the number of particles up to 20,000, where it is found that large cluster-cluster aggregates demonstrate pronounced multiscaling, *i.e.*, the power-law exponents in the pair-correlation function $p(r)$ are not constants, but depend on r and the number of particles in a cluster.

Enhanced Nonlinear-Optical Responses of Disordered Clusters and Composites

To appear in the *Proceedings of the Institute for Mathematics and Its Applications*, Edited by J.V. Moloney and J.E. Sipe (Springer, New York)

Mark I. Stockman, Lakshmi N. Pandey and Thomas F. George*

Office of the Chancellor / Departments of Chemistry and Physics & Astronomy - University of Wisconsin-Stevens Point

Stevens Point, WI 54481-3897

tgeorge@uwsp.edu

Clusters and nanocomposites belong to so-called nanostructured materials. Self-similar (fractal) systems, which (approximately) repeat themselves at different scales, are examined.

Viscosity and Ultrasonic Attenuation in ⁴He Below 0.6 K

To appear in *Fizika Nizkikh Temperatur*

Chung-In Um, Soo-Young Lee, Sahng-Kyoon Yoo, Lakshmi N. Pandey, Igor N. Adamenko and Thomas F. George*

Office of the Chancellor / Departments of Chemistry and Physics & Astronomy - University of Wisconsin-Stevens Point

Stevens Point, Wisconsin 54481-3897

tgeorge@uwsp.edu

Through a treatment of three-phonon processes, the wide-angle scattering rates and the absorption rates of phonons, which characterize viscosity and ultrasonic attenuation, respectively, are calculated for ⁴He below 0.6 K. These rates are obtained from the collision matrix which is constructed approximately from an integral eigenvalue equation for the collision operator.

Van der Waals interactions from density functional theories

in *Conceptual trends in Quantum Chemistry*, E. Kryachko Ed., Reidel Publ.(1997)

F.A. Gianturco*, F. Paesani

Department of Chemistry, The University of Rome, Città Universitaria, 00185 Rome, Italy.

The system He-CO has been analysed using different forms of correlation and exchange corrections from density functional theories.

Application of parallel computing to electron-molecule scattering processes

in *Photon and Electron Collisions with Atoms and Molecules*, P.G. Burke and C.J. Joachain Ed.s, Plenum Publ. Co., New York (1998)

F.A. Gianturco*, N. Sanna

Department of Chemistry, The University of Rome, Città Universitaria, 00185 Rome, Italy.

A general code for elastic and inelastic collisions of low energy electrons from polyatomic molecules is analysed in terms of its porting on several parallel platforms.

Low-energy electron scattering from Methane

J.Phys. B: at. mol. phys. (submitted)

F.A. Gianturco*, N. Sanna, C.T. Bundschu, J.C. Gibson, R.J. Gulley, M.J. Brunger and S.J. Buckman

Department of Chemistry, The University of Rome, Città Universitaria, 00185 Rome, Italy.

Several experimental results and theoretical calculations of elastic and inelastic cross sections, integral and differential, are compared and analysed.

Scattering of electrons from SO₂ molecules: elastic cross sections and rotational excitation

J.Phys. B: at. mol. phys. (submitted)

F.A. Gianturco*, P. Paiolletti, N. Sanna

Department of Chemistry, The University of Rome, Città Universitaria, 00185 Rome, Italy.

Several experimental results are shown to be well reproduced and explained by recent ab initio quantum calculations.

The role of vibrational coupling in positron scattering from molecular systems

J.Phys. B: at. mol. phys. (submitted)

F.A. Gianturco*, T. Mukherjee

Department of Chemistry, The University of Rome, Città Universitaria, 00185 Rome, Italy.

The effect of threshold coupling at the opening of the vibrational channels is analysed for positron scattering off a polyatomic system like CO₂.

Fragmentation of Ar₃⁺: the role of rotational and vibrational predissociation dynamics

Mol. Eng. (submitted)

F.A. Gianturco*, E. Buonomo

Department of Chemistry, The University of Rome, Città Universitaria, 00185 Rome, Italy.

