Welcome to the 68th
OSU International
Symposium on Molecular Spectroscopy

On behalf of the Executive Committee, Frank DeLucia, Anne B. McCoy, and myself, I extend a heartfelt welcome to all the attendees to the 68th Symposium and welcome you to The Ohio State University and Columbus.

The Symposium presents research in fundamental molecular spectroscopy and a wide variety of related fields and applications. The continued vitality and significance of spectroscopy is annually re-affirmed by the number of talks, their variety, and the fact that many are given by students. These presentations are the heart of the meeting and are documented by this Abstract Book. Equally important is the information flowing from informal exchanges and discussions. As organizers, we strive to provide an environment that facilitates both kinds of interactions.

The essence of the meeting lies in the scientific discussions and your personal experiences this week independent of the number of times that you have attended this meeting. It is our sincere hope that you will find this meeting informative and enjoyable both scientifically and personally, whether it is your first or 50th meeting. If we can help to enhance your experience, please do not hesitate to ask the Symposium staff or the Executive Committee.

Terry A. Miller
Symposium Chair

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Special Sessions

For the 68th Symposium, Wim Ubachs, Vrije Universiteit Amsterdam, and Tim Steimle, Arizona State University, are organizing a mini-symposium entitled, “Spectroscopy Tests of Fundamental Physics”. This mini-symposium will focus on experimental and theoretical efforts to characterize shifts in molecular quantum levels brought about by physics beyond the principles of General Relativity and the Standard Model. Invited speakers include Peter Schwerdtfeger, Massey University, and Wim Ubachs, Vrije Universiteit Amsterdam. A second mini-symposium is being organized by Vincent Boudon, CNRS/Universitie de Bourgogne and Peter Bernath, Old Dominion University on the subject of “Spectroscopy of Planetary Atmospheres.” This mini-symposium is dedicated to the spectroscopy of planetary atmospheres including observations, laboratory measurements and modeling for the Earth, planets of the Solar System, exoplanets and brown dwarfs. Invited talks for this mini-symposium will be given by Pierre-Francois Coheur, Universite Libre de Bruxelles; and Glenn Orton, JPL-California Institute of Technology, Jonathan Tennyson, University College London. A third mini-symposium is being organized by John Stanton, University of Texas at Austin entitled “Theory and Spectroscopy.” This symposium will focus on the development, and use of, theoretical tools for addressing spectroscopic problems. Invited speakers include Jon Hougen, NIST, and Horst Koeppel, Universitaet Heidelberg; Timothy Lee, NASA; and Cristina Puzzarini, Universita di Bologna.

Picnic

The Symposium picnic will be held on Wednesday evening, June 19, at the Fawcett Center. The cost of the picnic is included in your registration (at below cost to students), so that all may attend the event. The Coblenz Society is the host for refreshments at 6:30pm before the picnic which is scheduled to commence at 7:30pm at the Fawcett Center.
Sponsorship

We are pleased to announce the sponsorship for the 68th Symposium. Principal funding comes from the Army Office of Research (ARO). We are most grateful to ARO for their continued support. We also acknowledge the many efforts and contributions of The Ohio State University in hosting the meeting. Our Corporate sponsors are Elsevier, Coherent and the Journal of Physical Chemistry A. Please see the back of this book for their advertisements and the events they support. We are pleased to acknowledge Andor Technology, Block Engineering, Bristol Instruments, Bruker Optics, Clark-MXR, Continuum, CVI Laser Optics, Lockheed Martin/Aculight, MSquared Lasers, Newport/Spectra-Physics, Princeton Instruments, and Topica Photonics as Contributing sponsors. IOS Press has a special insert in your conference packet. Bruker Optics will have a special Tuesday lunch presentation. Look in your packet for fliers about that. Our sponsors will have exhibits at the Symposium and we encourage you to visit their displays.

Rao Prize

The three Rao Prizes for the most outstanding student talks at the 2012 meeting will be presented. The winners are Nils Bartels, Georg August Universitaet Gottingen; Andrew Petit, The Ohio State University; and Arron Wolk, Yale University. The Rao Prize was created by a group of spectroscopists who, as graduate students, benefited from the emphasis on graduate student participation, which has been a unique characteristic of the Symposium. This year three more Rao Prizes will be awarded. The award is administered by a Prize Committee chaired by Yunjie Xu, University of Alberta and comprised of Kevin Lehnmann, University of Virginia; Brooks Pate, University of Virginia; Rebecca Peebles, Eastern Illinois University; Brenda Winnewisser, The Ohio State University and Tim Zwier, Purdue University. Any questions or suggestions about the Prize should be addressed to the Committee. Anyone (especially post-docs) willing to serve on a panel of judges should contact Yunjie Xu (yunjie.xu@ualberta.ca).

Information

ACCOMMODATIONS: The check-in for dormitory accommodations is located in the Lane Avenue Residence Hall (LARH), 328 W. Lane Avenue, opens at 10 a.m. Sunday, June 16, and remains open 24 hours a day through the Symposium.

Other hotels close to campus include: The Blackwell, corner of Tuttle Park Place and Woodruff Avenue, 806-247-400; Red Roof Inn, State Route 315 & Ackerman Rd., 267-9941. NOTE: When making reservations with the Blackwell mention that you are with the Molspec Symposium and you will be given the OSU discount, if available.

MAIL: As in recent years, computer facilities for email will be available. Address your regular mail for delivery during the Symposium to: c/o MOLECULAR SPECTROSCOPY SYMPOSIUM, Department of Chemistry, The Ohio State University, 100 West 18th Avenue, Columbus, Ohio, 43210, U.S.A. FAX number - (614) 292-1948, Telephone number - (614) 292-2569.

PARKING: Parking permits, for the week, are available only from the check-in desk at the Lane Avenue Residence Hall. These permits allow you to park in any “C” parking space on campus. The permit must be displayed on the front windshield of your car. Please follow all traffic rules to avoid the issuance of tickets. NOTE: The Symposium takes place during Summer Session so parking on campus can be problematic.

REGISTRATION: The Registration Desk will be located in Room 2017 McPherson Lab. It will be open between 4:00-6:00 p.m. Sunday, and 8:00a.m. - 4:30p.m., Monday through Friday. Those who have prepaid their registration and who are staying in the dorms will receive their registration packet at LARH upon check-in. If you have prepaid your registration but are not staying at the dorms, pick up your packet at the Registration Desk. NOTE: If the dates of your stay change after Friday, June 7, please call the Symposium Office to find out your options.

LIABILITY: The Symposium fees DO NOT include provisions for the insurance of participants against personal injuries, sickness, theft or property damage. Participants and companions are advised to take whatever insurance they consider necessary. Neither the Symposium organizing committee, its sponsors, nor individual committee members assume any responsibility for loss, injury, sickness, or damages to persons or belongings, however caused. The statements and opinions stated during oral presentations or in written abstracts are solely the author’s responsibilities and do not necessarily reflect the opinions of the organizers.
**AUDIO/VIDEO INFORMATION:** Equipment for computer presentations, i.e. PowerPoint, will be available for each session. For computer presentations, you must go to the **Digital Presentation link** on our web site and follow the instructions. Your PowerPoint file and all supporting documents can be uploaded. These files must be submitted to the Symposium by **MIDNIGHT THE DAY BEFORE** your presentation session. All submitted files will be loaded on the presentation computer one half-hour prior to the beginning of the session.

Please make careful note of the username (p##) and password provided in the email confirming receipt of your abstract - this username/password combination will be required when you submit your digital presentation. If you are submitting multiple presentations you will need to log on separately with the appropriate username and password for each presentation.

**ACKNOWLEDGEMENTS:** The Symposium Chair wishes to acknowledge the hard work of numerous people who make this meeting possible. Key among these people are Becky Gregory, who solves everyone’s problems and keeps the meeting running smoothly; and my student assistants, Terrance Codd and Brennan Walder who ensure the sessions go well. We wish to acknowledge the hospitality of the Chemistry Department in tolerating our invasion this year. Sergey Panov originally wrote the script for the electronic aspects of the Symposium; Computer Support in Chemistry and Physics helps us modernize it as well as keep it and other aspects of our services operational. Finally, all the students in my group play vital roles in helping make sure nothing falls through the cracks.
MA. PLENARY
MONDAY, JUNE 17, 2013 – 8:45 AM
Room: AUDITORIUM, INDEPENDENCE HALL

Chair: FRANK C. DE LUCIA, The Ohio State University, Columbus, OH

Welcome 8:45
Caroline C. Whitacre, Vice President for Research
The Ohio State University

RAO AWARDS 10:50
Presentation of Awards by Yanjie Xu,
University of Alberta

2012 Rao Award Winners
Nils Bartels, Georg August Universitaet Goettingen
Andrew Petit, The Ohio State University
Arron Wolk, Yale University

MA01 40 min 9:00
LOW TEMPERATURE TRAPPING: FROM REACTIONS TO SPECTROSCOPY
S. SCHLEMMER, O. ASVANY, and S. BRÜNKEN, I. Physikalisches Institut,
Universität zu Köln, 50937 Köln, Germany.

MA02 40 min 9:45
DECODING THE EFFECTS OF LARGE AMPLITUDE VIBRATIONAL MOTIONS IN SPECTRA
ANNE B. MCCOY, LAURA C. DZUGAN, MENG HUANG, ZHOU LIN, BERNICE OPOKU-AGYEMAN, ANDREW S. PETIT, JASON FORD, and BETHANY A. WELLEN,
Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH 43210.

Intermission

MF. MINI-SYMPOSIUM: SPECTROSCOPY TESTS OF FUNDAMENTAL PHYSICS
MONDAY, JUNE 17, 2013 – 1:30 PM
Room: 160 MATH ANNEX

Chair: TIMOTHY STEIMLE, Arizona State University, Tempe, AZ

MF01 30 min 1:30
INVITED TALK
SEARCH FOR A VARIATION OF FUNDAMENTAL CONSTANTS
W. UBACHS, Department of Physics and Astronomy, VU University Amsterdam, De Boelelaan 1081, 1081 HV Amsterdam, Netherlands.
MF02 15 min 2:05
AN ALCOHOL TEST FOR DRIFTING CONSTANTS

P. JANSEN, J. BAGDONAITE, W. UBACHS and H. L. BETHLEM, Institute for Lasers, Life and Biophotonics, VU University Amsterdam, De Boelelaan 1081, 1081 HV Amsterdam, The Netherlands; I. KLEINER, Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA), CNRS UMR 7583 et Universités Paris Diderot et Paris Est, 61 av. Général de Gaulle, 94010 Créteil Cédex, France; L. H. XU, Department of Physics and Centre for Laser, Atomic, and Molecular Sciences, University of New Brunswick, Saint John, New Brunswick E2L 4L5, Canada.

MF03 15 min 2:22
SENSITIVITY OF TRANSITIONS IN INTERNAL ROTOR MOLECULES TO A POSSIBLE VARIATION OF THE PROTON-TO-ELECTRON MASS RATIO

P. JANSEN, W. UBACHS, H. L. BETHLEM, Institute for Lasers, Life and Biophotonics, VU University Amsterdam, De Boelelaan 1081, 1081 HV Amsterdam, The Netherlands; I. KLEINER, Laboratoire Interuniversitaire des Systèmes Atmosphériques, CNRS et Universités Paris Diderot et Paris Est, 61 av. Général de Gaulle, 94010, Créteil, France; L. H. XU, Department of Physics and Centre for Laser, Atomic and Molecular Sciences, University of New Brunswick, Saint John, New Brunswick E2L 4L5, Canada.

MF04 15 min 2:39
CH₃OH SUB-DOPPLER SPECTROSCOPY

GERMAN YU. GOLUBIATNIKOV, SERGEY P. BELOV and ALEXANDER V. LAPINOV, Institute of Applied Physics of RAS, 46 Ulyanov str., 603950 Nizhny Novgorod, Russia.

MF05 15 min 2:56
HIGH RESOLUTION MICROWAVE SPECTROSCOPY OF CH AS A SEARCH FOR VARIATION OF FUNDAMENTAL CONSTANTS

S. TRUPPE, R. J. HENDRICKS, S. K. TOKUNAGA, E. A. HINDS, M. R. TARBUtt, Centre for Cold Matter, Blackett Laboratory, Imperial College London, London, SW7 2BW.

MF06 15 min 3:13
SUB-DOPPLER AND FTMW SPECTROSCOPY OF HC₃N ISOTOPOLOGUES

A. V. LAPINOV, G. YU. GOLUBIATNIKOV, Institute of Applied Physics of RAS, 46 Ulyanov str., 603950 Nizhny Novgorod, Russia; A. P. VEL-MUZHOV, Institute of Metalloorganic Chemistry of RAS, 49 Tropinin str., 603950 Nizhny Novgorod, Russia; J. U. GRABOW, Institute of Physical Chemistry and Electrochemistry, Leibniz University of Hannover, Callinstrasse 3A, 30167 Hannover, Germany; and A. GUARNIERI, Technical Faculty of Christian Albrecht University of Kiel, Kaiserstrasse 2, 24143 Kiel, Germany.

MF07 15 min 3:30
THE CO A-X SYSTEM FOR CONSTRAINING COSMOLOGICAL DRIFT OF THE PROTON-ELECTRON MASS RATIO

M. L. NIU, E. J. SALUMBIDES, D. ZHAO, J. BAGDONAITE, Department of Physics and Astronomy, and LaserLaB, VU University, De Boelelaan 1081, 1081 HV Amsterdam, The Netherlands; N. DE OLIVEIRA, D. JOYEUX, L. NAHON, Synchrotron Soleil, Orme des Merisiers, St Aubin BP 48, 91192, GIF sur Yuette cedex, France; R. W. FIELD, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA, and W. UBACHS, Department of Physics and Astronomy, and LaserLaB, VU University, De Boelelaan 1081, 1081 HV Amsterdam, The Netherlands.

MF08 15 min 3:47
PRECISE MEASUREMENT OF ⁴⁰CaH⁺ VIBRATIONAL TRANSITION FREQUENCY


MF09 15 min 4:04
PRECISE MEASUREMENT OF VIBRATIONAL TRANSITION FREQUENCY OF OPTICALLY TRAPPED MOLECULES


Intermission
TOWARDS MORE ACCURATE MEASUREMENTS OF THE IONIZATION ENERGY OF MOLECULAR HYDROGEN

D. SPRECHER, M. BAYER, J. LIU, and F. MERKT, ETH Zürich, Laboratorium für Physikalische Chemie, Wolfgang-Pauli-Strasse 10, 8093 Zürich, Switzerland; E. SALUMBIDES, K. S. E. EIKEMA, W. UBACHS, Department of Physics and Astronomy, Vrije Universiteit, De Boelelaan 1081, 1081 HV Amsterdam, The Netherlands; CH. JUNGEN, Laboratoire Aimé Cotton, CNRS II, Bâtiment 505, Campus d’Orsay, 91405 Orsay Cedex, France.

NON-ADIABATIC ENERGIES OF THE HYDROGEN MOLECULE

KRZYSZTOF PACHUCKI, Faculty of Physics, University of Warsaw, Hoża 69, 00-681 Warsaw, Poland; JACEK KOMASA, Faculty of Chemistry, A. Mickiewicz University, Poznań 60-780 Poznań, Poland.

QED EFFECTS IN H₂

KRZYSZTOF PACHUCKI, Faculty of Physics, University of Warsaw, Hoża 69, 00-681 Warsaw, Poland; JACEK KOMASA, Faculty of Chemistry, A. Mickiewicz University, Poznań 60-780 Poznań, Poland.

PRECISION MEASUREMENT OF THE IONIZATION ENERGY OF THE G¹Σ⁺ (v = 1, N = 1) STATE OF MOLECULAR HYDROGEN.

M. BAYER, D. SPRECHER and F. MERKT, ETH Zürich, Laboratorium für Physikalische Chemie, Wolfgang-Pauli-Strasse 10, 8093 Zürich, Switzerland.

QED TESTS AND SEARCH FOR NEW PHYSICS IN MOLECULAR HYDROGEN

E. J. SALUMBIDES, M. L. NIU, G. D. DICKENSON, K. S. E. EIKEMA, Department of Physics and Astronomy, and LaserLaB, VU University, De Boelelaan 1081, 1081 HV Amsterdam, The Netherlands; J. KOMASA, Faculty of Chemistry, A. Mickiewicz University, Poznań 60-780 Poznań, Poland; K. PACHUCKI, Faculty of Physics, University of Warsaw, Hoża 69, 00-681 Warsaw, Poland and W. UBACHS, Department of Physics and Astronomy, and LaserLaB, VU University, De Boelelaan 1081, 1081 HV Amsterdam, The Netherlands.

MG. RADICALS AND IONS
MONDAY, JUNE 17, 2013 – 1:30 PM
Room: 170 MATH ANNEX

Chair: CHRISTOPHER NEESE, The Ohio State University, Columbus OH

COMBINATION BANDS BETWEEN 2900 AND 3600 CM⁻¹ OF CYCLIC O₄ CATION TRAPPED IN SOLID NEON

MARILYN E. JACOX and WARREN E. THOMPSON, Sensor Science Division, National Institute of Standards and Technology, Gaithersburg, MD 20899-8441.

FOURIER TRANSFORM FAR-INFRARED SPECTROSCOPY OF HN₂⁺ ON THE AILES BEAMLİNE OF SYNCHROTRON SOLEIL


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Also at: Institut des Sciences Moléculaires d’Orsay, UMR 8214 CNRS-Université Paris-Sud, Bât. 210, 91405 Orsay cedex, France.
MG03 15 min 2:04
SUB-DOPPLER SPECTROSCOPY OF ND₄⁺ ION IN THE NH STRETCHING MODE

CHIH-HSUAN CHANG, GRANT T. BUCKINGHAM, and DAVID J. NESBITT, JILA, National Institute of Standards and Technology University of Colorado, and Department of Chemistry and Biochemistry University of Colorado at Boulder, Colorado 80309.

MG04 15 min 2:21
INFRARED SPECTROSCOPY OF JET COOLED ND₄⁺ MOLECULAR IONS: THE SYMMETRIC AND ANTISYMMETRIC NH STRETCH MODES

CHIH-HSUAN CHANG and DAVID J. NESBITT, JILA, National Institute of Standards and Technology University of Colorado, and Department of Chemistry and Biochemistry University of Colorado at Boulder, Colorado 80309.

MG05 15 min 2:38
PRECISION LASER SPECTROSCOPY OF H⁺⁺

HSUAN-CHEN CHEN, Institute of Photonics Technologies, National Tsing Hua University, Hsinchu 30013, Taiwan; JIN-LONG FENG, Center for Measurement Standards, Industrial Technology Research Institute, Hsinchu 30011, Taiwan; T. AMANO, Department of Chemistry and Department of Physics and Astronomy, University of Waterloo, Waterloo, ON N2L 3G1, Canada; JOW-TSONG SHY, Institute of Photonics Technologies, National Tsing Hua University and Department of Physics, National Tsing Hua University, Hsinchu 30013, Taiwan.

