

Molecular Dynamics News

number 88, April 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 has been accepted - otherwise state *unpublished*).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 89 to Prof. V. Aquilanti (**You are encouraged to use electronic mail: AQUILA@HERMES.CHM.UNIPG.IT**). (Please keep line length less than 75 characters.) Editing time will be saved if submissions correspond to the formats found in this issue (#88). The closing date for issue number 89 is June 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.

Elsewhere: Your check for the equivalent of US \$20/year in any convertible currency should be paid out and sent to Prof. V. Aquilanti. **Amount enclosed**

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ANNOUNCING ELECTRONIC DELIVERY OF MDN

We offer to our subscribers several possibilities for electronic delivery of MDN:

1. Electronic mail to subscribers

In this case subscribers tell us if they want the newsletter automatically sent to them by electronic mail. The newsletter can be sent in two forms: raw LaTeX source file, or as a Postscript file. Subscribers may specify the desired form.

2. World Wide Web

Now anyone can access the newsletter as a LaTeX, dvi, HTML, pdf or Postscript file. A Web browser such as Mosaic or Netscape 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>

We periodically update the home page, and you can find links to Molecular Dynamics News subscribers' home pages at our WWW site. We will add a link to your home page if you send us the address by email or with the subscription form on the cover page of this issue. There is also a list of MDN subscribers that is linked to their email addresses.

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 continues, 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 in 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:

join molecular-dynamics-news John F Kennedy

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 also a 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:

join spectroscopy-group John Kennedy

a. Open Positions

FACULTY

BEN-GURION UNIVERSITY OF THE NEGEV, ISRAEL

The Chemistry Department of Ben-Gurion University of the Negev seeks outstanding candidates for a tenure track faculty position. Field of interest is open. Applicants with Ph.D obtained within the last 7 years should send current CV, outline of research interests and plans, and names of at least three references to Prof. James Y. Becker, Chair, Chemistry Department, Ben-Gurion University of the Negev, Beer Sheva, Israel 84120. Teaching in Hebrew is expected within three years. Deadline for applications is 6.30.97.

POST DOCTORAL AND VISITING

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.

NATIONAL TSING HUA UNIVERSITY, DEPARTMENT OF CHEMISTRY

Two postdoctoral positions starting August 1, 1997 (flexible) at the Department of Chemistry, National Tsing Hua University, TAIWAN. Possible projects include: (1) Two-color resonant four-wave mixing spectroscopy of free radicals in a supersonic jet, (2) Time-resolved Fourier-transform Spectroscopy with a step-scan FTIR - spectroscopy, kinetics, and dynamics after laser photolysis of gaseous molecules. (3) Photoionization spectroscopy and kinetic of free radicals using synchrotron radiation source or UVU laser. Extended experiences with excimer and Nd-YAG lasers preferred. Good salary with yearly renewable appointment. Applicants should arrange 2-3 letters of recommendation to be sent to Prof. Y. P. Lee, I-C. CChen, Department of Chemistry, National Tsing Hua University, TAIWAN 30043 (e-mail: yplee@net.nthu.edu.tw, icchen@net.nthu.edu.tw, FAX: 886-3-5722892).

CENTER FOR MOLECULAR REACTION DYNAMICS AND LASER CHEMISTRY, DENMARK

A number of postdoc positions or postdoc-like guest positions of one year duration, starting 1997 are open. The center consists of a group of scientists from different institutions in Denmark, representing both theoretical and experimental activities.

THEORY: The theoretical groups are the following:

Gert Due Billing (University of Copenhagen), Carl Nyeland (University of Copenhagen), Niels Engholm Henriksen (Technical University, Copenhagen), Flemming Yssing Hansen (Technical University, Copenhagen), Frank Jensen (Odense University), Kurt V. Mikkelsen (University of Copenhagen), Ole Sonnich Mortensen (Odense University)

The present theoretical activities are concentrated within the topics chemical reactions, photodissociation, laser induced processes, electron-proton transfer, reactions in solution, electronic structure calculations, semiclassical reactions, control of chemical reactions, transport properties etc.

The theoretical methods applied range from classical statistical mechanics to full scale quantum mechanical dynamics.