Calculations study of the quantum fragmentation dynamics using ab initio methods and comparing different coupling schemes are reviewed in detail.

On the low-energy rotationally inelastic collisions of H⁻ on H₂ molecules

J.Phys. B: at. mol. phys. (submitted)

F.A. Gianturco*, S. Kumar

Department of Chemistry, The University of Rome, Città Universitaria, 00185 Rome, Italy.

The rotational excitation of H₂ in collision with H⁻ projectiles is studied under different coupling schemes and compared with experiments.

On some possible mechanisms for Ar₄⁺ fragmentation: a computational modeling

Chem. Phys. Lett. (submitted)

F.A. Gianturco*, E. Buonomo, M.P. De Lara-Castells

Department of Chemistry, The University of Rome, Città Universitaria, 00185 Rome, Italy.

Possible mechanisms involving nuclear-excited ionic cores are suggested for explaining the experimental results on Argon tetramer ion fragmentations.

Positron scattering from polar molecules

Phys. Rev. A (submitted)

F.A. Gianturco*, T. Mukherjee, P. Paiolletti

Department of Chemistry, The University of Rome, Città Universitaria, 00185 Rome, Italy.

The rotovibrationally inelastic cross sections, integral and differential, are computed and analysed for the CO molecule.

Generalized potential harmonics and contracted Sturmians

Chem. Phys. Lett. December 1996

V. Aquilanti[†] and J. Avery*

[†] Dipartimento di Chimica dell'Università - 06123 Perugia, Italy

* Department of Physical Chemistry H.C. Ørsted Institute; University of Copenhagen, Denmark.

A formalism is described for choosing computationally manageable Sturmian basis set which are automatically adapted to the requirements of particular physical problems.

Bond Stabilization by Charge Transfer: the Transition from van der Waals Forces to the Simplest Chemical Bonds

Chem. Phys. Lett.

V. Aquilanti, D. Cappelletti and F. Pirani

Dipartimento di Chimica dell'Università - 06123 Perugia, Italy.

The passage is documented along the series of monohalides and monoxides of the rare gases, experimentally observed from molecular beam scattering of orbitally aligned oxygen and halogen atoms by rare gases and simple molecules. A correlation rule allows extension to excimer states and other (pseudo)-one-electron-bound systems, such as the rare-gas dimer ions.

c. Conferences

1. EXTRA TERRESTRIAL CHEMISTRY AND BIOLOGY - 25th Leermakers Symposium

Wesleyan University Middletown, CT 06459

Featured speakers will be Patrick Thaddeus, Harvard-Smithsonian Center for Astrophysics; William Klemperer, Department of Chemistry, Harvard University; Richard Zare, Department of Chemistry, Stanford University; Ralph Harvey, Geological Sciences, Case Western Reserve; Leslie Orgel, Department of Chemical Evolution, Salk Institute; and J. William Schopf, IGPP Center for the Study of Evolution and the Origin of Life, UCLA.

Those interested in receiving a mailing detailing this one-day symposium should contact Lucile Blanchard, at (860) 685-2572 or Stewart Novick at snovick@wesleyan.edu.

NB: I should have the titles of the talks by the end of January

2. XVII INTERNATIONAL SYMPOSIUM ON MOLECULAR BEAMS

Paris XI University, Orsay, June 2-6, 1997

The XVII INTERNATIONAL SYMPOSIUM ON MOLECULAR BEAMS will be held June 2-6, 1997, in Paris XI University at Orsay. It is organized by the Laboratoire Aime Cotton (CNRS, Orsay) and the Service des Photons, Atomes et Molecules (CEA, Saclay). The local Committee includes C.Collieux (Orsay), I.Dimicoli (Saclay), P.Luc (Orsay), I.Nenner (Chair, Saclay), A.Sarfati (Secretary, Orsay), R.Vetter (Chair, Orsay) and J.P.Visticot (Treasurer, Saclay).

Topics : manipulation of atoms and molecules, development of new techniques, time-resolved experiments, spectroscopy, fragmentation, reaction dynamics, metallic clusters, molecular clusters and large molecules, fullerenes, gas-liquid and gas-surface interactions.