MG06 15 min 2:55
SUB-DOPPLER SPECTROSCOPY OF H⁺⁺

JAMES N. HODGES, ADAM J. PERRY, BRIAN M. SILLER, Department of Chemistry, University of Illinois, Urbana, IL 61801; BENJAMIN J. MCCALL, Departments of Chemistry, Astronomy, and Physics, University of Illinois, Urbana, IL 61801.

MG07 15 min 3:12
HIGH PRECISION SPECTROSCOPY OF CH⁺⁺ USING NICE-OHVS

JAMES N. HODGES, ADAM J. PERRY, Department of Chemistry, University of Illinois, Urbana, IL 61801; BENJAMIN J. MCCALL, Departments of Chemistry, Astronomy, and Physics, University of Illinois, Urbana, IL 61801.

MG08 15 min 3:29
INFRARED SPECTROSCOPY OF THE MASS 43 CATION: ACETYL CATION AND PROTONATED KETENE

JONATHAN D. MOSLEY and MICHAEL A. DUNCAN, University of Georgia, Athens, GA 30683.

MG09 15 min 3:46
UBIQUITOUS INTERSTELLAR MOLECULES WITH RADICALLY DIFFERENT CATION STRUCTURES: INFRARED SPECTROSCOPY OF FORMALDEHYDE AND METHANOL CATIONS

JONATHAN D. MOSLEY and MICHAEL A. DUNCAN, University of Georgia, Athens, GA 30683.

Intermission

MG10 15 min 4:15
THE CORONENE VIBRONIC STATES ABOVE THE FIRST IONIZATION POTENTIAL INVESTIGATED THROUGH TPEPICO EXPERIMENTS

PH. BRECHIGNAC, C. FAILO, P. PARNEIX, T. PINO, O. PIRALI, Institut des Sciences Moléculaires d’Orsay, CNRS UMR8214, Univ Paris-Sud, Bât 210, F91405 Orsay Cedex, France; G. GARCIA, L. NAHON, Synchrtron SOLEIL, L’Orme des Merisiers, St Aubin, B.P. 48, 91192 Gif sur Yvette, France; C. JOBLIN, D. KOKKIN, A. BONAMMY, IRAP, Université de Toulouse [UPS], CNRS, Toulouse, France; G. MULAS, INAF-Osservatorio Astronomico di Cagliari-Astrochemistry Group, Strada 54, Località Poggio dei Pini, I-09012 Capoterra (CA), Italy.

MG11 15 min 4:32
MASS ANALYZED THRESHOLD IONIZATION OF LUTETIUM DIMER

LI WU, MOURAD ROUDJANE, YANG LIU AND DONG-SHENG YANG, Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055.

MG12 15 min 4:49
C-C BOND ACTIVATION AND COUPLING OF PROPENE INDUCED BY LA ATOM

DILRUISHI HEWAGE, Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055; HONG TAO, Department of Chemistry, Southwest Forestry University, Kunming 650224, PR China; RUCHIRA SILVA, SUDESH KUMARI, AND DONG-SHENG YANG, Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055.
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<td>UGO JACOVELLA, BÉRANGER GANS and FREDÉRIC MERKT, ETH Zürich, Labortorium für Physikalische Chemie, Wolfgang-Pauli-Strasse 10, 8093 Zürich, Switzerland.</td>
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<td>ANDREW F. DEBLASE and MARK A. JOHN-SON, Yale University, P.O. Box 208107, New Haven, CT 06520, USA; THOMAS LECTKA, Johns Hopkins University, 3400 North Charles Street, Baltimore, Maryland 21218, USA; XUN WANG and KENNETH D. JORDAN, University of Pittsburgh, 419 Parkman Avenue, Pittsburgh, PA 15260, USA; ANNE B. McCoy, The Ohio State University, Columbus, Ohio 43210, USA.</td>
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<tr>
<td></td>
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<td>RUCHIRA SILVA AND DONG-SHENG YANG, Department of Chemistry, University of Kent-ucky, Lexington, KY 40506-0055.</td>
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<td></td>
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<td>HEATHER L. ABBOTT, Department of Chemistry and Biochemistry, Kennesaw State University, Kennesaw, GA 30144; ANTO- NIO D. BRATHWAITE and MICHAEL A. DUNCAN, Department of Chemistry, University of Georgia, Athens, GA 30602-2256.</td>
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### MH. MICROWAVE

**Monday, June 17, 2013 – 1:30 PM**

**Room: 1000 MCPHERSON LAB**

**Chair: ELANGANNAN ARUNAN, Indian Institute of Science, Bangalore, India**

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<td>M. VARELA, C. CABEZAS, S. MATA, J. L. ALONSO, Grupo de Espectroscopia Molecular (GEM), Edificio Quimica, Laboratorias de Espectroscopia y Bioespectroscopia, Parque Cientifico, Universidad de Valladolid, 47011 Valladolid, Spain.</td>
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<td>H. V. L. NGUYEN, W. STAHL, Institut für Physikalische Chemie, RWTH Aachen University, Landoltweg 2, 52074 Aachen, Germany; and J.- U. GRABOW, Institut für Physikalische Chemie und Elektrochemie, Lehrgebiet A, Callinstrasse 3-3a, 30167 Hannover, Germany.</td>
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<th>MW SYSTEMATIC STUDY OF ALKALOIDS: THE DISTORTED TROPANE OF SCOPOLINE</th>
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<td>PATRICIA ECIA, EMILIO J. COCINERO, FRANCISCO J. BASTERRETXEA, JOSÉ A. FERNANDEZ, FERNANDO CASTANO, Departamento de Química Física, Facultad de Ciencia y Tecnología, Universidad del País Vasco (UPV/EHU), Ap.644, E-48940, Bilbao, Spain; ALBERTO LESARRI, Departamento de Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, E-47011 Spain.</td>
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MH04 15 min 2:16

STRUCTURAL STUDIES OF PYRROLE-BENZENE COMPLEXES BY CHIRPED-PULSE ROTATIONAL SPECTROSCOPY

SIMON LOBSIGER, CRISTOBAL PEREZ, DANIEL P. ZALESKI, NATHAN A. SEIFERT, BROOKS H. PATE, Department of Chemistry, University of Virginia, McCormick Rd., Charlottesville, VA 22904; CHANTEL PFAFFEN, MARIA A. TRACHSEL, SAMUEL LEUTWYLER, Departement für Chemie und Biochemie, Universität Bern, Freiestrasse 3, 3012 Bern, Switzerland.

MH05 15 min 2:33

A “WET DOG” TUNNELING MOTION AS THE CAUSE FOR THE DOUBLED ROTATIONAL SPECTRUM OF 1-IODONONAFLUOROBUTANE

W. C. BAILEY, Chemistry-Physics Department (Retired), Kean University, Union, New Jersey, USA 07083; R. K. BOHNI, Departments of Chemistry and Physics, University of Connecticut, Storrs, Connecticut, 06269-3060, USA.; G. S. GRUBBS II, Department of Chemistry, Wesleyan University, Hark-Atwater Laboratories, 52 Lawn Ave., Middletown, Connecticut, 06459-0180, USA.; Z. KISIEL, Institute of Physics, Polish Academy of Sciences, AL Lotnikow 32/46, 02-668 Warszawa, Poland.; S. A. COOKE, School of Natural and Social Sciences, Purchase College SUNY, 735 Anderson Hill Road, Purchase, NY 10577, USA.

MH06 15 min 2:50

TORSIONAL SPLITTING IN THE ROTATIONAL SPECTRUM FROM 8 TO 650 GHz OF THE GROUND STATE OF 1,1-DIFLUOROCETONE

L. MARGULÉS, R. A. MOTIYENKO, Laboratoire de Physique des Lasers, Atomes, et Molécules, UMR CNRS 8532, Université de Lille I, 59655 Villeneuve d’Ascq Cedex, France; P. GRÖNER, Department of Chemistry, University of Missouri-Kansas City, 5100 Rockhill Road, Kansas City, MO 64110-2399, USA; F. DE CHIRICO, A. TURK, S. A. COOKE, School of Natural and Social Sciences, Purchase College SUNY, 735 Anderson Hill Road, Purchase, NY 10577, USA.

MH07 15 min 3:07

AN IMPROVED ANALYSIS OF THE SEVOFLURANE-BENZENE STRUCTURE BY CHIRPED PULSE FTMW SPECTROSCOPY

NATHAN A. SEIFERT, CRISTOBAL PEREZ, DANIEL P. ZALESKI, JUSTIN L. NEILL, BROOKS H. PATE, Department of Chemistry, University of Virginia, McCormick Rd., Charlottesville, VA 22904-4319; ALBERTO LESARRI, MONTSERRAT VALLEJO, Departamento de Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, E-47011 Valladolid, Spain; EMILIO J. COCINERO, FERNANDO CASTANO, Departamento de Química Física, Facultad de Ciencia y Tecnología, Universidad del País Vasco (UPV/EHU), Campus de Leioa, Ap. 644, E-48080 Bilbao, Spain.

MH08 10 min 3:24

STRUCTURE DETERMINATION OF TWO STEREISOMERS OF SEVOFLURANE DIMER BY CHIRPED PULSE FTMW SPECTROSCOPY

NATHAN A. SEIFERT, CRISTOBAL PEREZ, DANIEL P. ZALESKI, JUSTIN L. NEILL, BROOKS H. PATE, Department of Chemistry, University of Virginia, McCormick Rd., Charlottesville, VA 22904-4319; ALBERTO LESARRI, MONTSERRAT VALLEJO, Departamento de Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, E-47011 Valladolid, Spain; EMILIO J. COCINERO, FERNANDO CASTANO, Departamento de Química Física, Facultad de Ciencia y Tecnología, Universidad del País Vasco (UPV/EHU), Campus de Leioa, Ap. 644, E-48080 Bilbao, Spain.

Intermission

MH09 15 min 3:50

THE COMPLETE MOLECULAR GEOMETRY OF SALICYL ALDEHYDE FROM ROTATIONAL SPECTROSCOPY

O. DOROSH, E. BALIKOWSKA-JAWORSKA, Z. KISIEL, L. PSZCZOLKOWSKI, Institute of Physics, Polish Academy of Sciences, Al. Lotnikow 32/46, 02-668 Warszawa, Poland; M. KANSKA, T. M. KRYGOWSKI, Department of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warszawa, Poland; H. MAEDER, Institut für Physikalische Chemie, Christian-Albrechts-Universität zu Kiel, Olshausenstrasse 40, D-24098 Kiel, Germany.
MH10 10 min 4:07
LABORATORY OBSERVATION OF THE ROTATIONAL SPECTRUM OF A POTENTIAL INTERSTELLAR SUGAR, ERYTHROSE
I. PENA, C. CABEZAS, A. M. DALY, S. MATA, J. L. ALONSO, Grupo de Espectroscopía Molecular (GEM), Edificio Quifima, Laboratorios de Espectroscopía y Bioespectroscopía, Parque Científico, Universidad de Valladolid, 47011 Valladolid, Spain.

MH11 15 min 4:19
ALDOPENTOSES IN THE GAS PHASE: ROTATIONAL SPECTRA OF D-XYLOSE, D-ARABINOSE, D-LYXOSE AND 2-DEOXY-D-RIBOSE

MH12 15 min 4:36
A ROTATIONAL STUDY OF D-MANNOSE AND D-GALACTOSE
I. PENA, A. M. DALY, C. CABEZAS, S. MATA, J. L. ALONSO, Grupo de Espectroscopía Molecular (GEM), Edificio Quifima, Laboratorios de Espectroscopía y Bioespectroscopía, Parque Científico, Universidad de Valladolid, 47011 Valladolid, Spain.

MH13 15 min 4:53
UNVEILING THE SWEET CONFORMATIONS OF KETOHEXOSES
C. BERMUDEZ, I. PENA, C. CABEZAS, A. M. DALY, S. MATA, J. L. ALONSO, Grupo de Espectroscopía Molecular (GEM), Edificio Quifima, Laboratorios de Espectroscopía y Bioespectroscopía, Parque Científico, Universidad de Valladolid, 47011 Valladolid, Spain.

MH14 15 min 5:10
ELUCIDATING THE STRUCTURE OF SUGARS: MW SPECTROSCOPY COMBINED WITH ULTRAFAST UV LASER VAPORIZATION
EMILIO J. COCINERO, PATRICIA ECJIA, FRANCISCO J. BASTERRETXEA, JOSÉ A. FERNANDEZ, FERNANDO CASTANO, Departamento de Química Física, Facultad de Ciencia y Tecnología, Universidad del País Vasco (UPV-EHU), Ap. 644, E-48080 Bilbao, Spain; ALBERTO LESARRI, Departamento de Química-Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, E-47011 Spain; JENS-UWE GRABOW, Institut für Physikalische Chemie, Lehrgebiet A, Universität Hannover, Callinstr. 3A, D-30167 Hannover, Germany; ALVARO CIMAS, Laboratoire Analyse et Modélisation pour la Biologie et l’Environnement, Université d’Évry Val d’Essonne, F-91025 Évry (France).

MH15 15 min 5:27
TOWARDS SOLVATION OF A CHIRAL ALPHA-HYDROXY ESTER: BROADBAND CHIRP AND NARROW BAND CAVITY FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF METHYL LACTATE-WATER CLUSTERS
JAVIX THOMAS, OLEKSANDR SUKHORUKOV, WOLFGANG JAEGER, YUNJIE XU, Department of Chemistry, University of Alberta, Edmonton, AB, T6G 2G2, Canada.

MI. ELECTRONIC
MONDAY, JUNE 17, 2013 – 1:30 PM
Room: 1015 MCPHERSON LAB

Chair: DAMIEN FORTHOMME, Brookhaven National Lab, Upton, NY

MI01 15 min 1:30
A DPF ANALYSIS YIELDS QUANTUM MECHANICALLY ACCURATE ANALYTIC POTENTIAL ENERGY FUNCTIONS FOR THE A1Σ+ AND X1Σ+ STATES OF NaH
ROBERT J. LE ROY, SADRU WALJI, KATHERINE SENTJENS, Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada.
MI02  15 min  1:47
UNCERTAINTIES IN PROPERTIES CALCULATED FROM FITTED POTENTIAL FUNCTIONS and DETERMINING POTENTIAL FUNCTIONS FROM FITS TO BOUND → CONTINUUM INTENSITY DATA

ROBERT J. LE ROY, Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada.

MI03  15 min  2:04
ASSIGNING COMPLEX VIBRATION-TUNNELING SPECTRA USING FRANCK-CONDON FINGERPRINTS

EDUARDO BERRIOS, PRAVEEN SUNDARADAVE and MARTIN GRUEBELE, Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, Il 61801.

MI04  15 min  2:21
OPTICAL-OPTICAL DOUBLE RESONANCE AND LIF SPECTROSCOPY OF THE JET-COOLED BORON CARBIDE (BC) FREE RADICAL

FUMIE X SUNAHORI, RAMYA NAGARAJAN, and DENNIS J. CLOUTHIER, Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055.

MI05  10 min  2:38
REINVESTIGATION OF THE EMISSION SPECTRA FOLLOWING THE 266 NM PHOTOLYSIS OF IODOMETHANES

CIAN-PING TU, HSIN-I CHENG, and BOR-CHEN CHANG, Department of Chemistry, National Central University, 300 Jhongda Road, Jhongli 32001, Taiwan.

MI06  15 min  2:50
CAVITY RINGDOWN ABSORPTION SPECTRUM OF THE T₁(n, π⁺) ← S₀ TRANSITION OF 2-CYCLOHEXEN-1-ONE

KATHERINE L. ZABRONSKY, MICHAEL O. MCANALLY, DANIEL J. STUPCA, NATHAN R. PILLSBURY, and STEPHEN DRUCKER, Department of Chemistry, University of Wisconsin-Eau Claire, Eau Claire, WI 54702.

MI07  15 min  3:07
COMPUTATIONAL INVESTIGATION OF THE T₁(n, π⁺) STATE OF 2-CYCLOHEXEN-1-ONE

MICHAEL O. MCANALLY and STEPHEN DRUCKER, Department of Chemistry, University of Wisconsin-Eau Claire, Eau Claire, WI 54702.

Intermission

MI08  15 min  3:40
PROBING COMPETITIVE NONCOVALENT INTERACTIONS: RESONANCE ENHANCED TWO-PHOTON IONIZATION (REMPI) SPECTROSCOPY OF HALOAROMATIC CLUSTERS

SILVER NYAMBO, LLOYD MUZANGWA, BRANDON UHLER and SCOTT A. REID, Department of Chemistry, Marquette University, Milwaukee, WI 53233.

MI09  15 min  3:57
NONLINEAR DUAL-COMB SPECTROSCOPY WITH TWO-PHOTON EXCITATION

S.A. MEEK, A. HIPKE, T. W. HÄNSCH, N. PICQUÉ, Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Straße 1, D-85748 Garching, Germany.

MI10  15 min  4:14
NEW DEVELOPMENTS OF BROADBAND CAVITY ENHANCED SPECTROSCOPIC TECHNIQUES

A. WALSH, D. ZHAO, H. LINNARTZ, Sackler Laboratory for Astrophysics, Leiden Observatory, University of Leiden, P.O. Box 9513, NL-2300 RA Leiden, the Netherlands; W. UBCACHS, LaserLab, VU University Amsterdam, De Boelelaan 1081, NL-1081 HV, Amsterdam, The Netherlands.

MI11  15 min  4:31
MEASURING THE QUENCHING OF NO FLUORESCENCE PRODUCED FROM THE EXCITATION OF PHOTO-FRAGMENTED NITROBENZENE USING A PICOSECOND LASER

CHRISTOPHER J. LUE, CHAKREE TANJAROON, J. BRUCE JOHNSON, SCOTT W. REEVE, Arkansas Center for Laser Applications and Science and Department of Chemistry and Physics, P.O. Box 419 State University, AR 72467; SUSAN D. ALLEN, Embyte Riddle Aeronautical University, 600 S. Clyde Morris Boulevard, Daytona Beach, FL 32114.

MI12  15 min  4:48
SPECTROSCOPY OF LUMINESCENT CRYSTALS CONTAINING RARE EARTH ELEMENTS

MENG-LING CHEN, KWANG-HWA LII, and BOR-CHEN CHANG, Department of Chemistry, National Central University, 300 Jhongda Road, Jhongli 32001, Taiwan.
DNA-ENHANCED DYE-SENSITIZED SOLAR CELLS

MARVIN POLUM and CARLOS E. CRESPO-HERNÁNDEZ. Department of Chemistry and Center for Chemical Dynamics, Case Western Reserve University, Cleveland, Ohio 44106.

SIMULATION OF FREE—FREE ABSORPTION SPECTRA AND THE CALCULATION OF INTERACTION POTENTIALS FOR ALKALI-RARE GAS ATOM PAIRS

J. DARBY HEWITT, THOMAS M. SPINKA, JASON. D. READLE, and J. GARY EDEN, Laboratory for Optical Physics and Engineering University of Illinois at Urbana Champaign, IL 61820.

SPECTROSCOPY OF 1,2-DIPHENYLETHANE-(H₂O)ₙ (n=1-3) CLUSTERS

JOSEPH R. GORD, EVAN G. BUCHANAN, PATRICK S. WALSH, and TIMOTHY S. ZWIER. Department of Chemistry, Purdue University, West Lafayette, IN 47907.