EXPERIMENT: The experimental groups are the following:

Robert Wilbrandt (Riso National Laboratory), Soren Rud Keiding (University of Aarhus), Nis Bjerre (University of Aarhus)

The present experimental activities are concentrated within the areas time-resolved optical spectroscopy and high-resolution spectroscopy, in particular structural and dynamical investigations of chemical intermediates in condensed phase by laser flash photolysis, resonance Raman scattering and quantum chemical

calculations; ultrafast laser spectroscopy and high resolution spectroscopy in molecular beams, THz-pulses and coherent control.

Salary according to guidelines for the University in question.

Potential applicants should contact

Prof. Gert Due Billing, tlf. +45 35320252 E-mail: gdb@moldyn.ki.ku.dk

Dr. Robert Wilbrandt, tlf. +45 46774248 E-mail: WILBRANDT@risoe.dk

Assoc. Professor Kurt V. Mikkelsen, tlf. +45 35320251 E-mail: kmi@teosgi2.ki.ku.dk

Assoc. Professor Niels Engholm Henriksen, tlf. +45 45252029 E-mail: neh@tkemi.klb.dtu.dk

Assoc. Professor Frank Jensen, tlf. +45 66158696-2507 E-mail: frj@dou.dk

Assoc. Professor Soren Rud Keiding, tlf. +45 89483333 E-mail: keiding@kemi.aau.dk

Formal application including a CV, list of publications and research areas of interest should be submitted in 5 copies by May 15'th to

Prof. Gert Due Billing, H. C. Oersted Institutet, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen, Denmark

Fax: +45 35320259

NORTHWESTERN UNIVERSITY, DEPARTMENT OF CHEMISTRY

I am looking for a theory postdoc to help me with a new project that falls at the interface of optical physics and materials chemistry. This is a collaborative project which involves my colleague Mark Ratner as well as several experimentalists (R. Van Duyne, J. Hupp, W. DeHeer, M. Jarrold, C. Mirkin, J. Ketterson), and the primary activity for this position is to develop and apply theories which are capable of describing the optical properties, both linear and nonlinear, of assemblies of clusters or nanoparticles. This would be an ideal position for someone with interests in light scattering theory and/or nonlinear optics, but I am willing to be flexible. There is also a connection with magnetic nanoparticles, so background in the magnetic properties of materials is another possibility. Some of our work would build on past studies in my lab of absorption spectra and Raman intensities using converged electrodynamics calculations. References to this past work are: W. -H. Yang, G. C. Schatz and R. P. Van Duyne, JCP 103, 869 (1995); W. -H. Yang, J. Hulteen, G. C. Schatz and R. P. Van Duyne, JCP 104, 4313 (1996) and A. C. R. Pipino, R. P. Van Duyne and G. C. Schatz, Phys. Rev. B53, 4162 (1996).

The position is available May 1, but a later starting date is possible.

Interested applicants should send their resume and two letters of recommendation to:

Prof. George C. Schatz, Department of Chemistry, Northwestern University, Evanston, IL 60208-3113

NATIONAL RESEARCH COUNCIL, STEACIE INSTITUTE

I am looking for a postdoctoral fellow to work with me on problems in theoretical physics or chemistry. My research interests include the interaction of molecules with intense fields, chemistry and photochemistry at interfaces, mathematical method development and condensed-phase dynamics.

The Steacie Institute of the National Research Council is located in downtown Ottawa, next to the Ottawa River. The annual salary is about \$40,000 CAN, commensurate with experience.

For more information please see <http://gold.nrc.ca/tamar> or contact me by phone, e-mail or Fax.

Tamar Seideman, Steacie Institute of Molecular Science, National Research Council of Canada, Ottawa K1A 0R6

Tel: 613-990-0945, e-mail: tamar.seideman@nrc.ca, Fax: 613-954-5242

INSTITUTE FOR MOLECULAR SCIENCE

Applications are invited for a postdoctr al position in the research group of Prof. Toshinori Suzuki at Institute for Molecular Science, Okazaki, Japan. The current research projects involve studies of photodissociation and reactive scattering of polyatomic molecules. Reaction dynamics is studied by state-resolved speed, angular, and alignment distributions of products and their time-evolution. Molecular beam methods are coupled with 2D ion imaging with nanosecond or femtosecond lasers. Interested candidates should send a