Invited speakers : M.N.R.Ashfold (Bristol), A.Aspect (Orsay), B.Brunetti (Perugia), P.Cahuzac (Orsay), C.Desfrancois (Villetaneuse), D.Dowek (Orsay), M.Faubel (Gottingen), M.Jarrold (Evanston), C.Jouvet (Orsay), D.A.King (Cambridge), A.W.Kleyn (Amsterdam), W.C.Lineberger (Boulder), K.Liu (Taipei), A.L'Huillier (Lund), T.D.Maerk (Innsbruck), T.P.Martin (Stuttgart), G.Meijer (Nijmegen), F.Merkt (Zurich), M.Mons (Saclay), R.Naaman (Rehovot), A.Perez (Lyon), H.Schmidt-Boking (Frankfurt), U.Schmitt (Zurich), G.Scoles (Princeton), T.Seideman (Ottawa), A.G.Suits (Berkeley), P.Tosi (Trento), J.Vigué (Toulouse), R.Weinkauff (Garching) and K.Yamanouchi (Tokyo). Short oral presentations of hot topics and two poster sessions are planned.

The symposium will take place in the Auditorium Pierre Lehmann at Orsay, from Monday June 2nd, 1997 at 9.00 to Friday June 6 after lunch. Registration and welcome buffet will take place in the Paris Quartier Latin on Sunday June 1st, from 16.00 to 22.00. A conference fee of 1,500 F.F. will be charged, including the book of abstracts, the welcome buffet and 5 lunches at Orsay. A conference dinner will be organized either on Wednesday June 4 or on Thursday June 5, in Paris, at a supplementary cost of 350 F.F. The participants will be accommodated in hotels of the Paris Quartier Latin, close to the RER B line which connects Paris to Orsay. Please, contact by fax the travel agency HAVAS and make room reservation before April 1st (Havas Communication Voyages, c/o Laure Dupont, fax : 33 1 47 96 77 32). Please, note that the whole journey between Paris and the Auditorium may last 1 hour and that Paris hotels are usually heavily crowded in June. For further information and application, contact Alain Sarfati (Secretary SMB17) by electronic mail (smb17@sun.lac.u-psud.fr) or by fax (33 1 69 35 20 04) or visit the WWW site (<http://www.lac.u-psud.fr/smb17>).

DEADLINE FOR APPLICATION, PAYMENT OF CONFERENCE FEES AND SUBMISSION OF ABSTRACTS: APRIL 1st, 1997 (later payments will be charged by a 400 F.F. extra)

3. The 9th International Congress of Quantum Chemistry

Emory University, Atlanta, Georgia (USA); June 9-14, 1997.

This is the largest international conference in quantum molecular sciences and held every three years around the world, this one following the 8th Congress at Prague in 1994. The Congress topics include (I) Methods: Parallel Computation-quantum chemistry code implementation, Density functional theory, Perturbation and Coupled Cluster, Multi-reference Approaches, Basis Sets and Corrections for Inadequacy, Hybrid Methods (QM/MM, etc.); (II) Applications: Photochemistry, Non-adiabatic Effects, Electronic Structure in Condensed Media, Intermolecular Interactions, Spectroscopy, Chemical Reactivity, Organic Reactions, Homogeneous Catalysts, Solid Surface and Heterogeneous Catalysis, Materials and Solid States, Biological Applications, Dynamics of Nuclear Motion, Statistical Applications, Industrial Applications. Plenary speakers are Reinhart Ahlrichs, Michele Parrinello and Martin Quack. Invited speakers include P. Armentrout, M. Bowers, S. Ceyer, E. Heller, J. C. Light, N. Makri, V. Bondybey, L. S. Cederbaum and many others. Organizing committee is Kieji Morokuma (Chair), Ernest R. Davidson and Henry F. Schaefer. Several satellite meetings are planned on Density-Functional Theory and Computation; Theoretical Chemistry in Biology - From Molecular Structure to Functional Mechanisms; Structural and Mechanistic Organic Chemistry; Coupled Cluster Theory and Electron Correlation Workshop; Interplay between Theory and Experiment in Molecular Spectroscopy and Dynamics. For the first circular and other information, visit the WWW site <http://www.chem.emory.edu/icqc/icqc.html>, send e-mail to icqc@euch4g.chem.emory.edu, Fax to Morokuma at (1)404-727-6586, or mail to Keiji Morokuma, Department of Chemistry, Emory University, Atlanta, GA 30322, USA.