MJ. ATMOSPHERIC SPECIES

MONDAY, JUNE 17, 2013 – 1:30 PM

Room: 2015 MCPHERSON LAB

Chair: CHRIS MCRAVEN, Brookhaven National Lab, Upton, NY

WATER BROADENING OF OXYGEN

BRIAN J. DROUN, VIVIENNE PAYNE, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr., Pasadena, CA 91109; ELI MLAWER, Atmospheric and Environmental Research, 131 Hartwell Avenue, Lexington, MA 02421.

AIR-BROADENING AND SHIFT PARAMETERS IN THE ν₁ BAND OF OZONE

M. A. H. SMITH, Science Directorate, NASA Langley Research Center, Hampton, VA 23681-2199; V. MALATHE DEVI and D. CHRIS BENNER, Department of Physics, The College of William and Mary, Williamsburg, VA 23187-8795.

LINE PARAMETERS FOR THE OXYGEN A BAND

D. CHRIS BENNER, V. MALATHE DEVI, JI-AJUN HOO, Department of Physics, College of William and Mary, Williamsburg, VA; KEEYOON SUNG, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA; JOSEPH T. HODGES, DAVID A. LONG, Material Measurement Laboratory, National Institute of Standards and Technology, Gaithersburg, MD; THINH BUI, PRIYANKA MILINDA RUPASINGHE, MITCHIO OKUMURA, California Institute of Technology, Pasadena, CA.

AIR-BROADENED LINE SHAPES IN THE 2ν₃ R BRANCH OF ¹³CH₄ BETWEEN 6014 AND 6100 CM⁻¹

MJ05 15 min 2:38
LINE BROADENING PARAMETERS OF METHANE AT 6000 CM⁻¹

VICTOR GORSHELEV, ANNA SERDYUCHENKO, M. BUCHWITZ, J. BURROWS, Institute of Environmental Physics, University of Bremen, Germany, NEIL HUMPHAGE, J. REMEDIOS, Earth Observation Science Group, University of Leicester, UK.

MJ06 15 min 2:55
EXAMINING CONTRIBUTIONS TO LINE SHAPES IN THE ν₁ + ν₃ BAND OF ACETYLENE

MATTHEW J. CICH, SALVATORE M. CAIOLA, STEPHEN W. LEE, GARY V. LOPEZ, TREVOR J. SEARS⁵, Department of Chemistry, Stony Brook University, Stony Brook, New York 11794; DAMIEN FORTHOMME, C. P. MCRAVEN, GREGORY E. HALL, Department of Chemistry, Brookhaven National Laboratory, Upton, New York 11973; A. W. MANTZ, Department of Physics, Astronomy, and Astrophysics, Connecticut College, New London, CT 06320.

⁵Also: Department of Chemistry, Brookhaven National Laboratory, Upton, New York 11973

Intermission

MJ07 15 min 3:30
REFINEMENT OF THE ROBERT-BONAMY FORMALISM: TAKING INTO ACCOUNT OF CONTRIBUTIONS FROM THE LINE COUPLING

Q. MA, NASA/Goddard Institute for Space Studies and Department of Applied Physics and Applied Mathematics, Columbia University, 2880 Broadway, New York, NY 10025; C. BOULET, Institut des Sciences Moléculaires d'Orsay (ISMO); CNRS (UMR8214) et Université Paris-Sud Bât 350 Campus d'Orsay F-91405 FRANCE; R. H. TIPPING, Department of Physics and Astronomy, University of Alabama, Tuscaloosa, AL 35487.

MJ08 15 min 3:47
UNDISCOVERED ERRORS OF VOIGT PROFILE BEYOND TINY W-SHAPED RESIDUALS

G. WAGNER, M. BIRK, DLR, D-82234 Wessling, Germany; S.A. CLOUGH, Clough Radiation Associates, 89 Hancock Street, Lexington, MA 02420, USA.

MJ09 15 min 4:04
WATER INTENSITIES: AB INITIO VS. EXPERIMENT

MANFRED BIRK, GEORG WAGNER, DLR, D-82234 Wessling, Germany; LORENZO LODI, JONATHAN TENNYSSEN, Department of Physics and Astronomy, University College London, London WC1E 6BT, UK.

MJ10 15 min 4:21
FT-IR MEASUREMENTS OF CROSS SECTIONS OF COLD C₃H₅ IN THE 7 - 15 μM FOR TITAN

KEEYOUNG SUNG, GEOFFREY C. TOON, LINDA R. BROWN, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr, Pasadena, CA 91109; ARLAN W. MANTZ, Dept. of Physics, Connecticut College, New London, CT 06320; MARY ANN H. SMITH, Science Directorate, NASA Langley Research Center, Hampton, VA 23681.

MJ11 15 min 4:38
QUANTITATIVE MEASUREMENT OF INTEGRATED BAND INTENSITIES OF ISOPRENE AND FORMALDEHYDE

CAROLYN S. BRAUER, TIMOTHY J. JOHNSTON, THOMAS A. BLAKE, ROBERT L. SAMS, Pacific Northwest National Laboratory, P.O. Box 999, Mail Stop K3-59, Richland, WA 99352.

MJ12 15 min 4:55
QUANTITATIVE INTENSITY STUDIES OF THREE GAS-PHASE MONOTERPENES IN THE INFRARED: α-PINENE, β-PINENE AND D-LIMONENE

CAROLYN S. BRAUER, TIMOTHY J. JOHNSTON, THOMAS A. BLAKE, ROBERT L. SAMS, Pacific Northwest National Laboratory, P.O. Box 999, Mail Stop K3-59, Richland, WA 99352.

MJ13 10 min 5:12
COMPARISON OF EXPERIMENTAL AND THEORETICAL ABSORPTION CROSS SECTIONS OF FBAm

PAUL J. GODIN, STEPHANIE CONWAY, Department of Physics, University of Toronto, 60 St. George St., Toronto, ON, M5S 1A7, Canada; ANGELA HONG, Department of Chemistry, University of Toronto, 80 St. George St., Toronto, ON, M5S 3H6, Canada; KARINE LE BRIS, Department of Physics, St. Francis Xavier University, Antigonish, Nova Scotia, B2G 2W5, Canada; SCOTT MABURY, Department of Chemistry, University of Toronto, 80 St. George St., Toronto, ON, M5S 3H6, Canada; and KIMBERLY STRONG, Department of Physics, University of Toronto, 60 St. George St., Toronto, ON, M5S 1A7, Canada.
INVESTIGATING ATMOSPHERIC OXIDATION WITH MOLECULAR DYNAMICS IMAGING AND SPECTROSCOPY

W. G. MERRILL, A. S. CASE, and F. N. KEUTSCH, Department of Chemistry, University of Wisconsin, Madison, WI 53706.

PHOTOCHEMISTRY OF ACETONE IN SIMULATED ATMOSPHERE

T. CHAKRABORTY, A. K. GHOSH and A. CHATTOPADHYAY, Department of Physical Chemistry, Indian Association for the cultivation of science, Calcutta 700032, India. E-mail: ptc@iacs.res.in.

PHOTODISSOCIATION DYNAMICS OF 2-BROMOETHYLNITRITE AT 351 NM AND C-C BOND FISSION IN THE β-BROMOETHOXY RADICAL PRODUCT

LEI WANG, Department of Chemistry, The University of Chicago, Chicago, IL 60637; RABI CHHANTYAL-PUN, Department of Chemistry, The Ohio State University, Columbus, OH 43210; MATT D. BRYNTESON, Department of Chemistry, The University of Chicago, Chicago, IL 60637; TERRY A. MILLER, Department of Chemistry, The Ohio State University, Columbus, OH 43210; and LAURIE J. BUTLER, Department of Chemistry, The University of Chicago, Chicago, IL 60637.

MARK, INFRARED/RAMAN

MONDAY, JUNE 17, 2013 – 1:30 PM

Room: 1153 SMITH LAB

Chair: JENNIFER VAN WIJNGAARDEN, University of Manitoba, Winnipeg MB, Canada

ROTATIONALLY-RESOLVED SPECTROSCOPY OF THE BENDING MODES OF DEUTERATED WATER DIMER

JACOB T. STEWART, Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801; BENJAMIN J. McCALL, Departments of Chemistry and Astronomy, University of Illinois at Urbana-Champaign, Urbana, IL 61801.

MAPPING CONFORMATIONAL ENERGY BARRIERS IN HYDRATED RUBIDIUM ION CLUSTERS

HAOCHEN KE, AMY L. NICELY, JAMES M. LISY, Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801.

IR SPECTROSCOPY OF [Ag(CO)₂₅]⁻ CLUSTERS: IMPLICATIONS FOR REDUCTIVE ACTIVATION OF CO₂

BENJAMIN J. KNURR, and J. MATTHIAS WEBER, JILA and Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO 80309.
HIGH-RESOLUTION INFRARED SPECTROSCOPY OF \( \text{Ge}_2\text{C}_3 \)

S. THORWIRTH, V. LUTTER, S. SCHLEMMER, I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany; T. F. GIESEN, Universität Kassel, Fachbereich 10 - Physik, 34122 Kassel, Germany; J. GAUSS, Institut für Physikalische Chemie, Universität Mainz, 55099 Mainz, Germany.

FIRST OBSERVATION OF CO TRIMER AND A NEW LOOK AT CO DIMER

M. REZAEI, S. SHEYBANI-DELOUI, N. MOAZZEN-AHMADI, Department of Physics and Astronomy, University of Calgary, 2500 University Dr., N.W., Calgary, AB T2N 1N4, Canada; K.H. MICHAELIAN, Natural Resources Canada, CanmetENERGY, 1 Oil Patch Drive, Suite A202, Devon, AB T9G 1A8, Canada; A.R.W. McKELLAR, National Research Council of Canada, Ottawa, ON K1A 0R6, Canada.

OBSERVATION OF COMBINATION BANDS INVOLVING INTERMOLECULAR VIBRATIONS OF \( \text{N}_2\text{O}-\text{N}_2, \text{N}_2\text{O}-\text{OCS} \) AND \( \text{N}_2\text{O}-\text{CO}_2 \) COMPLEXES USING AN EXTERNAL CAVITY QUANTUM CASCADE LASER

M. REZAEI, S. SHEYBANI-DELOUI, N. MOAZZEN-AHMADI, Department of Physics and Astronomy, University of Calgary, 2500 University Dr., N.W., Calgary, Alberta T2N 1N4, Canada; K.H. MICHAELIAN, Natural Resources Canada, CanmetENERGY, 1 Oil Patch Drive, Suite A202, Devon, Alberta T9G 1A8, Canada; A.R.W. McKELLAR, National Research Council of Canada, Ottawa, Ontario, K1A 0R6, Canada.

INFRARED SPECTRA OF THE \( \text{NE}_2\text{-N}_2\text{O}, \text{AR}_2\text{-N}_2\text{O} \) TRIMERS

M. REZAEI, N. MOAZZEN-AHMADI, Department of Physics and Astronomy, University of Calgary, 2500 University Dr., N.W., Calgary, Alberta T2N 1N4, Canada; K.H. MICHAELIAN, Natural Resources Canada, CanmetENERGY, 1 Oil Patch Drive, Suite A202, Devon, Alberta, T9G 1A8, Canada; A.R.W. McKELLAR, National Research Council of Canada, Ottawa, Ontario, K1A 0R6, Canada.

INFRARED SPECTRUM OF THE \( \text{(CO}_2\text{)}_2\text{-N}_2\text{O} \) TRIMER MEASURED IN \( \text{N}_2\text{O} \text{v}_1 \) AND \( \text{v}_3 \) REGIONS

J. NOROOZ OLLIAEE, N. MOAZZEN-AHMADI, Department of Physics and Astronomy, University of Calgary, 2500 University Dr., N.W., Calgary, Alberta T2N 1N4, Canada; A.R.W. McKELLAR, National Research Council of Canada, Ottawa, Ontario, K1A 0R6, Canada.
## TA. MINI-SYMPOSIUM: SPECTROSCOPY TESTS OF FUNDAMENTAL PHYSICS

**TUESDAY, JUNE 18, 2013 – 8:30 AM**

**Room: 160 MATH ANNEX**

**Chair: ANATOLY TITOV, St. Petersburg Nuclear Physics Institute, Gatchina, Russia**

<table>
<thead>
<tr>
<th>TA01</th>
<th>INVITED TALK</th>
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<tr>
<td><strong>TOWARDS THE FIRST MEASUREMENT OF PARITY VIOLATION IN CHIRAL MOLECULES &amp; NEW ATTEMPTS AND FUTURE PROSPECTIVE</strong></td>
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<tr>
<td><strong>PETER SCHWERDTFEGER</strong>, Centre for Theoretical Chemistry and Physics, The New Zealand Institute for Advanced Study, Massey University Auckland, Auckland, New Zealand.</td>
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<th>TA02</th>
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<tr>
<td><strong>RIGOROUS RELATIVISTIC METHODS FOR ADDRESSING P- AND T-NONCONSERVATION IN HEAVY-ELEMENT MOLECULES</strong></td>
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<tr>
<td><strong>TIMO FLEIG</strong>, Laboratoire de Chimie et Physique Quantiques, Université Paul Sabatier Toulouse 3, Toulouse, France.</td>
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<th>TA03</th>
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<tr>
<td><strong>PARITY VIOLATION IN CHIRAL MOLECULES: CURRENT STATUS OF THEORY AND SPECTROSCOPIC EXPERIMENT</strong></td>
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<tr>
<td><strong>MARTIN QUACK, GEORG SEYFANG, PHYSICAL CHEMISTRY, ETH ZURICH, CH-8093 ZURICH, SWITZERLAND.</strong></td>
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<th>TA04</th>
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<td><strong>A COMBINED SYNCHROTRON-BASED HIGH RESOLUTION FTIR AND DIODE LASER JET INFRARED SPECTROSCOPY STUDY OF THE CHIRAL MOLECULE CD₃BrClF</strong></td>
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<tr>
<td><strong>S. ALBERT, K. KEPLER ALBERT, M. QUACK, PHYSICAL CHEMISTRY, ETH ZURICH, CH-8093 ZURICH, SWITZERLAND; PH. LERCH, SWISS LIGHT SOURCE, PAUL-SCHERRER-INSTITUTE, CH-5232 VILLIGEN, SWITZERLAND; V. BOUDON, LABORATOIRE CARNO'T DE BOURGOGNE, UNIVERSITE DE BOURGOGNE, F-21078 DIJON, FRANCE.</strong></td>
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<th>TA05</th>
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<tr>
<td><strong>CAVITY-ENHANCED PARITY-NONCONSERVING OPTICAL ROTATION IN Hg, Xe, AND I</strong></td>
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<th>TA06</th>
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<td><strong>CHIRAL CAVITY RING-DOWN: ABSOLUTE MEASUREMENT OF OPTICAL ROTATION IN GASES AND LIQUIDS WITH SIGNAL REVERSALS</strong></td>
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<tr>
<td><strong>LYKOURGOS BOUGAS, G. E. KATSORI-NAKIS, T. P. RAKITZIS</strong>, Department of Physics, University of Crete, and Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas 71110 Heraklion-Crete, Greece.</td>
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### Intermission

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<td><strong>NEW PERSPECTIVES ON THE SEARCH FOR A PARITY VIOLATION EFFECT IN CHIRAL MOLECULES</strong></td>
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<tr>
<th>TA08</th>
<th>15 min</th>
<th>11:02</th>
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<tr>
<td><strong>TRAVELLING-WAVE DECELERATION OF HEAVY DI-ATOMIC MOLECULES</strong></td>
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TA09
DETECTING PARITY VIOLATION USING TRAPPED MOLECULES

TA10
A SLOW SOURCE OF MOLECULES FOR HIGH RESOLUTION SPECTROSCOPY
MARINA QUINTERO-PÉREZ, PAUL JANSEN, THOMAS E. WALL, WIM UBACHS and HENDRICK L. BETHLEM, LaserLaB, Department of Physics and Astronomy, VU University Amsterdam, De Boelelaan 1081, 1081 HV Amsterdam, The Netherlands.

TB. MINI-SYMPOSIUM: SPECTROSCOPY OF PLANETARY ATMOSPHERES
TUESDAY, JUNE 18, 2013 – 8:30 AM
Room: 170 MATH ANNEX

Chair: PETER BERNATH, Old Dominion University, Norfolk, Virginia

TB01
THE ROLE OF SPECTROSCOPY IN RESEARCH ON THE NEUTRAL ATMOSPHERES OF THE OUTER SOLAR SYSTEM
GLENN S. ORTON, JET PROPULSION LABORATORY, CALIFORNIA INSTITUTE OF TECHNOLOGY, PASADENA, CA 91109.

TB02
INTENSITY MODELING OF METHANOL IN THE TORSIONAL MANIFOLD
LI-HONG XU, Centre for Laser, Atomic and Molecular Sciences (CLAMS), Physics Department, University of New Brunswick, 100 Tucker Park Road, Saint John, NB, Canada E2L 4L5; ISABELLE KLEINER, Laboratoire Interuniversitaire des Systèmes Atmosphériques, CNRS et Universités Paris Diderot et Paris Est, 61 av. Général de Gaulle, 94010, Créteil, France.

TB03
THZ SPECTROSCOPY OF DEUTERATED ETHANE
BRIAN J. DROUIN, SHANSHAN YU, JOHN C. PEARSON, LINDA R. BROWN, KEEYOON SUNG, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr., Pasadena, CA 91109; PETER GRONER, Department of Chemistry, University of Missouri-Kansas City, Kansas City, MO 64110-2499.

TB04
OZONE RECOVERY IN THE PRESENCE OF O2(a1Δ) FOR ATMOSPHERIC STUDIES
MICHAEL C. HEAVEN, Department of Chemistry, Emory University, Atlanta, GA 30322; VALERIY N. AZYAZOV, P.N. Lebedev Physical Institute, Samara Branch, Samara, Russia, 443029.

Intermission

TB05
EXOMOL: MOLECULAR LINE Lists for EXOPLANET AND OTHER ATMOSPHERES
JONATHAN TENNYSON, Department of Physics and Astronomy, University College London, London, WC1E 6BT, UK.

TB06
A NEW GLOBAL FIT FOR 17O ENRICHED CO2
BEN M. ELLIOTT, CHARLES E. MILLER, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Drive, M/S 233-300, Pasadena, CA 91109.
TC01 10 min 8:30
ROTOR-L-1 MONOFUOROPYRIDINE VAN DER WAALS COMPLEXES
MAHDI KAMAE, MING SUN AND JENNIFER VAN WIJNAGARDEN, Department of Chemistry, University of Manitoba, Winnipeg MB R3T 2N2 Canada.

TC02 15 min 8:42
BROADBAND CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE SPECTROSCOPY AND MOLECULAR STRUCTURE OF THE ARGON-1-CHLORO-1-FLUOROETHYLENE COMPLEX
MARK D. MARSHALL AND HELEN O. LEUNG, Department of Chemistry, Amherst College, P.O. Box 5000, Amherst, MA 01002-5000.