CV and the names of two or three references to Toshinori Suzuki, Institute for Molecular Science, Myodaiji, Okazaki 444 Japan (e-mail suzuki@ims.ac.jp, FAX +81-564-54-2254)

CORNELL UNIVERSITY, Department of Chemistry

Two postdoctoral positions are available to work in the general area of photodissociation dynamics in the laboratory of Paul Houston at Cornell University. Successful applicants should have had significant experience with pulsed nanosecond dye lasers and, if possible, with pulsed molecular beams. One position is to investigate the photodissociation dynamics of ozone using photofragment imaging and Rydberg time-of-flight techniques. One position is to investigate the photodissociation dynamics of radical species.

Descriptions of the current research group and recently completed projects can be found on the web:

<http://www.msc.cornell.edu/plh2/group>

Applicants should send a curriculum vitae and arrange for letters from three references to be sent to Paul L. Houston, Department of Chemistry, Cornell University, Ithaca, New York 14850-1301 USA.

UNIVERSITY OF BRITISH COLUMBIA, THEORETICAL CHEMISTRY

A postdoctoral position in theoretical chemistry is available immediately in the group of Mark Thachuk for a period of one year, with an option to renew for a second year if mutually desirable. Areas of research include the interaction of molecular ions with intense laser fields, time-dependent semi-classical hopping methods, and gas phase reaction dynamics. Salary is within NSERC guidelines.

The University of British Columbia is located in the beautiful port city of Vancouver, nestled in the Rocky mountains with wonderful skiing and hiking nearby.

Interested applicants please send a curriculum vitae, and arrange for three letters of reference to be sent to: Mark Thachuk, Department of Chemistry, University of British Columbia, 2036 Main Mall, Vancouver, BC, Canada V6T 1Z1

Email: thachuk@chem.ubc.ca, Tel: (604) 822-2448, FAX: (604) 822-2847

Information about the Chemistry Department is available on the web at

<http://www.science.ubc.ca/departments/chem>.

IOWA STATE UNIVERSITY, DEPARTMENT OF CHEMISTRY

Postdoctoral positions are available summer or fall 1997 at salary: \$30,000/year. The applicants must have a physics or chemistry Ph.D., or related area after January 1994, with excellent background in fundamental quantum mechanics and electronic structure theory

The general goals of this research are to develop and apply new variational one-electron density functional theories that will allow direct computation of interaction potentials and forces in large complex systems. For more information, see <http://aztec.fi.ameslab.gov:80/depristo/>.

One can also work in two other areas: Cluster Structure and Reactivity and Thin film growth.

Applications must include: resume, publication list, unofficial photocopies of undergraduate and graduate transcripts, three letters of reference, a detailed description of your computer experience on PC's, workstations, vector and parallel supercomputers in 1 page or less, noting program, operating system and language expertise.

Send the above information to: Professor Andrew E. DePristo, 303 Wilhelm Hall, Ames Laboratory, Iowa State University, Ames, IA 50011. (e-mail to depristo@ameslab.gov for documents using MIME compliant mailers.)

Ames Lab and Iowa State University are equal opportunity employers.

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-phys.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

Time and frequency dependent charge carrier mobility on one-dimensional chains with energetic disorder.

Chem. Phys. Lett.

O. Hilt and L.D.A. Siebbeles

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

The thermally activated motion of a charge on a disordered chain in an oscillating external field is computer simulated. The frequency dependence of the mobility of the charge elucidates the charge transport mechanism.

The Kinetics of the Reaction $F + H_2 \rightarrow HF + H$. A Critical Review of Literature Data

Int. J. Chem. Kinet. 29, 67 (1997).

Avigdor Persky and Haya Kornweitz

Department of Chemistry, Bar-Ilan University, Ramat Gan, 52900, Israel

Published experimental results are critically reviewed and Arrhenius expressions are recommended for the $F+H_2$ and $F+D_2$ reactions for the temperature range 190-376 K.

Half- and full-collision VT energy transfer in the He-Br₂(B) system

Chem. Phys. Lett.

A. A. Buchachenko*, T. Gonzalez-Lezana, M. I. Hernandez, G. Delgado-Barrio, P. Villarreal, and N. F. Stepanov

Department of Chemistry, Moscow State University, Moscow 119899, Russia

The ability of model spectroscopic interaction potentials to reproduce the vibrationally-inelastic collision rate constants and van der Waals vibrational predissociation rates is examined for the He-Br₂(B) system.