4. Optical, electric and magnetic properties of molecules

Cambridge University, UK; 10-13 July 1997.

This conference is being organised to celebrate the career of Professor A. David Buckingham. Those interested in attending should write to Prof. David C Clary, Department of Chemistry, University College London, London WC1H OAJ, UK or Professor Brian J. Orr, School of Chemistry, Macquarie University, NSW 2109, Australia. The Keynote Lecturers will be: D.P. Craig, N.C. Handy, J.-P. Hansen, D.R. Herschbach, D.A. King, W. Klemperer, R.A. Marcus, J.A. Pople, A.H. Zewail. Invited Speakers: L. D. Barron, C. A. de Lange, P. W. Fowler, J. M. Hutson, D. M. Neumark, G. L. D. Ritchie, J.-L. Rivail, R. J. Saykally, P. J. Stephens. Principal Organisers: D. C. Clary (UCL, UK) and B. J. Orr (Macquarie, Australia). Conference Secretary: M. J. T. Jordan (Cambridge, UK).

The conference will start after lunch, at 2pm, on Thursday 10 July 1997 and finish with breakfast on Sunday 13 July. Lectures will be held in the Department of Chemistry, University of Cambridge and accommodation will be in Pembroke College Cambridge. Cambridge is easy to get to from London by rail and from Stansted and Heathrow Airports by bus. Sponsors for the conference include Elsevier, Taylor and Francis, Shell and CCP6. The total cost for registration and accommodation will be close to 240 pounds. There will be a limited capacity for contributed poster papers. More details will be sent out in 1997 to those who register their interest now. The www site for the meeting is : <http://nickel.chem.ucl.ac.uk/adb.conference/>

If you would like to take part in the conference, please email the form below to: Dr Meredith Jordan, Conference Secretary, Department of Chemistry, University of Cambridge, Lensfield Rd Cambridge, CB2 1EW, UK. Email: mjtj2@cus.cam.ac.uk Fax: [44]-(1223)-336 362

I would like to attend the conference:

OPTICAL, ELECTRIC AND MAGNETIC PROPERTIES OF MOLECULES: A conference to celebrate the career of Professor A. D. Buckingham
July 10-13 1997 Cambridge, UK

Name:

Email:

Fax:

Address:

Suggested Poster Title (optional):