TC03 15 min 8:59
MICROWAVE SPECTRA AND MOLECULAR STRUCTURES OF 2-CHLORO-1,1-DIFLUOROETHYLENE AND ITS COMPLEX WITH ARGON
JOSEPH P. MESSINGER, GREGORY S. KNOWLTON, KATHRYN M. SUNDEHEIM, HELEN O. LEUNG, AND MARK D. MARSHALL, Department of Chemistry, Amherst College, P.O. Box 5000, Amherst, MA 01002-5000.

TC04 15 min 9:16
ROTOR-L-1 TRIFLUORO ETHANOL (TFE) - WATER CLUSTERS AND THE TFE DIMERS
JAVOX THOMAS, YUNJIE X U, Department of Chemistry, University of Alberta, Edmonton, AB, T6G 2G2, Canada.

TC05 15 min 9:33
STRUCTURE FOR THE PROPIONIC ACID - FORMIC ACID COMPLEX FROM MICROWAVE SPECTRA FOR MULTIPLE ISOTOPOLOGUES
STEPHEN G. KUKOLICH, ERIK G. MITCHELL, SPENCER J. CAREY, MING SUN, AND BRYAN M. SARGUS, Department of Chemistry and Biochemistry, The University of Arizona, Tucson, Arizona 85721.

"Supported by THE NATIONAL SCIENCE FOUNDATION"
THE EFFECT OF PROTIC ACID IDENTITY ON THE STRUCTURES OF COMPLEXES WITH VINYL CHLORIDE: FOURIER TRANSFORM MICROWAVE SPECTROSCOPY AND MOLECULAR STRUCTURE OF THE VINYL CHLORIDE-ACETYLENE COMPLEX

HELEN O. LEUNG, MARK D. MARSHALL, AND FAN FENG, Department of Chemistry, Amherst College, P.O. Box 5000, Amherst, MA 01002-5000.

Intermission

THE MICROWAVE STUDIES OF GUIACOL (2-METHOXYPHENOL) ISOTOPOLOGUES AND VAN DER WAALS COMPLEXES

RANIL M. GURUSINGHE, ASHLEY FOX, and MICHAEL J. TUBERGEN, Department of Chemistry, Kent State University, Kent, OH 44242.

AN IMPROVED CHIRPED PULSE FTMW ANALYSIS OF THE STRUCTURES OF PHENOL DIMER AND TRIMER

NATHAN A. SEIFERT, CRISTÓBAL PÉREZ, AMANDA L. STEBER, DANIEL P. ZALESKI, JUSTIN L. NEILL, BROOKS H. PATE, Department of Chemistry, University of Virginia, McCormick Rd., Charlottesville, VA 22904-4319; ALBERTO LESARRI, Departamento de Quimica Fisica y Quimica Inorganica, Facultad de Ciencias, Universidad de Valladolid, E-47011 Valladolid, Spain.

OLIGOMERS BASED ON A WEAK HYDROGEN BOND NETWORK: THE ROTATIONAL SPECTRUM OF THE TETRAMER OF DIFLUOROMETHANE

GANG FENG, LUCA EVANGELISTI, and WALther CAMINATI, Dipartimento di Chimica "G. Ciamicnan" dell'Università, Via Selmi 2, I-40126 Bologna, Italy; IVO CACELLI, and LAURA CARBONARO, Dipartimento di Chimica e Chimica Industriale, Università di Pisa, Via Risorgimento 35, I-56126 Pisa, Italy; GIACOMO PRAMPOLINI, Istituto per i Processi Chimico-Fisici (IPCF-CNR), Area della Ricerca, Via G. Moruzzi 1, I-56124 Pisa, Italy.

ROTATIONAL SPECTRA OF ADDUCTS OF FORMALDEHYDE WITH FREONS

GOU QIAN, GANG FENG, LUCA EVANGELISTI, and W. CAMINATI, Dipartimento di Chimica "G. Ciamicnan" dell'Università, Via Selmi 2, I-40126 Bologna, Italy; MONTserrat VALLEJO LÓPEZ, ALBERTO LESARRI, Departamento de Quimica Fisica y Quimica Inorganica, Facultad de Ciencias, Universidad de Valladolid, E-47011 Valladolid, Spain; EMILIO COCJERO, Departamento de Quimica Fisica, Facultad de Ciencia y Tecnologia, Universidad del Pais Vasco, E-48080 Bilbao, Spain.

MICROWAVE SPECTROSCOPIC INVESTIGATIONS OF THE C-H-...π CONTAINING COMPLEXES CHF₂-...PROPYLE AND CH₂F-...PROPYLE

REBECCA A. PEEBLES, SEAN A. PEEBLES, CORI L. CHRISTENHOLZ, ANTHONY A. ERNST, and YASER J. DHAHIR, Department of Chemistry, Eastern Illinois University, 600 Lincoln Ave., Charleston, IL 61920.

OBSERVATION OF A C-H-...AROMATIC INTERACTION IN THE FLUOROBENZENE-...HCCH WEAKLY BOUND COMPLEX

NATHAN W. ULRICH, SEAN A. PEEBLES, REBECCA A. PEEBLES, and YASER J. DHAHIR, Department of Chemistry, Eastern Illinois University, 600 Lincoln Ave., Charleston, IL 61920; NATHAN A. SEIFERT, CRISTÓBAL PÉREZ, and BROOKS H. PATE, Department of Chemistry, University of Virginia, McCormick Rd., PO Box 400319, Charlottesville, VA 22904.

TD. RADICALS AND IONS
TUESDAY, JUNE 18, 2013 – 8:30 AM
Room: 1015 MCPHERSON LAB
Chair: YUAN-PERN LEE, National Chiao Tung University, Hsinchu, Taiwan

TD01  15 min  8:30
THE ROLES OF ATOMIC OXYGEN AND NITRIC OXIDE IN LOW TEMPERATURE PLASMAS

SHERRIE S. BOWMAN, DAVID BURNETTE, IGOR V. ADAMOVICH, and WALTER R. LEMPERT, M.A. Chassey Laboratory, The Ohio State University, Columbus, Ohio 43210.

TD02  15 min  8:47
SUB-DOPPLER SPECTROSCOPY OF trans-HOCO RADICAL IN THE OH STRETCHING MODE

CHIH-HSUAN CHANG, GRANT BUCKINGHAM, and DAVID J. NESBITT, JILA, National Institute of Standards and Technology University of Colorado, and Department of Chemistry and Biochemistry University of Colorado at Boulder, Colorado 80309.

TD03  15 min  9:04
VIBRATIONAL ANALYSIS FOR B - X TRANSITION OF ISOPROPANOXY RADICAL

RABI CHHANTYAL-PUN and TERRY A. MILLER, Laser Spectroscopy Facility, Department of Chemistry, The Ohio State University, 120 W. 18th Avenue, Columbus OH 43210.

TD04  15 min  9:21
ANALYSIS OF THE ROTATIONAL STRUCTURE OF B2A' --> X2A' TRANSITION OF ISOPROPANOXY RADICAL: ISOLATED STATE vs. COUPLED STATES MODEL

DIMITRY G. MELNIK and TERRY A. MILLER, Laser Spectroscopy Facility, Department of Chemistry, The Ohio State University, 120 W. 18th Avenue, Columbus, Ohio 43210; JINJUN LIU, Department of Chemistry, University of Louisville, 2320 South Brook Street, Louisville, Kentucky 40292.

TD05  15 min  9:38
HIGH-RESOLUTION LASER-INDUCED FLUORESCENCE SPECTROSCOPY OF CYCLOHEXENOXY: ROTATIONAL AND FINE STRUCTURE OF MOLECULES IN NEARLY DEGENERATE ELECTRONIC STATES

JINJUN LIU, Department of Chemistry, University of Louisville, 2320 S. Brook St., Louisville, Kentucky 40292; DIMITRY G. MELNIK, and TERRY A. MILLER, Laser Spectroscopy Facility, Department of Chemistry, The Ohio State University, 120 W. 18th Ave., Columbus, Ohio 43210.

TD06  15 min  9:55
ANOMALOUS A-DOUBLING IN THE INFRARED SPECTRUM OF THE HYDROXYL RADICAL IN HELIUM NANO-DROPLETS

P. RASTON, T. LIANG, and G. E. DOUBERLY, Department of Chemistry, University of Georgia, Athens, Georgia 30602, USA.

TD07  15 min  10:12
HELIUM NANO-DROPLET ISOLATION SPECTROSCOPY AND AB INITIO CALCULATIONS OF HO2(O2)N CLUSTERS (N=0-4)

T. LIANG, P. RASTON, and G. E. DOUBERLY, Department of Chemistry, University of Georgia, Athens, Georgia 30602, USA.

Intermission

TD08  15 min  10:45
FOURIER TRANSFORM INFRARED SPECTROSCOPY OF CH3OO RADICAL IN MID-INFRARED RANGE

KUO-HSIANG HSU and YUAN-PERN LEE, Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu 30010, Taiwan and Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617; MENG HUANG and TERRY A. MILLER, Laser Spectroscopy Facility, Department of Chemistry, The Ohio State University, 120 W. 18th Avenue, Columbus, Ohio 43210.

TD09  15 min  11:02
FARADAY ROTATION SPECTROSCOPY OF HO2 FROM AN ATMOSPHERIC FLOW REACTOR

BRIAN BRUMFIELD, GERARD WYSOCKI, Department of Electrical Engineering, Princeton University, Princeton, NJ 08544; WENTING SUN, YIGUANG JU, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ 08544.

TD10  15 min  11:19
OBSERVATION OF THE A' - X ELECTRONIC TRANSITION OF C6H10 PEROXY RADICALS

NEAL D. KLINE and TERRY A. MILLER, Laser Spectroscopy Facility, Department of Chemistry, The Ohio State University, 120 W. 18th Avenue, Columbus, Ohio 43210.
TD11 15 min 11:36
STRUCTURE IN THE VISIBLE ABSORPTION BANDS OF JET-COOLED PHENYL PEROXY RADICALS

MICHAEL N. SULLIVAN, KEITH FREELE, J. PARK, M.C. LIN, and MICHAEL C. HEAVEN, Department of Chemistry, Emory University, Atlanta, GA 30322.

TD12 15 min 11:53
TERAHERTZ ROTATIONAL SPECTROSCOPY OF THE SO RADICAL

M. A. MARTIN-DRUEDE, A. CUISSET, S. ELIET, G. MOURET, F. HINDLE, Laboratoire de Physico-Chimie de l’Atmosphère, EA 4493, Université du Littoral Côte d’Opale, 59140 Dunkerque, France; O. PIROLI, Institut des Sciences Moléculaires d’Orsay, CNRS, UMR 8214, Université Paris XI, bât. 210, 91405 Orsay Cedex, France; SOLEIL Synchrotron, AILES beamline, L’orner des Merisiers, Saint-Aubin, 91192 Gif-Sur-Yvette, France.

TE. MATRIX/CONDENSED PHASE

TUESDAY, JUNE 18, 2013 – 8:30 AM
Room: 2015 MCPHERSON LAB

Chair: MARILYN JACOX, NIST, Gaithersburg, MD

TE01 15 min 8:30
INFRARED SPECTROSCOPY OF HNO AND NOH SUSPENDED IN SOLID PARAHYDROGEN

DAVID T. ANDERSON AND MAHMUT RUZI, Department of Chemistry, University of Wyoming, Laramie, WY 82071-3838.

TE02 15 min 8:47
COLD CHEMICAL REACTIONS OF H-ATOMS AND N₂O IN SOLID PARAHYDROGEN AT 2 K

DAVID T. ANDERSON AND FREDRICK M. MUTUNGA, Department of Chemistry, University of Wyoming, Laramie, WY 82071-3838.

TE03 15 min 9:04
RYDBERG STATES OF Rb AND Cs ATOMS ON HELIUM NANODROPLETS: A RYDBERG-RITZ ANALYSIS

FLORIAN LACKNER, GÜNTER KROIS and WOLFGANG E. ERNST, Institute of Experimental Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria.

TE04 15 min 9:21
DYNAMICS OF CH₃F-(ortho-H₂)ₙ CLUSTERS IN SOLID para-H₂ CRYSTAL STUDIED BY PUMP AND PROBE SPECTROSCOPY USING TWO CW-QUANTUM CASCADE LASERS

H. KAWASAKI and A. MIZOGUCHI, H. KANAMORI, Department of Physics, Tokyo Institute of Technology, Tokyo, JAPAN 152-8551.

TE05 15 min 9:38
TERAHERTZ TIME DOMAIN SPECTROSCOPY OF SIMPLE ASTROPHYSICALLY RELEVANT Ices: THE STRUCTURE OF THE ICE

SERGIO IOPPOLO, Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, CA 91125; MARCO A. ALLODI, BRETT A. McGUIRE, MATTHEW J. KELLEY, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125; GEOFFREY A. BLAKE, Division of Chemistry and Chemical Engineering and Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, CA 91125.

TE06 15 min 9:55
FIRST OBSERVATION OF A VIBRATIONAL FUNDAMENTAL OF SiC₄Si TRAPPED IN SOLID Ar

T. H. LE, C.M. L. RITTBY and W.R.M. GRAHAM, Department of Physics and Astronomy, Texas Christian University, Fort Worth, TX 76129.

TE07 15 min 10:12
NIR LASER RADIATION INDUCED CONFORMATIONAL CHANGES AND TUNNELING LIFETIMES OF HIGH-ENERGY CONFORMERS OF AMINO ACIDS IN LOW-TEMPERATURE MATRICES

GÁBOR BÁZSÓ, ESZTER E. NAJBÄUER, GÁBOR MAGYARFALVI and GYÖRGY TARCSAY, Laboratory of Molecular Spectroscopy, Institute of Chemistry, Eötvös University, PO Box 32, H-1518, Budapest 112, Hungary.

Intermission
CHARACTERIZATION OF A 1:1 METHANOL-BENZENE COMPLEX USING MATRIX ISOLATION INFRARED SPECTROSCOPY

JAY C. AMICANGELO, NATALIE C. ROMANO, AND GEOFFREY R. DEMAY. School of Science, Penn State Erie, Erie, PA 16563.

VUV PHOTOLOGY OF NH3: A MATRIX ISOLATION STUDY OF THE MOLECULAR INTERACTIONS BETWEEN AMIDOGEN RADICAL AND AMMONIA MOLECULES

L. KRIM, and E. L. ZINS, Laboratoire de Dynamique, Interactions et Réactivité, LADIR, CNRS, UMR 7075, Université Pierre et Marie Curie, 4 place Jussieu, 75252 Paris cedex 05, France.

HOT SPOT GENERATION IN ENERGETIC MATERIALS BY APPLYING WEAK ENERGIES

MING-WEI CHEN, SIZHU YOU, KENNETH S. SUSLICK, DANA D. DLOTT, School of Chemical Sciences, University of Illinois at Urbana-Champaign, Urbana, IL 61801.

THERMAL DECOMPOSITION MECHANISM OF BUTYRALDEHYDE

COURTNEY D. HATTEN, BRIAN WARNER, EMILY WRIGHT, KEVIN KASKEY, LAURA R. McCUNN. Department of Chemistry, Marshall University, Huntington, WV 25755.

THE PECULIARITIES OF THE NMR SPIN-LATTICE RELAXATION IN PROTON EXCHANGED LINBO3

IGOR VERTEGEL, Institute of Physics NAS of Ukraine, Prospect Nauki 46, 03680 Kiev, Ukraine; EUGENY CHESNOKOV, Institute of Physics NAS of Ukraine, Prospect Nauki 46, 03680 Kiev, Ukraine; ALEXANDER OVCARENKO, Institute of Physics NAS of Ukraine, Prospect Nauki 46, 03680 Kiev, Ukraine; and IVAN VERTEGEL, The Faculty of Mechanics and Mathematics, National Tams Shevchenko University of Kiev, Ukraine.

TF. MINI-SYMPHOSIUM: SPECTROSCOPY TESTS OF FUNDAMENTAL PHYSICS

TUESDAY, JUNE 18, 2013 – 1:30 PM

Room: 160 MATH ANNEX

Chair: WIM UBACHS, Vrije Universiteit, Amsterdam, The Netherlands

AN OVERVIEW OF PNC RELATED STUDIES INVOLVING HEAVY POLAR MOLECULES

TIMOTHY C. STEIMLE, Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287.

THE MOLECULAR FRAME ELECTRIC DIPOLE MOMENT AND HYPERFINE INTERACTIONS IN HAFNIUM FLUORIDE, HfF

ANH LE AND TIMOTHY C. STEIMLE, Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287; LEONID SKRIPNIKOV AND ANATOLY V. TITOY, Petersburg Nuclear Physics Institute, Gatchina, 188300, Russia and Quantum Mechanics Division, St. Petersburg State University, St. Petersburg 198904, Russia.

ThF+ AS A CANDIDATE FOR eEDM MEASUREMENTS

MICHAEL C. HEAVEN, JOSHUA H. BARTILETT, Department of Chemistry, Emory University, Atlanta, GA 30322.
A CONCEPT OF EFFECTIVE STATE OF ATOMS-IN-COMPOUNDS TO DESCRIBE PROPERTIES DETERMINED BY THE VALENCE Electron's DENSITIES IN ATOMIC CORES

A.V. TITOV, Yu.V. LOMACHUK, L.V. KRIPNIKOV, A.N. PETROV, N.S. MOSYAGIN, B.P. Konstantinov Petersburg Nuclear Physics Institute, Gatchina, Leningrad district 188300; Department of Physics, Saint Petersburg State University, Petrodvorets 198904, RUSSIA.

*SPbU Fundamental Science Research grant from Federal budget N.038.652.2013 and RFBR grant 13-02-01406 are gratefully acknowledged

VOLTAGE CONTROLLED GEOMETRIC PHASE ROTATION IN $^{208}$Pb,$^{19}$F.

J.E. FURNEAUX, NEIL SHAFER-RAY, J. COKER, P. M. RUPASINGHE, Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma, Norman, OK 73019; and C. P. McRAVEN, Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973.

MEASUREMENT OF THE ELECTRON'S ELECTRIC DIPOLE MOMENT IN THORIUM MONOXIDE

J. BARON, Harvard University; D. DEMILLE, Yale University; J. DOYLE, G. GABRIELSE, P. HESS, N. HUTZLER, Harvard University; B. OLEARY, Yale University; C. PANDA, E. PETRIK, B. SPAUN, Harvard University.

*ACME COLLABORATION

BROADBAND VELOCITY MODULATION SPECTROSCOPY OF MOLECULAR IONS FOR USE IN THE JILA ELECTRON EDM EXPERIMENT

DANIEL N. GRESH, KEVIN C. COSSEL, ERIC A. CORNELL, and JUN YE, JILA, National Institute of Standards and Technology and University of Colorado Department of Physics, University of Colorado, Boulder, Colorado 80309-0440, USA.

PROGRESS OF THE JILA ELECTRON EDM EXPERIMENT

HUANQIAN LOH, KEVIN C. COSSEL, MATT GRAU, DANIEL N. GRESH, KANG-KUEN NI, JUN YE, and ERIC A. CORNELL, JILA, National Institute of Standards and Technology and University of Colorado Department of Physics, University of Colorado, Boulder, Colorado 80309-0440, USA.