First-order intermolecular DIM potentials. Potential energy surfaces, spectra, and fragmentation dynamics of the Ne...Cl₂ complex

J. Chem. Phys.

A. A. Buchachenko and N. F. Stepanov

The novel efficient semiempirical approach to the intermolecular potentials, based on the perturbative treatment of the diatomics-in-molecule expansion of the electronic Hamiltonian, is shown to provide very accurate description of the structure, vibronic spectra, and predissociation rates of the Ne...Cl₂ van der Waals complex

Measurement of the rate constant $k(E)$ of the unimolecular H₂ elimination from ethane radical cations in a Reflectron mass spectrometer.

Ber. Bunsenges. Phys. Chem., 101, (1997), 484

Felix Guethe and Karl-Michael Weitzel*

Institut fuer Physikalische und Theoretische Chemie, Freie Universitaet Berlin, Takustr. 3, 14195 Berlin, Germany

Direct measurements in a Reflectron show that $k(E)$ of the title reaction increases by three orders of magnitude within less than 100 meV of ion internal energy.

Distinguishing the formation of C₂D₄⁺ ions from C₂D₆⁺ (by D₂ loss) and from C₂D₅H⁺ (by HD loss) in a Reflectron spectrometer.

unpublished

Felix Guethe, Marcus Malow, Karl-Michael Weitzel* and Helmut Baumgaertel

Institut fuer Physikalische und Theoretische Chemie, Freie Universitaet Berlin, Takustr. 3, 14195 Berlin, Germany

The setup of a Reflectron optimized for coincidence experiments is described and illustrated by an investigation of the D₂ and HD loss reaction from C₂D₆⁺ and C₂D₅H⁺ ions respectively.

The Formation of ArCO⁺ Ions by Dissociative Ionization of Argon / Carbonmonoxide Clusters.

unpublished

Joachim Maehner, Helmut Baumgaertel and Karl-Michael Weitzel*

Institut fuer Physikalische und Theoretische Chemie, Freie Universitaet Berlin, Takustr. 3, 14195 Berlin, Germany

The kinetic energy released in the dissociative formation of ArCO⁺ ions has been investigated experimentally and compared to predictions from phase space theory.

Photofragment imaging by sections for measuring angle-velocity differential cross sections

J. Chem. Phys.

J. A. Syage

The Aerospace Corporation, P.O. Box 92957, Mail Stop M5-754, Los Angeles, CA 90009

A technique for measuring state-selected "slices" of the 3D velocity distribution of photofragments and products is described and the simple relationship to differential cross sections for reactive and unreactive scattering described.

State-to-state proton tunneling probabilities: A study in molecular clusters

Femtochemistry, edited by M. Chergui (World Scientific Press, 1996)

J. A. Syage

The Aerospace Corporation, P.O. Box 92957, Mail Stop M5-754, Los Angeles, CA 90009

A model for proton tunneling in clusters is presented that treats the rate as dependent on specific vibrational modes, in terms of modulating the barrier width and in bridging energy gaps between reactants and products.

State-specific, angle-velocity-resolved measurements of photodissociations in clusters: I atom escape from (CH₃I)_n (n=1,2,3)

Chem. Phys.

J. A. Syage

The Aerospace Corporation, P.O. Box 92957, Mail Stop M5-754, Los Angeles, CA 90009

State-angle-velocity resolved measurements from bimolecular collisions initiated in aligned van der Waals complexes are presented.

Size-specific photodissociation of (CH₃I)_n⁺ cluster ions

J. Mass Spectrom. and Ion Proc.

J. A. Syage* and J. Steadman

The Aerospace Corporation, P.O. Box 92957, Mail Stop M5-754, Los Angeles, CA 90009

Photodissociation and electron-induced dissociation spectra were recorded for size-specific cluster ions, and physical properties such as excitation cross sections and energy-dependent branching ratios reported.

Ozone decomposition on alumina: Implications for solid rocket motor exhaust

Geophys. Res. Lett.