Please email this completed form to mjtj2@cus.cam.ac.uk

5. 1997 Conference on the Dynamics of Molecular Collisions

Gull Lake, Minnesota USA, July 20-25, 1997

The Dynamics of Molecular Collisions (DMC) Conference is the major conference in the United States on the topic of molecular collisions and related phenomena. This conference was begun as a Gordon Conference in 1965, and has been held every two years since then. In recent years it has been held at major resorts around the country, most recently (1995) at the Asilomar Conference Center in Pacific Grove, California (Dan Neumark, chair). The Asilomar Meeting attracted over 300 participants from around the world, with 23 invited talks and about 235 poster talks. The 1997 Conference will be held at Cragun's Resort on Gull Lake near Brainerd Minnesota. This resort is located in the central lakes district of Minnesota in a region of beautiful pine forests and many thousands of lakes. The conference was last held at Cragun's in 1983. Since then the resort has been substantially improved, with increased space for poster and oral talks, modernized sleeping rooms, and many new recreational facilities including an indoor sports center. In addition, Cragun's has its own beach, sail and motor boats, tennis courts and golf course, and nearby are hiking and biking trails and other attractions. Cragun's is about a 2.5 hour drive from the Minneapolis airport; we plan to arrange for ground transportation to and from the conference. Alternatively, if you fly on Northwest airlines to Minneapolis, the extra fare to fly to the Brainerd airport is about \$40 roundtrip. The scientific program will be international and will cover all aspects of molecular collisions, including reactive and nonreactive collisions, and related photochemistry and surface processes. Both experimental and theoretical topics will be included. Suggestions for specific areas or speakers are welcome and should be addressed to the conference chair. The meeting will follow a Gordon Conference format, i.e., morning and evening sessions from Monday morning to Friday noon, with afternoons free for informal discussions, recreation, and relaxation. Time will be set aside for formal presentation of poster papers and long discussion periods after invited talks. The conference program committee consists of chair George C. Schatz, Northwestern University and vice-chair James J. Valentini, Columbia University. Further details will be announced in the fall of 1996. This conference has generally included at least one representative of almost every major experimental and theoretical group studying molecular collision dynamics in the United States, as well as a very good representation from foreign groups. We hope that you will be able to attend the 1997 meeting and urge you to mark off the week of July 20-25 on your calendar now.

IMPORTANT INFORMATION: If you are interested in receiving additional information concerning this conference (such as the second announcement), please send your name, address, phone, fax and email to: George C. Schatz, Department of Chemistry, Northwestern University, Evanston IL 60208-3113, phone: 1-847-491-5657, fax: 1-847-491-7713, email: dmc@chem.nwu.edu

Web site for conference: <http://www.chem.nwu.edu:80/schatz/index.html> (This web site repeats the information in this announcement right now, but it will eventually contain information about speakers, lists of attendees, information about Cragun's, registration and housing forms, etc.)

6. 1997 TWENTY-THIRD INTERNATIONAL SYMPOSIUM ON FREE RADICALS

Taellberg, Dalarna, Sweden, August 17-22, 1997

Organizing committee:

Mats Larsson (chairman), Physics Department I, KTH, Stockholm (larsson@atom.kth.se)

Bosse Lindgren, Physics Department, Stockholm University, Stockholm

Lars-Erik Berg, Physics Department I, KTH, Stockholm (berg@atom.kth.se)

Sven Mannervik, Atomic Physics, Stockholm University, Stockholm

The 1997 Twenty-third International Symposium on Free Radicals will be held Aug 17- 22, 1997 at Green Hotel, Taellberg, Dalarna, Sweden. The Symposium will address the physical and chemical properties of FREE RADICALS, including paramagnetic molecules, ions, molecules in excited states and short-lived species. A wide variety of topics will be covered by papers and discussions: Spectroscopy of radicals; Dynamics and reaction kinetics, theory and experiment; Structure of free radicals; Molecular ions and molecules in excited states; Free radicals and atmospheric chemistry; Interstellar spectroscopy and chemistry; Free radicals as reaction intermediates; Free radicals in applied research; Production and observation techniques.

There will be several invited talks covering the listed topics above. Contributed papers will be presented in poster sessions with a brief introduction by the author. The conference will be held at Green Hotel, Taellberg near Lake Siljan in Dalarna, Sweden. It is located 280 km from Stockholm. Taellberg is easy accessible from Stockholm (3 1/2 hours by train or car, 40 min by flight to Dala airport and then car transportation). This part of Dalarna is one of the most attractive tourist sites in Sweden. There are many activities and places of interest around Lake Siljan. Further information can soon be obtained from the conference home page on <http://www.atom.kth.se>

7. GORDON RESEARCH CONFERENCE MOLECULAR ELECTRONIC SPECTROSCOPY AND DYNAMICS

Queens College, Oxford, UK, Aug. 31 - Sept. 5, 1997

The 1997 Gordon Research Conference on Molecular Electronic Spectroscopy and Dynamics will be held at Queens College, Oxford, England from August 31 - September 5, 1997, on the High Street. In keeping with the international venue, and the traditions of the meeting, a wide variety of topics relating to electronic spectroscopy and its applications to studies of molecular structure and dynamics in both the gas phase and the condensed phase will be discussed. An active social program also is planned. Program details, application procedures, and travel and accommodation information will be provided at a later date.