HYPERFINE INTERACTION IN DIATOMICS AS A TOOL FOR SUPPRESSION OF SYSTEMICS AND VERIFICATION OF THEORETICAL VALUES FOR THE EFFECTIVE ELECTRIC FIELD ON ELECTRON FOR THE ELECTRON EDM EXPERIMENTS

A.N. PETROV, L.V. KRIPNIKOV, N.S. MOSYAGIN, A.V. TITOV, B.P. Konstantinov Petersburg Nuclear Physics Institute, Gatchina, Leningrad district 188300; Department of Physics, Saint Petersburg State University, Petrodvorets 198904, RUSSIA.

*SPbU Fundamental Science Research grant from Federal budget N.038.652.2013 and RFBR grant 13-02-01406 are gratefully acknowledged

ROTATIONAL SPECTRA IN SERVICE OF PARTICLE PHYSICS — ZEEMAN & HYPERFINE EFFECTS

RICHARD J MAWHORTER, ALEXANDER L. BAUM, ZACHARY GLASSMANN, BENJAMIN GIRODAS, Dept of Physics & Astronomy, Pomona College, Claremont, CA 91711; TREVOR SEARS, Chemistry Dept, Brookhaven National Laboratory, Upton, NY 11973; NEIL E. SHAFER-RAY, Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma, Norman, OK; LUKAS ALPHEI, JENS-UWE GRABOW, Institut für Physikalische Chemie und Elektrochemie, Gottfried-Wilhelm-Leibniz-Universität, 30167 Hannover, Germany.

PRECISE THEORETICAL STUDY OF SPECTROSCOPIC CONSTANTS IN DIATOMICS

L.V. KRIPNIKOV, A.N. PETROV, A.V. TITOV, N.S. MOSYAGIN, B.P. Konstantinov Petersburg Nuclear Physics Institute, Gatchina, Leningrad district 188300; Department of Physics, Saint Petersburg State University, Petrodvorets 198904, RUSSIA.

*SPbU Fundamental Science Research grant from Federal budget N.038.652.2013 and RFBR grant 13-02-01406 are gratefully acknowledged

Intermission
DETERMINATION OF THE BOLTZMANN CONSTANT BY MEANS OF DOPPLER-ENHANCED THERMOMETRY ON WATER AT 1.39 µm.

L. MORETTI, A. CASTRILLO, E. FASCI, M.D. DE VIZIA, Dipartimento di Matematica e Fisica, Seconda Università di Napoli, Caserta, Italy. G. GALZERANO, P. LAPORTA, Dipartimento di Fisica, Politecnico di Milano and IFN-CNR, Milano, Italy. A. MERLONE, INRIM, Istituto Nazionale di Ricerca Metrologica, Torino, Italy and L. GIANFRANI, Dipartimento di Matematica e Fisica, Seconda Università di Napoli, Caserta, Italy.

ULTRA-LOW PHASE NOISE, HIGH RESOLUTION SPECTROMETER USING COMB-ASSISTED QUANTUM CASCADE LASERS

ANDREW A. MILLS, CHRISTIAN MOHR, JIE JIANG, IMRA America, Ann Arbor, MI. DAVIDE GATTI, MARCO MARANGONI, Dipartimento di Fisica del Politecnico di Milano, Milano, Italy. LIVIO GIANFRANI, Seconda Università Di Napoli, Caserta, Italy. INGMAR HARTL, Deutsches Elektronen-Synchrotron, Hamburg, Germany. MARTIN FERMANN, IMRA America, Ann Arbor, MI.

NARROW OPPOSITE-PARITY LEVEL CROSSINGS IN A DIATOMIC RADICAL

S. B. CAHN, J. AMMON, Y. GUREVICH, E. ALTUNTAS, D. DEMILLE, Yale University, Dept. of Physics, New Haven, CT, USA. R. PAOLINO, US Coast Guard Academy, New London, CT, USA. M. G. KOZLOV, Petersburg Nuclear Physics Institute, Gatchina, Russia.

PHOTOELECTRON SPECTROSCOPY STUDIES OF URANIUM FLUORIDE

WEI-LI LI, TIAN JIAN, GARY V. LOPEZ, AND LAI-SHENG WANG, Brown University, Chemistry Department, 924 Brook St, Providence, RI, 02912.

TG. MINI-SYMPOSIUM: THEORY AND SPECTROSCOPY
TUESDAY, JUNE 18, 2013 – 1:30 PM
Room: 170 MATH ANNEX

Chair: JOHN STANTON, The University of Texas at Austin, Austin, TX

INVITED TALK 30 min 1:30
DIABATIC VERSUS ADIABATIC CALCULATION OF TORSION-VIBRATION INTERACTIONS

JON T. HOUGEN, Sensor Science Division, NIST, Gaithersburg, MD 20899-8441, USA.

AB INITIO AND MODEL-HAMILTONIAN STUDY OF THE TORSIONAL VARIATION OF THE THREE CH STRETCHING NORMAL MODES IN METHANOL

LI-HONG XU, RONALD M. LEES, Centre for Laser, Atomic and Molecular Sciences (CLAMS), Physics Department, University of New Brunswick, 100 Tucker Park Road, Saint John, NB, Canada E2L 4L5. JON T. HOUGEN, Sensor Sciences Division, National Institute of Standards and Technology, Gaithersburg, MD 20899-8441.
TG03 15 min 2:22
EXTENDING DIFFUSION MONTE CARLO TO INTERNAL COORDINATES
ANDREW S. PETITT and ANNE B. McCOY, Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH 43210.

TG04 15 min 2:39
PATTERNS OF BROKEN PATTERNS
R. W. FIELD, G. B. PARK, P. B. CHANGALA, J. H. BARABAN, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139, USA; J. F. STANTON, Institute for Theoretical Chemistry, Departments of Chemistry and Biochemistry, The University of Texas at Austin, Austin, Texas 78712; A. J. MERER, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan, Department of Chemistry, University of British Columbia, Vancouver, B.C., Canada V6T 1Z1.

TG05 15 min 2:56
ISOMERIZATION, PERTURBATIONS, CALCULATIONS AND THE S1 STATE OF C2H2
J. H. BARABAN, P. B. CHANGALA, J. R. P. BEER, R. W. FIELD, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139, USA; J. F. STANTON, Institute for Theoretical Chemistry, Departments of Chemistry and Biochemistry, The University of Texas at Austin, Austin, Texas 78712; A. J. MERER, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan, Department of Chemistry, University of British Columbia, Vancouver, B.C., Canada V6T 1Z1.

TG06 15 min 3:13
REDUCED DIMENSION ROVIBRATIONAL VARIATIONAL CALCULATIONS OF THE S1 STATE OF C2H2
P. B. CHANGALA, J. H. BARABAN, R. W. FIELD, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139, USA; J. F. STANTON, Institute for Theoretical Chemistry, Departments of Chemistry and Biochemistry, The University of Texas at Austin, Austin, Texas 78712; A. J. MERER, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan;

TG07 15 min 3:30
LEAST SQUARES FITTING OF PERTURBED VIBRATIONAL POLYADS NEAR THE ISOMERIZATION BARRIER IN THE S1 STATE OF C2H2
A. J. MERER, Department of Chemistry, University of British Columbia, Vancouver, B.C., Canada V6T 1Z1 AND Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan; J. H. BARABAN, P. B. CHANGALA, and R. W. FIELD, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139, USA.

Intermission

TG08 15 min 4:00
COLLISIONAL LINE MIXING IN PARALLEL AND PERPENDICULAR BANDS OF LINEAR MOLECULES BY A NON-MARKOVIAN APPROACH
JEANNA BULDYREVA, Institut UTINAM, UMR CNRS 6213, Université de Franche-Comté, 16 route de Gray, 25030 Besançon cedex, France.

TG09 15 min 4:17
TUNNELING AND TUNNELING SWITCHING DYNAMICS IN PHENOL AND ORTHO-D-PHENOL: FTIR SPECTROSCOPY WITH SYNCHROTRON RADIATION AND THEORY
S. ALBERT, R. PRENTNER, M. QUACK, PHYSICAL CHEMISTRY, ETH ZURICH, CH-8093 ZURICH, SWITZERLAND; PH. LERCH, SWISS LIGHT SOURCE, PAUL-SCHERRER-INSTITUTE, CH-5232 VILLIGEN, SWITZERLAND.

TG10 15 min 4:34
ANHARMONIC VIBRATIONAL MÖLLER-PLESSET PERTURBATION THEORIES USING THE DYSON EQUATION
MATTHEW R. HERMIES and SO HIRATA, Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801.
**THG11**

**15 min 4:51**

PERTURBATIVE CORRECTIONS TO THE CALCULATED TRANSITION FREQUENCY AND OSCILLATOR STRENGTH OF THE HYDROGEN BONDED OH-OSCIILLATOR IN THE DONOR WATER MOLECULE IN WATER DIMER

KASPER MACKEPRANG, HENRIK G. KJAERGAARD, Department of Chemistry, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen, DENMARK; TEEMU SALMI, LAURI HALONEN, Laboratory of Physical Chemistry, Department of Chemistry, P.O. Box 55, A. I. Virtanen auki 1, FI-00014, University of Helsinki, Helsinki, Finland.

**THG12**

**15 min 5:08**

VIBRATIONAL CONSTANS TO TRIATOMIC MOLECULES FROM FOURTH-ORDER PERTURBATION THEORY

DEVIN A. MATTHEWS, JUSTIN Z. GONG, and JOHN F. STANTON, Department of Chemistry and Biochemistry, Institute for Theoretical Chemistry, The University of Texas at Austin, Austin, Texas 78712.

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**TH. MICROWAVE**

TUESDAY, JUNE 18, 2013 – 1:30 PM

Room: 1000 MCPHERSON LAB

**Chair:** GILLES ADANDE, University of Arizona, Tucson, AZ

**TH01**

**15 min 1:30**

THE SUB-MILLIMETER WAVE SPECTROSCOPY OF MONODUTERATED AMIDOXAN RADICAL (NHD)

YUTA MOTOKI, HIROYUKI OZEKI, Department of Environmental Science, Toho University, 2-2-1 Miyama, Funabashi, 274-8510, Japan; KAORI KOBAYASHI, Department of Physics, University of Tohoku, 3190 Gofuku, Tohoku, 920-8555, Japan.

**TH02**

**15 min 1:47**

FOURIER TRANSFORM MICROWAVE SPECTRUM OF N2-(CH2)nO

YOSHIYUKI KAWASHIMA, Department of Applied Chemistry, Faculty of Engineering, Kanagawa Institute of Technology, Atsugi, Kanagawa 243-0292, JAPAN; EIZI HIROTA, The Graduate University for Advanced Studies, Hayama, Kanagawa 248-0193, JAPAN.

**TH03**

**15 min 2:04**

THE BROADBAND ROTATIONAL SPECTRUM AND GEOMETRY OF N2–ICF3

N R WALKER, D. HIRD, School of Chemistry, Bedson Building, Newcastle University, Newcastle-upon-Tyne, NE1 7RU, U.K.; A. C. LEGON, School of Chemistry, University of Bristol, Bristol, BS8 1TS, U.K.

**TH04**

**15 min 2:21**

UNEXPECTED GENERATION AND OBSERVATION OF A T-SHAPED COMPLEX OF H2C2•AgCCH

N. R. WALKER, School of Chemistry, Bedson Building, Newcastle University, Newcastle-upon-Tyne, NE1 7RU, U.K.; S. L. STEPHENS, W. MIZUKAMI, D. P. TEW AND A. C. LEGON, School of Chemistry, University of Bristol, Bristol, BS8 1TS, U.K.
TH05 15 min 2:38
STRUCTURES OF THE CAGE, PRISM, AND BOOK HEXAMER WATER CLUSTERS FROM MULTIPLE ISOTOPE SUBSTITUTION

SIMON LOBSIGER, CRISTOBAL PEREZ, DANIEL P. ZALESKI, NATHAN SEIFERT, BROOKS H. PATE, Department of Chemistry, University of Virginia, McCormick Rd., Charlottesville, VA 22904-4319; ZBIGNIEW KISIEL, Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warszawa, Poland; BERHANE TEMELSO, GEORGE C. SHIELDS, Dean’s Office, College of Arts and Sciences, and Department of Chemistry, Bucknell University, Lewisburg, PA 17837.

TH06 15 min 2:55
CHARACTERIZATION OF LARGE WATER CLUSTERS BY BROADBAND ROTATIONAL SPECTROSCOPY

CRISTOBAL PEREZ, DANIEL P. ZALESKI, NATHAN A. SEIFERT, BROOKS H. PATE, Department of Chemistry, University of Virginia, McCormick Rd., Charlottesville, VA 22904-4319; ZBIGNIEW KISIEL, Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warszawa, Poland; BERHANE TEMELSO, GEORGE C. SHIELDS, Dean’s Office, College of Arts and Sciences, and Department of Chemistry, Bucknell University, Lewisburg, PA 17837; STEVEN T. SHIPMAN, IAN FINNEMAN, Division of Natural Sciences, New College of Florida, Samsota, FL 34243.

TH07 15 min 3:12
HYDROGEN BOND NETWORK ISOMERS OF THE WATER NONAMER AND DECAFER OBSERVED BY BROADBAND ROTATIONAL SPECTROSCOPY

CRISTOBAL PEREZ, DANIEL P. ZALESKI, NATHAN A. SEIFERT, BROOKS H. PATE, Department of Chemistry, University of Virginia, McCormick Rd., Charlottesville, VA 22904-4319; ZBIGNIEW KISIEL, Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warszawa, Poland; BERHANE TEMELSO, GEORGE C. SHIELDS, Dean’s Office, College of Arts and Sciences, and Department of Chemistry, Bucknell University, Lewisburg, PA 17837.

TH08 15 min 3:29
STRUCTURES OF THE LOWEST ENERGY NONAMER AND DECAFER WATER CLUSTERS FROM CHIRP-PULSE ROTATIONAL SPECTROSCOPY

CRISTOBAL PEREZ, BROOKS H. PATE, Department of Chemistry, University of Virginia, McCormick Rd., Charlottesville, VA 22904-4319; ZBIGNIEW KISIEL, Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warszawa, Poland; BERHANE TEMELSO, GEORGE C. SHIELDS, Dean’s Office, College of Arts and Sciences, and Department of Chemistry, Bucknell University, Lewisburg, PA 17837.

Intermission

TH09 15 min 4:00
MILLIMETER WAVE SPECTRA OF THE INTERNAL ROTATION EXCITED STATES OF (α)H₂-H₂O AND (α)H₂-D₂O

K. HABADA, Y. IWASAKI, T. GIESEN, and K. TANAKA, Department of Chemistry, Faculty of Science, Kyushu University, Hakozaki, Higashiku, Fukuoka, 812-8581 JAPAN.

TH10 15 min 4:17
THE PERFORMANCE OF THE THIRD GENERATION OF CP-FTMW SPECTROMETERS ILLUSTRATED BY THE ANALYSIS OF THE WATER HEPTAMER STRUCTURE

CRISTOBAL PEREZ, DANIEL P. ZALESKI, NATHAN A. SEIFERT, SIMON LOBSIGER, BROOKS H. PATE, Department of Chemistry, University of Virginia, McCormick Rd., Charlottesville, VA 22904-4319; ZBIGNIEW KISIEL, Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warszawa, Poland; BERHANE TEMELSO, GEORGE C. SHIELDS, Dean’s Office, College of Arts and Sciences, and Department of Chemistry, Bucknell University, Lewisburg, PA 17837; STEVEN T. SHIPMAN, Division of Natural Sciences, New College of Florida, Samsota, FL 34243; DAVID W. PRATT, Department of Chemistry, The University of Vermont, Cook Physical Sciences Building, 82 University Place, Burlington, VT 05405.

TH11 10 min 4:34
THE CYTOSINE WATER COMPLEX

TH12  10 min  4:46
EXPERIMENTAL EVIDENCE OF LONE PAIRS - \( \pi \) SYSTEM INTERACTION: THE ROTATIONAL SPECTRUM OF CHLOROTRIFLUOROETHYLENE - WATER COMPLEX

L. EVANGELISTI, Q. GOU, G. FENG and W. CAMINATI, Dipartimento di Chimica "G. Ciamician" dell'Università, Via Selmi 2, I-40126 Bologna, Italy.

TH13  15 min  4:58
MICROWAVE SPECTRA AND STRUCTURE OF H\(_2\)-CuF: OVERVIEW OF THE COMPLEXES OF HYDROGEN WITH METAL-CONTAINING DIATOMICS

G. S. GRUBBS II, DANIEL J. FROHMAN, Department of Chemistry, Wesleyan University, 52 Lawn Avenue, Middletown, CT, 06459 – 0180, USA; ZHENHONG YU, Aerodyne Research, Inc. 45 Manning Road, Billerica, MA 01821; STEWART E. NOVICK, Department of Chemistry, Wesleyan University, 52 Lawn Avenue, Middletown, CT, 06459-0180, USA (email to SEN: smovick@wesleyan.edu).

TH14  15 min  5:15
EFFECTS OF A REMOTE BINDING PARTNER ON THE ELECTRIC FIELD AND ELECTRIC FIELD GRADIENT AT AN ATOM IN A WEAKLY BOUND TRIMER: MICROWAVE SPECTROSCOPY AND QUANTUM MECHANICAL COMPUTATIONS ON Kr-SO\(_3\) AND Kr-SO\(_2\)-CO

REBECCA B. MACKENZIE, BROOKE A. TIMP, KENNETH R. LEOPOLD, Department of Chemistry, University of Minnesota, 207 Pleasant St., SE, Minneapolis, MN 55455; YIRONG MO, Department of Chemistry, Western Michigan University, Kalamazoo, MI 49008.

TH15  15 min  5:32
MICROWAVE SPECTRUM AND STRUCTURE OF THE 2,6-DIFLUOROPYRIDINE-CO\(_2\) COMPLEX

CHRISTOPHER T. DEWBERY, Department of Chemistry, University of Minnesota, 207 Pleasant St., SE, Minneapolis, MN 55455; JESSICA L. MUELLER, MARK D. MARSHALL, HELENE O. LEUNG, Department of Chemistry, Amherst College, P.O. Box 5000, Amherst, MA 01002-5000; KENNETH R. LEOPOLD, Department of Chemistry, University of Minnesota, 207 Pleasant St., SE, Minneapolis, MN 55455.

TH16  15 min  5:49
OBSERVATION OF A MODERATE STRENGTH INTERACTION OF HYDROGEN WITH A COINAGE METAL HALIDE: THE ROTATIONAL SPECTRUM AND STRUCTURE OF THE p-H\(_2\)-CuCl AND o-H\(_2\)-CuCl COMPLEXES

HERBERT M. PICKETT, DANIEL A. OBENCHAIN, G. S. GRUBBS II, and STEWART E. NOVICK, Department of Chemistry, Wesleyan University, 52 Lawn Avenue, Middletown, CT, 06459-0180, USA.