M. A. Hanning-Lee, B. B. Brady, L. R. Martin, and J. A. Syage*

The Aerospace Corporation, P.O. Box 92957, Mail Stop M5-754, Los Angeles, CA 90009

The rate of ozone decomposition on various phases and surface preparations of aluminum oxide particles was measured using traditional flow tube methods and a new technique based on real-time absorption spectroscopy; predicted ozone depletions due to this reaction are calculated in rocket plumes and in the ambient stratosphere.

An assessment of the total ozone mapping spectrometer for measuring ozone levels in solid rocket plumes

Geophys. Res. Lett.

J. A. Syage* and M. A. Ross

The Aerospace Corporation, P.O. Box 92957, Mail Stop M5-754, Los Angeles, CA 90009

The adequacy of TOMS for measuring ozone depletion in rocket plumes is examined, as are the factors that could perturb the measurements, such as the presence of molecules and particles in the plume that are not included in the TOMS analysis algorithm.

Angle-velocity-resolved measurements of photodissociation in clusters

Proc. QELS (1996)

J. A. Syage

The Aerospace Corporation, P.O. Box 92957, Mail Stop M5-754, Los Angeles, CA 90009

Results are presented for the photoexcitation of O_3-H_2O complex and the state-resolved angle-velocity detection of unreactive O and reactive OH scattering

Laser chemistry moves toward smaller and faster probes

Photonics Spectra

J. A. Syage

The Aerospace Corporation, P.O. Box 92957, Mail Stop M5-754, Los Angeles, CA 90009

A brief sidebar highlighting some recent experiments in ultrafast spectroscopy in elementary reactions and in clusters.

Production, characterization and scattering of a beam of sulphur monoxide radicals: the SO-rare gas interactions.

J. Phys. Chem.

Vincenzo Aquilanti, Daniela Ascenzi, Elisabetta Braca, David Cappelletti, Giorgio Liuti, Emilio Luzzatti and Fernando Pirani Dipartimento di Chimica dell'Università I-06123, Perugia, Italy

An intense and stable continuous beam of SO radicals has been produced with a microwave discharge source operating in the Torr range in a mixture of SO_2 with various gases. The beam emerging from the plasma source is velocity analyzed and detected by a quadrupole mass filter. Stern-Gerlach magnetic analysis shows SO radicals mainly in the electronic ground state and provides an upper limit on the concentration of electronic metastable states. Total integral cross section measurements for the scattering of SO radicals by Ne, Ar and Kr have also been performed to characterize the interaction potential features.

Tracks of Symmetric Top Molecules in Hexapole Electric Fields

J. Phys. Chem. (submitted)

Roger W. Anderson

Department of Chemistry, University of California, Santa Cruz, CA 95064 and Zentrum fuer

Interdisziplinäre Forschung, Universität Bielefeld, Bielefeld, Germany

Trajectories of symmetric top molecules are computed in hexapole electric fields assuming the exact Stark effect instead of the usual linear Stark effect. Hyperfine interactions and cylindrical rod approximations for ideal hexapole fields also have significant effects on the trajectories. Results are also presented for the electric field magnitude for various choices for the cylindrical rod radius to the hexapole radius.

UV photodissociation of oxalyl chloride yields four fragments from one photon absorption

J. Chem. Phys.

Musahid Ahmed, David Blunt, Daniel Chen and Arthur G. Suits*

Chemical Sciences Division, Ernest Orlando Lawrence Berkeley National Laboratory, Berkeley, CA

c. Conferences

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

Wesleyan University Middletown, CT 06459, May 5, 1997

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.Colliex (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 (Göttingen), 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-Böking (Frankfurt), U.Schmitt (Zurich), G.Scoles (Princeton), T.Seideman (Ottawa), A.G.Suits (Berkeley), P.Tosi (Trento), J.Vigu (Toulouse), R.Weinkauff (Garching) and K.Yamanouchi (Tokyo). Short oral presentations of hot topics and poster sessions are planned. The symposium will take place in the Auditorium Pierre Lehmann at Orsay, from Monday June 2nd at 9.00 to Friday June 6 after lunch. 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. A conference fee of 1,500 F.F. will be charged if received by April 1st, 1997 and 1,900 F.F. if received later. It includes the book of abstracts, the registration and welcome buffet, five lunches and one dinner at Orsay. The registration and welcome buffet will take place on Sunday June 1st from 16.00 to 22.00, in the hall of the Ecole Nationale Supérieure de Chimie de Paris, 11 rue Pierre et Marie Curie, Paris V, in the heart of the Quartier Latin, near the 'Luxembourg' station of the RER B line. The conference dinner is planned on Thursday June 5 at 20.30, in the Hotel Intercontinental, 3 rue de Castiglione, Paris I, near the Tuileries gardens and the Louvre museum. A supplementary cost of 350 F.F. will be charged. For application or further information, 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>).