David W. Pratt (Chair; pratt+@pitt.edu), Robert W. Field (Vice-Chair; rwfield@mit.edu), John P. Simons (Chair. Local Organizing Committee; jpsimons@vax.ox.ac.uk).

8. THEORETICAL CHEMISTRY

University of Sussex, Brighton, U.K., 5th December 1997

A one-day meeting has been organised to celebrate the contribution Professor J.N. Murrell has made to Theoretical Chemistry. The programme will consist of contributions from former students, including P. Madden, J. Tennyson, D. Clary, D. Bosanac, A. Varandas, and H. Guo, and will be followed by dinner in the evening. Friends and former colleagues wishing to attend should contact Prof. A.J. Stace, School of Chemistry, Physics and Environmental Science, University of Sussex, Falmer, Brighton BN1 9QJ, U.K.

9. Faraday Division, Royal Society of Chemistry - Faraday Discussion 108 "The Dynamics of Electronically-Excited States in Gaseous, Cluster and Condensed Media"

University of Sussex, UK, 15-17 December 1997

Organising Committee: G S Beddard, R J Donovan, R Grice, J M Hutson, A Orr-Ewing, B Soep, A J Stace, J C Whitehead (Chairman)

There are now a wide range of experiments being performed that can study various aspects of the dynamics of electronically-excited states in gaseous, cluster and condensed phases. The aim of the Discussion will be to explore the similarities and differences between these processes in the different media focusing on the effect of the medium. The processes involved include energy transfer processes, chemical reaction, decomposition to neutral and ionic fragments, proton and electron transfer. Contributions are invited for consideration by the Organising Committee. Titles and abstracts should be submitted by 20th DECEMBER 1996 to Dr J C Whitehead, Chemistry Department, Manchester University, Manchester, M13 9PL (j.c.whitehead@man.ac.uk). Full papers for publication in the Faraday General Discussion 108 will be

required by August 1997. Further details about the Discussion can be obtained from Ms Shazia Riaz, riazs@rsc.org.

10. Faraday Division, Royal Society of Chemistry - Faraday Discussion 110 ” CHEMICAL REACTION THEORY”

University of St Andrews, Scotland, 1-3 July 1998

CALL FOR ABSTRACTS

This will be the first Faraday Discussion devoted purely to the theory of chemical reactions, one of the most rapidly developing areas of theoretical chemistry. Predictions on the dynamics of the reactions of small molecules can now be as reliable as experimental measurements and the accuracy of calculations on more complicated problems ranging from reactions of organic molecules to reactions on surfaces and in solution is improving at a very fast pace.

The committee specially welcomes theoretical or computational papers in the following areas:

* ab initio calculation of accurate potential energy surfaces for chemical reactions

scattering theory for the accurate treatment of the reactions of small molecules

extension of theory to dynamics and kinetics of larger molecules

reactions of molecules on solid surfaces and in solution

The papers chosen for the Discussion will be concerned with theory or calculations that can be tested by comparison with experiment. St Andrews University on the east coast of Scotland is over 500 years old and is a beautiful place to hold the meeting (especially in July). The accommodation facilities there are excellent. There are good connections to St Andrews from the international airport at Glasgow and also from Edinburgh. Contributions are invited for consideration by the Organising Committee. Titles and abstracts of about 300 words should be submitted no later than 1 JUNE 1997 to Professor D C Clary, Department of Chemistry, University College London, London WC1H OAJ (email: d.c.clary@ucl.ac.uk). Full papers for publication in the Faraday General Discussion 110 volume will be required by February 1998. Organising Committee: D C Clary (Chairman), J N L Connor, I H Hillier, S Holloway, W C Mackrodt, D E Manolopoulos, M A Robb

11. 15th International Symposium on Gas Kinetics

The 15th International Symposium on Gas Kinetics will be held in Bilbao, Spain, during the week 12-19th September 1998. Further details from Prof. F. Castano (qfpcalf@lgdx02.lg.ehu.es)