TI. ASTRONOMICAL SPECIES AND PROCESSES
TUESDAY, JUNE 18, 2013 – 1:30 PM
Room: 1015 MCPHERSON LAB

Chair: ERIC HERBST, University of Virginia, Charlottesville, VA

TI01  15 min  1:30  TI02  15 min  1:47
LARGE PICTURE OF THE GALACTIC CENTER STUDIED BY H\(_{\alpha}\); HIGH IONIZATION RATE, PREVAILING WARM AND DIFFUSE GAS, AND NON-ROTATING EXPANDING MOLECULAR RING

TAKESHI OKA, Department of Astronomy and Astrophysics, Department of Chemistry, the Enrico Fermi Institute, University of Chicago, Chicago, IL 60637; THOMAS R. GEBALLE, Gemini Observatory, Hilo, HI 96720; NICK INDRIOLO, Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD 21218.

EXPLORING SHOCK CHEMISTRY IN ORION-KL WITH MID-J MOLECULAR TRANSITIONS

JULIE K. ANDERSON and LUCY M. ZIURYS, Department of Chemistry and Biochemistry, The University of Arizona, Tucson, AZ 85719.
FORMATION OF CH⁺: SHOCK CHEMISTRY IN NGC 7027

JULIE K. ANDERSON, Department of Chemistry and Biochemistry, The University of Arizona, Tucson, AZ 85719; LUCY M. ZIURYS, Department of Chemistry and Biochemistry, The University of Arizona, Tucson, AZ 85719; FABRICE HERPIN, LAB-OASU, France.

WARMT, DENSE GAS NEAR THE MASSIVE PROTO-STAR AFGL 2136 IRS 1 AS REVEALED BY ABSORPTION FROM THE \( v_1, v_2, \) AND \( v_3 \) BANDS OF WATER

NICK INDRIGLO, DAVID A. NEUFELD, Department of Physics & Astronomy, Johns Hopkins University, Baltimore, MD 21218; ANDREAS SEIFAHRT, Department of Astronomy and Astrophysics, University of Chicago, Chicago, IL 60637; MATT J. RICHTER, Department of Physics, University of California Davis, Davis, CA 95616.

NEW RESULTS FROM A SPECTRAL-LINE SURVEY OF Sgr B2(N): INSIGHT INTO GAS-PHASE PROCESSES

D. T. HAHNEN and L. M. ZIURYS, Department of Chemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, AZ 85721.

CSO BROADBAND MOLECULAR LINE SURVEYS I: BENCHMARKING GOBASIC ANALYSIS SOFTWARE

MARY L. RADHUBER, JAMES L. SANDERS III, JACOB C. LAAS, BRIAN M. HAYS, SUSANNA L. WIDICUS WEAVER, Department of Chemistry, Emory University, Atlanta, GA 30322; DAREK C. LIS, Division of Physics, Mathematics, and Astronomy, California Institute of Technology, Pasadena, CA 91125.

CSO BROADBAND MOLECULAR LINE SURVEYS II: INITIAL CORRELATION ANALYSIS RESULTS FOR COMPLEX ORGANIC MOLECULES

JAMES L. SANDERS III, MARY L. RADHUBER, JACOB C. LAAS, BRIAN M. HAYS, DAREK C. LIS and SUSANNA L. WIDICUS WEAVER, Emory University, Department of Chemistry, Atlanta, Georgia 30322.

DETECTION AND FORMATION OF INTERSTELLAR c-C₃D₂

SILVIA SPEZZANO, SANDRA BRÜNNKEN, PETER SCHILKE, I. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany; KARL M. MENTEN, Max-Planck-Institut für Radioastronomie, Auf dem Hügel 69, 53121 Bonn, Germany; PAOLA CASELLI, School of Physics and Astronomy, University of Leeds, Leeds LS2 9JT, UK; MICHAEL C. MCCARTHY, Harvard-Smithsonian Center for Astrophysics, 60 Garden St., Cambridge, MA 02138, and School of Engineering & Applied Sciences, Harvard University, 29 Oxford St., Cambridge, MA 02138; LUCA BIZZOCCHI, Centro de Astronomía e Astrofísica, Observatório Astronómico de Lisboa, Terceira do Ajudá, 1349-018 Lisboa, Portugal; SANDRA TREVINIO, IRAM, 18012, Granada, Spain; YURI AIKAWA, Department of Earth and Planetary Sciences, Kobe University, Kobe 657-8501, Japan; and STEPHAN SCHLEMMER, I. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany.

Intermission

TERAEHRZ TIME DOMAIN SPECTROSCOPY OF COMPLEX ORGANIC MOLECULES IN ASTROPHYSICALLY RELEVANT ICES

BRET A. MCGUIRE, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125; SERGIO IOPPOLO, Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, CA 91125; MARCO A. ALLODI, MATTHEW J. KELLEY, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125; GEOFFREY A. BLAKE, Division of Chemistry and Chemical Engineering and Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, CA 91125.

THE ANALYSIS OF ACETONITRILE (CH₃CN) USING 3-D SUBMILLIMETER SPECTROSCOPY

JAMES P. MCMILLAN, SARAH M. FORTMAN, CHRISTOPHER F. NEESE, FRANK C. DE LUCIA, Department of Physics, The Ohio State University, Columbus, OH 43210.
THE COMPLETE, TEMPERATURE RESOLVED EXPERIMENTAL SPECTRUM OF METHANOL BETWEEN 560 AND 654 GHZ
SARAH M. FORTMAN, CHRISTOPHER F. NEESE, and FRANK C. DE LUCIA, Department of Physics, The Ohio State University, 191 W. Woodruff Ave., Columbus, OH 43210.

SPECTROSCOPY OF ISOCYANIDES AND THEIR SEARCH IN INTERSTELLAR MEDIUM
L. MARGULÈS, R. A. MOTIYENKO, Laboratoire PhLAM, CNRS UMR 8523, Université de Lille 1, 59655 Villeneuve d’Ascq Cedex, France; B. TERCERO, J. CERNICHARO, Centro de Astrobiología (CSIC-INIA). Laboratory of Molecular Astrophysics, Department of Astrophysics, Ctra de Ajalvir Km 4, 28850 Torrelodones, Madrid, Spain; and J.-C. GUILLEMIN, Sciences Chimiques de Rennes, UMR 6226 CNRS-ENSCR, Avenue du Général Leclerc, CS 50837, 35708 Rennes Cedex 7, France.

SUBMILLIMETER WAVE SPECTROSCOPY OF HIGHLY ASTROPHYSICAL INTEREST MOLECULE: HYDROXYACETONITRILE
L. MARGULÈS, R. A. MOTIYENKO, Laboratoire PhLAM, CNRS UMR 8523, Université de Lille 1, 59655 Villeneuve d’Ascq Cedex, France; and J.-C. GUILLEMIN, Sciences Chimiques de Rennes, UMR 6226 CNRS-ENSCR, Avenue du Général Leclerc, CS 50837, 35708 Rennes Cedex 7, France.

LABORATORY MEASUREMENTS AND ASTRONOMICAL OBSERVATIONS OF H$_2$NCO$^+$
HARSHAL GUPTA, Morristown Astrodome Laboratory, California Institute of Technology, Pasadena, CA 91125; CARL A. GOTTLIEB AND MICHAEL C. MCCARTHY, Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138.

MILLIMETER AND SUBMILLIMETER WAVE SPECTRA OF THE HCOO$^{18}$CH$_2$ ISOTOPOLOG OF METHYLFORMATE IN THE GROUND STATE AND IN THE FIRST EXCITED TORSIONAL STATE.
I. HAYKAL, L. MARGULÈS, T. R. HUET, R. A. MOTIYENKO, Laboratoire PhLAM, UMR8523 CNRS-Université Lille 1, F-59655 Villeneuve d’Ascq Cedex, France; M. CARVALHAL, Unidade Associada IEM-CSIC-Dpto. de Física Aplicada, Universidad de Huelva, Spain; I. KLEINER, LISA, CNRS et Université Paris Est et Paris Diderot, 61 av. Général de Gaulle, 94010, Créteil, France; J. C. GUILLEMIN, ENS de Chimie de Rennes - CNRS - 35700 Rennes, France; B. TERCERO, J. CERNICHARO, Centro de Astrobiología (CSIC-INIA), Ctra de Ajalvir, Km 4, 28850 Torrelodones, Madrid, Spain.

TJ. INFRARED/RAMAN
TUESDAY, JUNE 18, 2013 – 1:30 PM
Room: 2015 MCPHERSON LAB

Chair: BRIAN BRUMFIELD, Princeton University, Princeton, NJ
TJ03  15 min  2:04
ACCURATE DETERMINATION OF ROTATIONAL ENERGY LEVELS IN THE GROUND STATE OF $^{13}$CH$_4$

M. ABE, K. IWAKUNI, S. OKUBO and H. SASADA, Department of Physics, Faculty of Science and Technology, Keio University, Yokohama, Japan.

TJ04  10 min  2:21
IR/THZ DOUBLE RESONANCE SPECTROSCOPY IN THE PRESSURE BROADENED REGIME: A PATH TOWARDS ATMOSPHERIC GAS SENSING

S. SREE HARSHA, Aegis Technologies, 410 Jan Davis Drive, Huntsville, Alabama 35806; DANE J. PHILLIPS, IERUS Technologies, 2904 Westcort Blvd, Ste 210, Huntsville, AL 35805; FRANK C. DE LUCIA, Department of Physics, 191 Woodruff Ave., Ohio State University, Columbus, OH 43210; HENRY O. EVERITT, Army Aviation and Missile RDE Center, Redstone Arsenal, AL 35989.

TJ05  15 min  2:33
DETECTION OF NO AND S-NITROSOCOMPOUNDS USING MID-IR CAVITY RING-DOWN SPECTROSCOPY

VITALI STSIAPURA, VINCENT K. SHUALL, ANGELA ZIEGLER, KEVIN K. LEHMANN, Chemistry Department, University of Virginia, Charlottesville, VA 22904; and BENJAMIN M. GASTON, Case Western Reserve University, Cleveland, Ohio 44106.

TJ06  15 min  2:50
DIFFERENTIAL OPTICAL DISPERSION SPECTROSCOPY FOR COMPARATIVE MOLECULAR QUANTIFICATION

MICHAL NIKODEM, BRIAN BRUMFIELD, GERARD WYSOCKI, Department of Electrical Engineering, Princeton University, Princeton, NJ, 08544, USA.

Intermission

TJ07  5 min  3:30
STUDY OF UTILIZATION OF AUTOMOTIVE DIESEL GLOW PLUG AS AN IR SOURCE

ALLEN R. WHITE, Department of Mechanical Engineering, Rose-Hulman Institute of Technology, 5500 Wabash Ave., Terre Haute, IN 47803.

TJ08  10 min  3:37
FTIR STUDY OF COMBUSTION SPECIES IN SEVERAL REGIONS OF A CANDLE FLAME

ALLEN R. WHITE, Department of Mechanical Engineering, Rose-Hulman Institute of Technology, 5500 Wabash Ave., Terre Haute, IN 47803.

TJ09  15 min  3:49
SPONTANEOUS RAMAN SCATTERING MEASUREMENTS OF NITROGEN VIBRATIONAL DISTRIBUTION FUNCTION IN NANOSECOND PULSED DISCHARGE

A. ROETTGEN, I.V. ADAMOVICH, W.R. LEMPERT, Michael A. Chaszycka Nonequilibrium Thermodynamics Laboratory, Dept. of Mechanical and Aerospace Engineering, The Ohio State University, Columbus, OH 43210.

TJ10  15 min  4:06
STIMULATED INFRARED EMISSION OF C$_2$H$_2$ NEAR 3000 cm$^{-1}$ WITH CONTINUOUS-WAVE LASERS

MIKAEL SILTANEN, MARKUS METSÄLÄ, MARKKI VAINIO, and LAURI HALONEN, Department of Chemistry, University of Helsinki, P.O. Box 55, FIN-00014 Helsinki, Finland.

TJ11  15 min  4:23
CONTINUOUS WAVE STIMULATED RAMAN SPECTROSCOPY INSIDE A HOLLOW CORE PHOTONIC CRYSTAL FIBER

JOSÉ L. DOMÉNECH and MAITE CUETO, Instituto de Estructura de la Materia (IEM-CSIC), Serrano 123, E-28006 Madrid, Spain. (email to J.L.D.: jdomezech@csic.es).

TJ12  15 min  4:40
DEVELOPMENT OF AN EXTERNAL CAVITY QUANTUM CASCADE LASER SPECTROMETER FOR HIGH-RESOLUTION SPECTROSCOPY OF MOLECULAR IONS

JACOB T. STEWART, BRADLEY M. GIBSON, Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801; BENJAMIN J. McCall, Departments of Chemistry and Astronomy, University of Illinois at Urbana-Champaign, Urbana, IL 61801.
TK13  15 min  4:57

FELION: A CRYOGENIC TRAP APPARATUS FOR SPECTROSCOPIC STUDIES WITH FELIX

S. BRÜNKEN, L. KLUGE, S. FANGHÄNEL, A. POTAPOV, O. ASVANY, and S. SCHLEMMER, Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany. J. OOMENS, B. REDLICH, Radboud University Nijmegen, Institute for Molecules and Materials, FELIX Facility, 6525 ED Nijmegen, Netherlands; A. STOFFELS, Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany, and Radboud University Nijmegen, Institute for Molecules and Materials, FELIX Facility, 6525 ED Nijmegen, Netherlands.

TK14  15 min  5:14

DEVELOPMENT OF A SHEATH-FLOW SUPERCRITICAL FLUID EXPANSION SOURCE FOR VAPORIZATION OF NONVOLATILES AT MODERATE TEMPERATURES

BRADLEY M. GIBSON and JACOB T. STEWART, Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801; BENJAMIN J. MccALL, Department of Chemistry and Astronomy, University of Illinois at Urbana-Champaign, Urbana, IL 61801.

TK15  15 min  5:31

A NEW FAR-IR (THz) AND IR SPECTROMETER FOR THE STUDY OF ASTROCHEMICAL ICES

MARCO A. ALLODI, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125; SERGIO IOPPOLO, Division of Geology and Planetary Science, California Institute of Technology, Pasadena, CA 91125; BRET A. MCGUIRE, MATTHEW J. KELLEY, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125; and GEORGE A. BLAKE, Division of Geology and Planetary Science, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125.

TK16  15 min  5:48

DEVELOPMENT AND APPLICATION OF A HIGHER RESOLUTION TERAHERTZ TIME-DOMAIN SPECTROMETER

DANIEL B. HOLLAND, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125 (email to D.B.H.: holland@caltech.edu); GEOFFREY A. BLAKE, Division of Geological and Planetary Sciences, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125.

TK. ELECTRONIC

TUESDAY, JUNE 18, 2013 – 1:30 PM
Room: 1153 SMITH LAB

Chair: SCOTT REID, Marquette University, Milwaukee, WI

TK01  15 min  1:30

THE CHARACTER OF THE LONG-LIVED STATE FORMED FROM S1 OF PHENYLACETYLENE

PHILIP M. JOHNSON and TREVOR J. SEARS, Department of Chemistry, Stony Brook University, Stony Brook, New York 11794.

*also: Department of Chemistry, Brookhaven National Laboratory, Upton, New York 11973

TK02  15 min  1:47

TWO-PROTON PHOTOTAUTOMERIZATION DYNAMICS OF 7-AZAINDOLE COMPLEXES

T. CHAKRABORTY, M. MUKHERJEE and S. KARMAKAR, Department of Physical Chemistry, Indian Association for the cultivation of science, Calcutta 700032, India. E-mail: pete@iacs.res.in.

TK03  15 min  2:04

STRUCTURE DETERMINATION AND EXCITED STATE PROTON TRANSFER REACTION OF 1-NAPHTHOL-AMMONIA CLUSTERS IN THE S1 STATE STUDIED BY UV-IR-UV MID-IR SPECTROSCOPY

SHUNPEI YOSHIKAWA, MITSUHIKO MIYAZAKI, WEILER MARTIN, Chemical Resources Laboratory, Tokyo Institute of Technology, 4259 Nagatsuta-cho, Midori-ku, Yokohama 226-8503 Japan; HARUKI ISHIKAWA, Department of Chemistry, School of Science, Kita-Sen University, Minami-ku, Sapporo 060-8510, Japan; MASAAKI FUJI, Chemical Resources Laboratory, Tokyo Institute of Technology, 4259 Nagatsuta-cho, Midori-ku, Yokohama 226-8503 Japan.
TK04 15 min 2:21
LASER DESORPTION SUPERSONIC JET SPECTROSCOPY OF HYDRATED TYROSINE
HIKARI OBA, YOKO SHIMOZONO, SHUN-Ichi ISHUCHI, MASAKI FUKUI, Chemical Resources Lab., Tokyo Tech., 255 Nagatsuta-cho, Midori, Yokohama, 226-8503, Japan; PIERRE CARCABAL, ISMO, Université Paris Sud XI Bâtiment 210, 91405, Orsay, Paris, France.

TK05 15 min 2:38
EXCITED-STATE DYNAMICS IN FOLIC ACID AND 6-CARBOXYPYRERIN UPON UVA EXCITATION
HUIHUA HUANG, R. AARON VOIGT and CARLOS E. CRESCO-HERNÁNDEZ, Department of Chemistry and Center for Chemical Dynamics, Case Western Reserve University, Cleveland, Ohio 44106.

TK06 15 min 2:55
RESONANCE ENHANCED MULTI-PHOTON IONIZATION (REMPI) AND DOUBLE RESONANCE (UV-UV AND IR-UV) SPECTROSCOPIC INVESTIGATION ISO-CYTOSINE
HEUNG JIN LEE, AHREUM MIN, AHREUM AHN, CHEOL JOO MOON, MYONG YONG CHO, Department of Chemistry and Research Institute of Natural Science, Gyeongsang National University, Jinju 660-701, Korea; SHUN-Ichi ISHUCHI, MITSUHIKO MIYAZAKI, MASAKI FUKUI, Tokyo Institute of Technology, Chemical Resources Laboratory, Japan.

TK07 15 min 3:12
RESONANCE ENHANCED MULTI-PHOTON IONIZATION AND UV-UV HOLE-BURNING SPECTROSCOPIC STUDIES OF JET-COOLED ACETANILIDE DERIVATIVES
CHEOL JOO MOON and AHREUM MIN, AHREUM AHN, SEUNG JUN LEE, MYONG YONG CHO, Department of Chemistry, Gyeongsang National University, Jinju 660-701, South Korea; SEONG KEUN KIM, Department of Chemistry and Biophysics & Biophysical Chemistry (WCW) Seoul National University, Seoul 151-747, South Korea.

TK08 15 min 3:29
TAILOR MADE SYNTHESIS OF T-SHAPED AND π-STACKED DIMERS IN THE GAS PHASE: CONCEPT FOR EFFICIENT DRUG DESIGN AND MATERIAL SYNTHESIS
SUMIT KUMAR and ALOKE DAS, Indian Institute of Science Education and Research (IISER), 900 NCL Innovation Park, Dr. Homi Bhabha Road, Pune-411008, Maharashtra, India.