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 Kiejji 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. CONDENSED PHASE QUANTUM DYNAMICS: APPLICATION TO CHEMICAL AND BIOLOGICAL SYSTEMS

Lausanne, Switzerland 28-30 August 1997

Chaipersons: Prof. M. Chergui and Dr M. T. Portella-Oberli

The scientific programme of this meeting will emphasize the various aspects of condensed phase dynamics as probed by conventional and ultrafast laser techniques. The topics that will be covered during the meeting include photoinduced dynamics in solids and liquids, interfaces and surfaces, biological molecules and polymers. Contributions, by both experimentalists and theoreticians, will be made to an audience of not more than 80 people. This format will allow intense discussions and a fruitful exchange of ideas. A poster session is also planned. This conference precedes the Femtochemistry Conference in Lund (1-4/9/1997)

Speakers that have confirmed participation include: A. H. Zewail (USA), V.S. Letokhov (R), M.

Aeschlimann (CH), J.-Y. Bigot (F), R.D. Coalson (USA), H. Girault (CH), M. Gruebele (USA), J.-E. Moser (CH), A. Rebane (USA), Y.Tanimura (J), M. Wulff (F)

For further information and registration forms:

Dr Marcia T. Portella-Oberli

Inst. de Physique Experimentale,

Faculty des Sciences, BSP

University of Lausanne

1015 Lausanne-Dorigny

tel.: xx-41-21-692 3676 fax: xx-41-21-692 3635

email: QD@ipe.unil.ch also available on the web site: <http://www.unil.ch/ipe/>

8. 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).

9. Symposium on Dynamics in Molecular Systems

214th ACS National Meeting in Las Vegas, Nevada September 7 - 11, 1997

Tim Zwier and I are organizing a special Symposium at the Las Vegas ACS Meeting. The symposium will run for four days, September 8 - 11, with morning and afternoon oral sessions, and one or two poster sessions. There are seven different sessions listed below with the invited speakers, who have agreed to attend:

PHOTODISSOCIATION

Keiji Morokuma, Alberto Beswick, Hanna Reisler and Fleming Crim.

REACTION DYNAMICS AND COHERENT CONTROL

Herschel Rabitz, Robert Gordon, Jim Valentini and Joel Bowman.

IONS

John Maier, Rob Continetti, Peter Hackett and Kent Ervin.

INTRA- INTERMOLECULAR PROCESSES

Tom Rizzo, Bob Field, Marek Zgierski and Hai-Ping Cheng.

CLUSTERS

Peter Felker, Birgitta Whaley, Dan Neumark, Will Castleman, Ken Leopold, Friedrich Huisken, Stephen Gray and Sherwin Singer.

SURFACES AND SOLIDS

Manfred Kappes, Phillipe Guyot-Sionnest, Barbara Garrison and Ara Apkarian.

We plan to have a number of contributed oral presentations in addition to the invited speakers. If you would like to participate in the Symposium, please send a completed ACS Abstract Form to:

Prof. James M. Lisy Department of Chemistry, Box 7-6 University of Illinois at Urbana-Champaign 600 S. Mathews Ave. Urbana, IL 61801

If you need an abstract form, please contact me by e-mail: j-lisy@uiuc.edu or by telephone: 217-333-2898.

There are a limited number of graduate student travel fellowships (up to \$300) to offset conference fees, travel or local expenses. Please direct these applications (Abstract Form and Supporting Letter indicating our Symposium) to:

Dr. Ellen Stechel, Program Chair Sandia National Laboratories P.O. Box 5800 MS-1421 Albuquerque, NM 87185-1421

We hope to see you in Las Vegas. Don't forget to bring your favorite good luck charm(s).

10. 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.

11. 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.

12. 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

13. 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)