TK09 15 min 4:00
ROTATIONALLY RESOLVED HIGH-RESOLUTION LASER SPECTROSCOPY OF THE S0 -- S1 TRANSITION OF NAPHTHALENE AND CN-NAPHTHALENE
SHUNJI KASAHARA, RYO YAMAMOTO, KOHEI TADA, Molecular PhotoScience Research Center, Kobe University, Kobe 657-8501, Japan.

TK10 15 min 4:17
VIBRIONIC SPECTROSCOPY OF 4-ISOCYANOBENZONITRILE
JOSEPH A. KORN, DEEPAI N. MEHTA-HURT and TIMOTHY S. ZWIER, Department of Chemistry, Purdue University, West Lafayette, IN 47907.

TK11 15 min 4:34
STEPWISE SOLVATION EFFECTS ON THE EXCITED STATES OF A WEAKLY COUPLED BICHROMOPHORE 1,2-DIPHENOXYETHANE-(H2O)N (N=2-4) CLUSTERS
PATRICK S. WALSH, EVAN G. BUCHANAN, JOSEPH R. GORD and TIMOTHY S. ZWIER, Department of Chemistry, Purdue University, 560 Oval Drive, West Lafayette, IN 47907.

TK12 15 min 4:51
PLANT SUNSCREENS IN NATURE: UV AND IR SPECTROSCOPY OF SINAPATE DERIVATIVES
JACOB C. DEAN, PATRICK S. WALSH, and TIMOTHY S. ZWIER, Department of Chemistry, Purdue University, West Lafayette, IN 47907; FLORENT ALLAIS, AgroParistech, Paris, France.

TK13 15 min 5:08
FLUORESCENCE EXCITATION SPECTRA OF PHOTO-UNSTABLE NITROBENZENE USING A PICOSECOND LASER: POTENTIAL EVIDENCE FOR NO PRODUCED BY TWO DISTINCT CHANNELS
CHRISTOPHER J. LEE, CHAKREE TANJAROON, J. BRUCE JOHNSON, SCOTT W. REEVE, Arkansas Center for Laser Applications and Science and Department of Chemistry and Physics, P.O. Box 419 State University, AR 72756; SUSAN D. ALLEN, Embry Riddle Aeronautical University, 600 S. Clyde Morris Boulevard, Daytona Beach, FL 32114.

TK14 15 min 5:25
SPECTROSCOPIC CHARACTERIZATION OF A NATURAL PRODUCT: ANETHOLE
VICTORIA P. BARBER and JOSHD NEWBY, Department of Chemistry and Biochemistry, Swarthmore College, Swarthmore, PA 19081.

Intermission
WA. PLENARY
WEDNESDAY, JUNE 19, 2013 – 8:30 AM
Room: AUDITORIUM, INDEPENDENCE HALL
Chair: ANNE MCCOY, The Ohio State University, Columbus, OH

WA01 40 min 8:30
CHARGE TRANSFER REACTIONS INDUCE BORN-OPPENHEIMER BREAKDOWN IN SURFACE CHEMISTRY: APPLICATIONS OF DOUBLE RESONANCE SPECTROSCOPY IN MOLECULE-SURFACE SCATTERING

ALEC M. WODTKE, Georg-August University of Göttingen and the Max-Planck-Institute for Biophysical Chemistry, Göttingen, Germany.

WA02 40 min 9:15
ULTRA SENSITIVE CAVITY RING DOWN SPECTROSCOPY OF MAJOR ATMOSPHERIC SPECIES BETWEEN 1.20 AND 1.71 µm

A. CAMPARGUE, S. KASSI, and D. MONDELAIN, Université Grenoble 1/CNRS, UMR5588 LIPhy, Grenoble, F-38041, France.

Intermission

WA03 40 min 10:20
INFRARED STUDIES OF METAL CATION-DIHYDROGEN COMPLEXES

EVAN BIESKE, School of Chemistry, University of Melbourne, 3010, Australia.

WA04 40 min 11:05
SPECTROSCOPIC ENGINEERING IN THE SUBMILLIMETER

FRANK C. DE LUCIA, DEPARTMENT OF PHYSICS, OHIO STATE UNIVERSITY, COLUMBUS, OH 43210.

WF. ASTRONOMICAL SPECIES AND PROCESSES
WEDNESDAY, JUNE 19, 2013 – 1:30 PM
Room: 160 MATH ANNEX
Chair: SANDRA BRUENKEN, University of Cologne, Koeln, Germany

WF01 15 min 1:30
RADIATIVE LIFETIME FOR NUCLEAR SPIN CONVERSION OF WATER-ION, H20+

KEICHI TANAKA, Department of Applied Chemistry, National Chiao Tung University, Hsinchu, 30010, TAIWAN and Department of Chemistry, Faculty of Sciences, Kyushu University, Fukuoka, 812-8581 JAPAN; KENSHUKE HARADA, Department of Chemistry, Faculty of Sciences, Kyushu University, Fukuoka, 812-8581 JAPAN; TAKESHI OKA, Department of Astronomy and Astrophysics and Department of Chemistry, the Enrico Fermi Institute, the University of Chicago, Chicago, Illinois, 60637, USA.

WF02 15 min 1:47
A MM/SMBM WAVE SPECTROMETER TO QUANTIFY ASTROCHEMICAL REACTION RATES

JACOB C. LAAS and SUSANNA L. WIDICUS WEAVER, Department of Chemistry, Emory University, Atlanta, GA 30322.

WF03 15 min 2:04
UNIFIED MICROSCOPIC-MACROSCOPIC MONTE CARLO SIMULATION OF ICE FORMATION ON INTERSTELLAR GRAINS

QIANG CHANG, Department of Chemistry, University of Virginia, Charlottesville, Virginia, USA; ERIC HERBST, Department of Chemistry, Physics and Astronomy, University of Virginia, Charlottesville, Virginia, USA.
WF04 15 min 2:21

THE LOW-TEMPERATURE NUCLEAR SPIN EQUILIBRIUM OF H$_2^+$ IN COLLISIONS WITH H$_2$

FLORIAN GRUSSEI, MAX H. BERG, ANDREAS WOLF, and HOLGER KRECKEL. Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany. KYLIE N. CRABTREE* and BENJAMIN J. MCCALL, Department of Chemistry, University of Illinois, Urbana, IL, 61801; SABRINA GÄRTNER and STEPHAN SCHLEMMER, I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany.

*Present address: Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, 02138

WF05 15 min 2:38

MOLECULAR HYDROGEN FORMATION: EFFECT OF DUST GRAIN TEMPERATURE FLUCTUATIONS

EMERIC-BRON, JACQUES LE BOURLOT and FRANCK LE PETIT. LUTH - Observatoire de Paris, CNRS UMR 8102, Université Paris Diderot. e-mail: emeric.bron@obspm.fr

WF06 15 min 2:55

REVISED TERM VALUES FOR THE A - X ($v'$ = 0-9, $v''$ = 0) BANDS IN $^{13}$C$^{18}$O FROM HIGH-RESOLUTION SPECTRA ACQUIRED AT THE SOLEIL SYNCHROTRON

L. GAVILAN, J. L. LEMAIRE, M. EIDELBERG, Observatoire de Paris, Paris, France; S. R. FEDERMAN, Department of Physics and Astronomy, University of Toledo, Toledo, OH 43606; G. STARK, A. N. HEAYS, Department of Physics, Wellesley College, Wellesley, MA 02481; J. H. FILLION, Université PVI UMPAC, Paris, France; J. R. LYONS, IGPP, University of California, Los Angeles, CA 90095; N. DE OLIVEIRA, Synchrotron SOLEIL, Saint Aubin, France.

WF07 15 min 3:30

PHOTOIONIZATION AND RECOMBINATION OF Ne IV AND EXCITATION OF NeV IN NEBULAR PLASMAS

SULTANA N. NAHAR, ETHAN PALAY, ANIL K. PRADHAN, Department of Astronomy, The Ohio State University, Columbus, OH 43210.

WF08 15 min 3:47

THE 4050 Å GROUP OF THE $\lambda^1\Pi_u - \chi^1\Sigma_g^+$ TRANSITION SYSTEM OF C$_3$

D. ZHAO, H. LINNARTZ, Sackler Laboratory for Astrophysics, Leiden Observatory, University of Leiden, P.O. Box 9513, NL-2300 RA Leiden, the Netherlands; M. A. HADDAD, W. UBAHKS, LaserLaB, VU University Amsterdam, De Boelelaan 1081, NL-1018 HV, Amsterdam, The Netherlands; M. R. SCHMIDT, Department of Astrophysics, N. Copernicus Astronomical Center, ul. Raciborska 8, 00-447 Puskal, Poland; J. KRELOWSKI, Centre for Astronomy, Nicolaus Copernicus University, Gagarina 11, 87-100 Toruń, Poland; G. A. GALAZUTDINOV, Instituto de Astronomia, Universidad Catolica del Norte, Av. Angamos 0610, Antofagasta, Chile.

WF09 15 min 4:04

A NEW METHODOLOGY FOR THE DETECTION OF LOW-ABUNDANCE SPECIES IN THE ISM: DETECTION OF INTERSTELLAR CARBODIIMIDE (HNCNH)

BRETT A. MCCUIRE, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125; RYAN A. LOOMIS, Department of Chemistry, University of Virginia, Charlottesville, VA 22903; CAMERON M. CHARNES, JOANNA F. CORBY, Department of Astronomy, University of Virginia, Charlottesville, VA 22901; GEOFFREY A. BLAKE, Division of Chemistry and Chemical Engineering and Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, CA 91125; JAN M. HOLLIS, NASA Goddard Space Flight Center, Greenbelt, MD 20771; FRANK J. LOVAS, National Institute of Standards and Technology, Gaithersburg, MD 20899; PHILIP R. JEWELL, and ANTHONY J. REMILIAN, National Radio Astronomy Observatory, Charlottesville, VA 22903.

Intermission

WF10 15 min 4:21

INDIRECT ROTATIONAL SPECTROSCOPY OF HCO$^+$

ADAM J. PERRY, JAMES N. HODGES, BRIAN M. SILLER, Department of Chemistry, University of Illinois, Urbana, IL 61801; BENJAMIN J. MCCALL, Departments of Chemistry, Astronomy, and Physics, University of Illinois, Urbana, IL 61801.
WF11  
15 min 4:38
SLIT-JET DISCHARGE STUDIES OF POLYACETYLENIC MOLECULES: SYNTHESIS AND HIGH RESOLUTION INFRARED SPECTROSCOPY OF DIACETYLENE

CHIH-HSUAN CHANG, MELANIE A. ROBERTS, and DAVID J. NESBITT, JILA, National Institute of Standards and Technology University of Colorado, and Department of Chemistry and Biochemistry University of Colorado at Boulder, Colorado 80309.

WF12  
15 min 4:55
SUB-DOPPLER SLIT JET DISCHARGE SPECTROSCOPY OF JET COOLED POLYACETYLENES: THE ANTI-SYMMETRIC CH STRETCH MODE OF TRIACETYLENE

CHIH-HSUAN CHANG, MELANIE A. ROBERTS, and DAVID J. NESBITT, JILA, National Institute of Standards and Technology University of Colorado, and Department of Chemistry and Biochemistry University of Colorado at Boulder, Colorado 80309.

WF13  
15 min 5:12
A LINE LIST FOR HYDROGEN SULFIDE

ALA'A A. A. AZZAM, SERGEI N. YURCHENKO, JONATHAN TENNYSON, Department of Physics and Astronomy, University College London, London, WC1E 6BT, UK.

WF14  
15 min 5:29
ANALYSIS OF THE SUB-MILLIMETER ROTATIONAL SPECTRUM OF UREA

JESSICA R. THOMAS, ALYSSA M. FOS-NIGHT, IVAN R. MEDVEDEV, Department of Physics, Wright State University, 3640 Colonel Glenn Highway, Dayton, OH 45435, USA.

WF15  
10 min 5:46
THE ROTATIONAL SPECTRUM OF COMPLEX ORGANIC MOLECULES: 2(N)-METHYLAminoETHANOL

S. MELANDRi, A. MARIS and C. CAL-ABRESE, Dipartimento di Chimica, Università di Bologna, via Selmi 2, 40126 Bologna, Italy.

WG. MINI-SYMPOSIUM: THEORY AND SPECTROSCOPY
WEDNESDAY, JUNE 19, 2013 – 1:30 PM
Room: 170 MATH ANNEX

Chair: G. BARNEY ELLISON, University of Colorado, Boulder, CO

WG01  
INVITED TALK  
30 min 1:30
COMBINING THEORY AND EXPERIMENT TO COMPUTE HIGHLY ACCURATE LINE LISTS FOR STABLE MOLECULES, AND PURELY AB INITIO THEORY TO COMPUTE ACCURATE ROTATIONAL AND ROVIBRATIONAL LINE LISTS FOR TRANSIENT MOLECULES

TIMOTHY J. LEE, XINCHUAN HUANG, RYAN C. FORTENBERRY, Space Science and Astrobiology Division, NASA Ames Research Center; DAVID W. SCHVENKE, NASA Ames Research Center.

WG02  
15 min 2:05
A NEW POTENTIAL ENERGY SURFACE FOR H$_2$–N$_2$O AND PMC SIMULATION PROBING SUPERFLUIDITY AND VIBRATIONAL FREQUENCY SHIFTS IN DOPED para-H$_2$ CLUSTERS

LECHENG WANG, ROBERT J LE ROY AND PIERRE-NICHOLAS ROY, Guelph-Waterloo Centre for Graduate Work in Chemistry and Biochemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada; DAIQIAN XIE, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing, Jiangsu, China.

WG03  
15 min 2:22
SUPERFLUIDITY HIDDEN IN A FORGOTTEN CORNER

TAO ZENG, GREGOIRE GUILLON, and PIERRE-NICHOLAS ROY, Department of Chemistry, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1.
WG04  15 min  2:39
COMPUTATIONAL FRAMEWORK FOR STUDYING H-
BONDING IN THE OH STRETCH REGION OF VIBRA-
TIONAL SPECTRA

LAURA C. Dzugan and ANNE B. McCoy,
Department of Chemistry and Biochemistry, The
Ohio State University, Columbus, OH 43210.

WG05  15 min  2:56
ESR SPECTRA OF ALKALI-METAL ATOMS ON HELI-
UM NANODROPLETS: A THEORETICAL MODEL
FOR THE PREDICTION OF HELIUM INDUCED HY-
PERFINE STRUCTURE SHIFTS

ANDREAS W. HAUSER, Institute of Experi-
mental Physics, Graz University of Technol-
ogy, Petersgasse 16, A-8010 Graz, Austria;
MICHAEL FILATOV, Muliken Center for Theo-
retical Chemistry, Institut für Physikalische und Theoretische Chemie, Univer-
sität Bonn, Beringstrasse 4, 53115 Bonn, Ger-
many; WOLFGANG E. ERNST, Institute of Ex-
perimental Physics, Graz University of Technol-
y.9y, Petersgasse 16, A-8010 Graz, Austria.

WG06  15 min  3:13
Xe and Rb Atoms on Helium Nanodroplets:
Is the Van der Waals Attraction Strong
Enough to Form a Molecule?

JOHANNES POMS, ANDREAS W. HAUSER
and WOLFGANG E. ERNST, Institute of Exper-
imental Physics, Graz University of Technology,
Petersgasse 16, A-8010 Graz, Austria.

Intermission

WG07  15 min  3:45
REN-NER-TELLER COUPLING IN OPEN SHELL DI-
HYDRIDES: A COMPARISON OF THEORY WITH
OPTICAL SPECTRA OF NEUTRAL AND IONIC
MOLECULES

G. Duxbury, Department of Physics, SUPA,
John Anderson Building, University of Strath-
clyde, 107 Rottenrow, Glasgow G4 0NG, Scot-
lund, UK; Ch. Jungen, LAC; 1Laboratoire Aime Cotton du CNRS, Université de Paris-Sud,
91405 Orsay, France; A. Aliajha, GSMA, UMR
CNRS 6089, Université de Reims Champagne-
Ardenne, B.P. 1039, 51687 Reims Cedex 2, France.

WG08  15 min  4:02
REN-NER-TELLER AND SPINORBIT COUPLING IN
H2S+ AND AsH2

G. Duxbury, Department of Physics, SUPA,
John Anderson Building, University of Strath-
clyde, 107 Rottenrow, Glasgow G4 0NG, Scot-
land, UK; Ch. Jungen, LAC; 1Laboratoire Aime Cotton du CNRS, Université de Paris-Sud,
91405 Orsay, France; A. Aliajha, GSMA, UMR
CNRS 6089, Université de Reims Champagne-
Ardenne, B.P. 1039, 51687 Reims Cedex 2, France.

WG09  15 min  4:19
COMPUTING ROVIBRATIONAL LEVELS OF POLY-
ATOMIC MOLECULES WITH CURVILINEAR IN-
TERNAL VIBRATIONAL COORDINATES AND AN
ECKART FRAME

XIAO-GANG WANG and TUCKER CARRING-
TON, JR., Chemistry Department, Queen's Uni-
versity, Kingston, Canada.

WG10  15 min  4:36
AN ACCURATE POTENTIAL ENERGY SURFACE FOR
METHANE

XIAO-GANG WANG and TUCKER CARRING-
TON, JR., Chemistry Department, Queen's Uni-
versity, Kingston, Canada.

WG11  15 min  4:53
THEORETICAL CALCULATIONS AND SIMULA-
TIONS OF INTERACTION OF X-RAYS WITH HIGH-Z
NANOMOITIES FOR USE IN CANCER RADIO-
THERAPY

Sara N. Lim, Biophysics Graduate Program;
Anil K. Pradhan, Biophysics Graduate Pro-
gram, Chemical Physics Program and Depart-
ment of Astronomy, The Ohio State University;
Sultana N. Nahar, Astronomy, The Ohio State
University.

WG12  15 min  5:10
SUPERIORITY OF LOW ENERGY 160 KV X-RAYS
COMARED TO HIGH ENERGY 6 MV X-RAYS IN
HEAVY ELEMENT RADIOSENSITIZATION FOR CANCER TREATMENT

Sara N. Lim, Biophysics Graduate Program;
Anil K. Pradhan, Biophysics Graduate Pro-
gram, Departments of Astronomy and Chem-
istry, Sultana N. Nahar, Department of As-
tronomy; Rolf F. Barth, Wellian Yang,
Robin J. Nakkula, Pathology, The Ohio State
University; Alycia Palmer and Claudia
Turro, Department of Chemistry, The Ohio
State University.
WK13 15 min 5:27
ALKYL CH STRETCH VIBRATIONS AS A PROBE OF
CONFORMATIONAL PREFERENCES

EDWIN L. SIBERT III, Department of
Chemistry and Theoretical Chemistry Insti-
tute, University of Wisconsin-Madison,
WI 53706. EVAN G. BUCHANAN AND TIM-
OTHY S. ZWIER, Department of Chemistry,
Purdue University, West Lafayette, IN 47907-
2084.

WK14 15 min 5:44
THEORETICAL STUDY OF THE VIBRATIONAL
SPECTROSCOPY OF THE ETHYL RADICAL

DANIEL P. TABOR and EDWIN. L. SIB-
ERT III, Department of Chemistry and Theoreti-
cal Chemistry Institute, University of Wiscon-
sin-Madison, Madison, WI 53706.

WK15 15 min 6:01
SIMULATION OF HIGH RESOLUTION VIBRATIONAL
AND ELECTRONIC SPECTRA WITH A MULTIFRE-
QUENCY VIRTUAL SPECTROMETER

MALGORZATA BICZYSKO, Center for Nano-
technology Innovation, Institute of Technol-
yng, Piazza San Silvestro 12, I-56127 Pisa, Italy; JULIEN BLOINO, Consiglio
Nazionale delle Ricerche, Istituto di Chimica dei
Composti Organometallici (ICCOM-CNR), UOS
di Pisa, Area della Ricerca CNR, Via G. Moruzzi
1, I-56124 Pisa, Italy; VINCENZO BARONE,
Scuola Normale Superiore, Piazza dei Cavaliere
7, I-56126 Pisa, Italy.

WH. MICROWAVE
WEDNESDAY, JUNE 19, 2013 – 1:30 PM
Room: 1000 MCPHERSON LAB

Chair: NICHOLAS WALKER, Newcastle University, Newcastle-upon-Tyne, United Kingdom

WH01 15 min 1:30
THE LATEST REVISION OF THE ERHAM CODE

P. GRONER, Department of Chemistry, Univer-
sity of Missouri-Kansas City, Kansas City, MO
64110-2499.

WH02 10 min 1:47
GENERALIZED EQUATIONS FOR THE INERTIAL
TENSOR OF A WEAKLY BOUND COMPLEX

KENNETH R. LEOPOLD, Department of
Chemistry, University of Minnesota, 207 Pleas-
ant St., SE, Minneapolis, MN 55455.

WH03 15 min 1:59
SECOND MOMENTS (PLANAR MOMENTS) AND
THEIR APPLICATION IN SPECTROSCOPY

ROBERT K. BOHN, Dept. of Chemistry,
Univ. of Connecticut, Storrs, CT 06269-3060;
JOHN A. MONTGOMERY, JR., H. HAR-
VEY MICHELS, JASON N. BYRD, Dept. of
Physics, Univ. of Connecticut, Storrs, CT 06269-
3040.

WH04 15 min 2:16
AN EMPIRICAL APPROACH TO OBTAINING ACCU-
RATE MOLEULAR ROTATIONAL CONSTANTS FOR
ISOTOPICALLY-SUBSTITUTED SPECIES FROM AB
INITIO CALCULATIONS

BRETT A. McGUIRE, P. BRANDON CAR-
ROLL, Division of Chemistry and Chemical
Engineering, California Institute of Technol-
y, Pasadena, CA 91125; GEOFFREY A.
BLAKE, Division of Chemistry and Chemical En-
gineering and Division of Geological and Plan-
etary Sciences, California Institute of Technology,
Pasadena, CA 91125.

WH05 15 min 2:33
SINGULAR VALUE DECOMPOSITION-BASED MOD-
ELING OF TIME DOMAIN SIGNALS IN BROADBAND
MICROWAVE SPECTROSCOPY

A.J. MINEI, Department of Chemistry and Bio-
chemistry, Division of Natural Sciences, College
of Mountain Saint Vincent, 6301 Riverdale Avenue,
Riverdale, New York, 10471; S.A. COOKE,
School of Natural and Social Sciences, Purchase
College SUNY, 735 Anderson Hill Road, Pur-
chase, NY 10577, USA.
WH06  15 min  2:50
PURE ROTATIONAL SPECTROSCOPY OF ASYMMETRIC TOPS IN THE UNDERGRADUATE CLASSROOM OR LABORATORY
A. J. MINEL, Department of Chemistry and Biochemistry, Division of Natural Sciences, College of Mount Saint Vincent, 6301 Riverdale Avenue, Riverdale, New York 10471; S. A. COOKE, School of Natural and Social Sciences, Purchase College SUNY, 735 Anderson Hill Road, Purchase, NY 10577, USA.

WH07  15 min  3:07
A NEW E-BAND (60 - 90 GHz) FOURIER TRANSFORM MILLIMETER-WAVE SPECTROMETER
D. T. HALFEN and L. M. ZIURYS, Department of Chemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, AZ 85721.

WH08  15 min  3:24
THE FOURIER TRANSFORM MICROWAVE/MILLIMETER SPECTRUM OF ScO (X^2Sigma^+)
D. T. HALFEN, J. MIN, and L. M. ZIURYS, Department of Chemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, AZ 85721.

Intermission

WH09  15 min  4:00
SUBMILLIMETER SPECTROSCOPIC DIAGNOSTICS IN A SEMICONDUCTOR PROCESSING PLASMA
YASER H. HELAL, CHRISTOPHER F. NEESE, JENNIFER A. HOLT, FRANK C. DE LUCIA, Department of Physics, The Ohio State University, Columbus, OH 43210; PAUL R. EWING, Applied Materials, Austin, TX 78724; PHILLIP J. STOUT, MICHAEL D. ARMACOST, Applied Materials, Sunnyvale, CA 94085.

WH10  15 min  4:17
IR/THZ DOUBLE RESONANCE SPECTROSCOPY APPROACH FOR REMOTE CHEMICAL DETECTION AT ATMOSPHERIC PRESSURE
ELIZABETH A. TANNER and DANE J. PHILLIPS, JERUS Technologies, 2901 Westcort Blvd Ste 210, Huntsville, AL 35805; FRANK C. DE LUCIA, Department of Physics, 191 Woodruff Ave, Ohio State University, Columbus, OH 43210; HENRY O. EVERITT, Army Aviation and Missile RD&E Center, Redstone Arsenal, AL 35898.

WH11  15 min  4:34
A MICRO-CANTILEVER BASED PHOTOACOUSTIC DETECTOR OF TERAHERTZ RADIATION FOR CHEMICAL SENSING
NATHAN E. GLAVITZ, RONALD A. COUTU JR., Department of Electrical and Computer Engineering, Air Force Institute of Technology, 2950 Hobson Way, Wright-Patterson AFB, OH 45433, USA; MICHAEL N. KISTLER, RYAN F. HAMILTON, DOUGLAS T. PETKIE, IVAN R. MEDVEDEV, Department of Physics, Wright State University, 3670 Colonel Glenn Highway, Dayton, OH 45433, USA.

WH12  15 min  4:51
A TWO-COLOR FOURIER TRANSFORM MM-WAVE SPECTROMETER FOR GAS ANALYSIS OPERATING FROM 260-295 GHZ
AMANDA L. STEBER, BRENT J. HARRIS, KEVIN K. LEHMANN, and BROOKS H. PATE, Department of Chemistry, University of Virginia, Charlottesville, VA 22904.

WH13  15 min  5:08
GAS ANALYSIS BY FOURIER TRANSFORM MM-WAVE SPECTROSCOPY
BRENT J. HARRIS, AMANDA L. STEBER, KEVIN K. LEHMANN, and BROOKS H. PATE, Department of Chemistry, University of Virginia, Charlottesville, VA 22904.

WH14  15 min  5:25
A SEGMENTED CHIRPED-PULSE FOURIER TRANSFORM MM-WAVE SPECTROMETER (260-295 GHZ) WITH REAL-TIME SIGNAL AVERAGING CAPABILITY
BRENT J. HARRIS, AMANDA L. STEBER, and BROOKS H. PATE, Department of Chemistry, University of Virginia, Charlottesville, VA 22904.

WH15  15 min  5:42
COHERENT SYNCHROTRON RADIATION FOR ROTATIONAL SPECTROSCOPY: APPLICATION TO THE ROTATIONAL SPECTRUM OF PROPYNAL IN THE 200-750 GHZ RANGE
J. BARROS, P. ROY, Synchrotron SOLEIL, L’Orme des Merisiers Saint-Aubin, 91192 Gif-sur-Yvette, France; D. APPADOO, D. Mc NAUGHTON, Australian Synchrotron Light Source, 800 Blackburn Road Victoria 3168 and Monash University, School of Chemistry, Clayton, Victoria 3800 Australia.; E. ROBERTSON, La Trobe University, Department of Chemistry, Victoria, 3086, Australia; L. MANCERON, Laboratoire LADIR, CNRS, Université Pierre et Marie Curie, 75252 Paris Cedex, France.
DEVELOPMENT OF A REDUCED-COST CHIRPED PULSE MICROWAVE SPECTROMETER

IAN A. FINNERAN, DANIEL B. HOLLAND, P. BRANDON CARROLL, Department of Chemistry, California Institute of Technology, Pasadena, CA 91125; and GEOFFREY A. BLAKE, Divisions of Geological & Planetary Sciences and Chemistry & Chemical Engineering, California Institute of Technology, Pasadena, CA 91125.

WI. INFRARED/RAMAN
WEDNESDAY, JUNE 19, 2013 – 1:30 PM
Room: 1015 MCPHERSON LAB

Chair: REBECCA PEEBLES, Eastern Illinois University, Charleston, IL

WI01 15 min 1:30
INFRARED SPECTROSCOPIC INVESTIGATION ON HIGH ACIDITY OF DIETHYLETHER CATION
TOMOYA ENDO, YOSHIYUKI MATSUDA, ASUKA FUJII, Department of Chemistry, Graduate School of Science, Tohoku University, Sendai 980-8578, Japan KAITO TAKAHASHI, Institute of Atomic and Molecular Sciences, Academia Sinca, Taipei 10617, Taiwan.

WI02 15 min 1:47
STRUCTURAL, CONFORMATIONAL AND VIBRATIONAL STUDIES OF ISOCYANOCYCLOPENTANE FROM INFRARED, RAMAN SPECTRA AND AB INITIO CALCULATIONS
DATTATRAY K. SAWANT, JOSHUA J. KIAASSEN, JAMES R. DURIG, DEPARTMENT OF CHEMISTRY, UNIVERSITY OF MISSOURI-KANSAS CITY, MO 64110 USA.

WI03 15 min 2:04
MICROWAVE AND INFRARED SPECTRA, ADJUSTED R0 STRUCTURAL PARAMETERS, CONFORMATIONAL STABILITIES, VIBRATIONAL ASSIGNMENTS, AND AB INITIO CALCULATIONS OF CYCLOBUTYL CARBOXYLIC ACID CHLORIDE
JOSHUA J. KIAASSEN, PETER GRONER, JAMES R. DURIG, Department of Chemistry, University of Missouri-Kansas City, Kansas City, MO 64110 USA.

WI04 15 min 2:21
LOWERING OF KETO-ENOL TAUTOMERIZATION BARRIER OF CYCLIC DIKETONES VIA CH...O INTERACTION
T. CHAKRABORTY, B. BANDYOPADHYAY, P. BANERJEE and P. PANDEY, Department of Physical Chemistry, Indian Association for the cultivation of science, Calcutta 700032, India. E-mail: pete@iacs.res.in

WI05 15 min 2:38
A SPECTROSCOPIC AND THEORETICAL STUDY OF WEAK INTRAMOLECULAR OH...π INTERACTIONS IN ALKYL CARBINOL AND METHALLYL CARBINOL
SIDSELD S. SCHROEDER, KASPER MACKEPRANG, HENRIK G. KJAERGAARD, Department of Chemistry, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen.

Intermission
VIBRATIONAL SPECTROSCOPIC INVESTIGATION AND CONFORMATIONAL ANALYSIS OF 1-HEPTYLAMINE: A COMPARATIVE DENSITY FUNCTIONAL STUDY

MAHIR TURSAN, Department of Physics, Dumuljinar University, Katahya, 43100, Turkey, and GURKAN KESAN, Institute of Physics and Biophysics, Faculty of Science, University of South Bohemia, BrnisionukAq 31, CeskAlik BudAřoves, 370 05, Czech Republic, and CEMAL PARLAK, Department of Physics, Dumuljinar University, Katahya, 43100, Turkey, MUSTAFA SENER, Science Faculty, Department of Physics, Anadolu University, Eskisehir, Turkey 26/70.

LOWEST ENERGY VIBRATIONAL MODES OF NINE NAPHTHALENE DERIVATIVES: EXPERIMENT AND THEORY

M. A. MARTIN-DREMEL, O. PIRALI, Y. LAQUAIS*, Institut des Sciences Moléculaires d’Orsay, CNRS, UMR 8214, Université Paris XI, bat. 210, 91405 Orsay Cedex, France; SOLEIL Synchrotron, AILES beamline, L’orme des Merisiers, Saint-Aubin, 91192 Gif-Sur-Yvette, France; C. FALVO, P. PARNEIX and PH. BRECHIGNAC, Institut des Sciences Moléculaires d’Orsay, CNRS, UMR 8214, Université Paris XI, bat. 210, 91405 Orsay Cedex, France.

*Present address: LPCA, EA 4493, Université du Littoral Côte d’Opale, 59140 Dunkerque, France

Present address: CEA, IRAMIS, SPAM, Lab. Francis Perrin, 91192 Gif-Sur-Yvette, France

TOWARD COMPUTATIONAL SPECTROSCOPY STUDIES FOR LARGE MOLECULAR SYSTEMS

MALGORZATA BICZYSKO, Center for Nanotechnology Innovation @ NEST, Istituto Italiano di Tecnologia, Piazza San Silvestro 12, 1-56127 Pisa, Italy; JULIEN BLOINO, Consiglio Nazionale delle Ricerche, Istituto di Chimica dei Composti OrganoMetallici (ICCOM-CNR), UOS di Pisa, Area della Ricerca CNR, Via G. Moruzzi 1, I-56124 Pisa, Italy; VINCENZO BARONE, Scuola Normale Superiore, Piazza dei Cavalieri 7, I-56126 Pisa, Italy.

DETERMINATION OF STRUCTURAL AND VIBRATIONAL PROPERTIES OF 5-QUINOLINECARBOXALDEHYDE USING EXPERIMENTAL FT-IR, FT-RAMAN TECHNIQUES AND THEORETICAL HF AND DFT METHODS

MUSTAFA KUMRU, MUSTAFA KOCADEMIR, TAYYIBE BARDAKCI, Department of Physics, Faculty of Arts and Sciences, Rah University, 34500 Buyukcekmece, Istanbul, Turkey.

CYCLIC CONSTRAINTS ON CONFORMATIONAL FLEXIBILITY IN γ-PEPTIDES: CONFORMATION-SPECIFIC IR AND UV SPECTROSCOPY

PATRICK S. WALSH, RYOJI KUSAKA and TIMOTHY S. ZWIER, Department of Chemistry, Purdue University, West Lafayette, IN 47907; BRIAN F. FISHER and SAMUEL H. GELLMAN, Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706.

CONFORMATION-SPECIFIC UV AND IR SPECTROSCOPY OF CONFORMATIONALLY CONFINED α/γ PEPTIDE FOLDAMERS

RYOJI KUSAKA, Department of Chemistry, Purdue University, West Lafayette, IN 47907, and Department of Chemistry, Graduate School of Science, Hiroshima University, Hiroshima, 739-8556, Japan; DI ZHANG, PATRICK WALSH, JOSEPH GORD, and TIMOTHY S. ZWIER, Department of Chemistry, Purdue University, West Lafayette, IN 47907; BRIAN F. FISHER, and SAMUEL H. GELLMAN, Department of Chemistry, University of Wisconsin, Madison, WI 53706.

MIXED CYCLIC CONSTRAINTS ON CONFORMATIONAL FLEXIBILITY IN β/γ-PEPTIDES: CONFORMATION SPECIFIC IR AND UV SPECTROSCOPY

JOSEPH R. GORD, PATRICK S. WALSH, and TIMOTHY S. ZWIER, Department of Chemistry, Purdue University, West Lafayette, IN 47907; BRIAN F. FISHER and SAMUEL H. GELLMAN, Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706.
WI13  15 min  5:04
ACTION IRMPD SPECTROSCOPY OF B₂ FRAGMENT IONS FROM QAXIG AND NAXIG PENTAPEPTIDES

L. MORRISON, Department of Chemistry, The Ohio State University, Columbus, OH 43210; J. CHAMOT-ROOKE, Department of Mass Spectrometry and Proteomics Research, Pasteur Institute, Paris, France; V. WYSOCKI, Department of Chemistry, The Ohio State University, Columbus, OH 43210.

WI14  15 min  5:21
MODIFICATION OF THE PROLYL RING OF VAL-PRO-LA AND THE IMPACT OF THIS MODIFICATION ON B₂ ION STRUCTURE

MATTHEW C. BERNIER, VICKI H. WYSOCKI, THE OHIO STATE UNIVERSITY, COLUMBUS, OH; ASHLEY GUCINSKI, U. S. FDA, SAINT LOUIS, MO; JULIA CHAMOT-ROOKE, INSTITUT PASTEUR, PARIS, FRANCE.

WJ. RADICALS AND IONS
WEDNESDAY, JUNE 19, 2013 – 1:30 PM
Room: 2015 MCPHERSON LAB

Chair: MITCHIO OKUMURA, California Institute of Technology, Pasadena, CA

WJ01  15 min  1:30
THE INFRARED AND NEAR-INFRARED SPECTRUM OF HNO TRAPPED IN SOLID NEON

MARILYN E. JACOX and WARREN E. THOMPSON, Sensor Science Division, National Institute of Standards and Technology, Gaithersburg, MD 20899-8441.

WJ02  15 min  1:47
A NEW TYPE OF VIBRONIC INTERACTION IN THE NITRATE FREE RADICAL NO₃

E. HIROTA, The Graduate University for Advanced Studies, Hayama, Kanagawa 240-0193, Japan.

WJ03  15 min  2:04
DISPERSED FLUORESCENCE SPECTROSCOPY OF THE B ²E⁻ → X ²A₂⁺ TRANSITION OF JET COOLED ¹⁴NO₃ AND ¹⁵NO₃

MASARU FUKUSHIMA and TAKASHI ISHIWATA, Faculty of Information Sciences, Hiroshima City University, Asa-Minami, Hiroshima 731-3194, Japan.

WJ04  15 min  2:21
ROTATIONALLY-RESOLVED HIGH-RESOLUTION LASER SPECTROSCOPY AND MAGNETIC EFFECT OF THE B → X TRANSITION OF NO₃ RADICAL

K. TADA, W. KASIHARA, S. KASAHARA, Graduate School of Science, Kobe University, Kobe 657-8501, Japan; M. BABA, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan; T. ISHIWATA, Graduate School of Information Sciences, Hiroshima City University, Hiroshima 731-3194, Japan; and E. HIROTA, The Graduate University for Advanced Studies, Kanagawa 240-0193, Japan.

WJ05  15 min  2:38
VIBRONIC ANALYSIS OF THE Ā²E'' STATE OF NO₃ RADICAL

TERRANCE J. CODD, MOURAD ROUDJANE, MING-WEI CHEN, and TERRY A. MILLER, Laser Spectroscopy Facility, The Ohio State University, Columbus, Ohio 43210.

*Present address: University of Illinois at Urbana-Champaign, Urbana, IL 61801

WJ06  15 min  2:55
HIGH RESOLUTION CAVITY RING DOWN SPECTROSCOPY OF THE 3₁₀ and 3₁₀ 4₁₀ BANDS OF THE Ā²E'' STATE OF NO₃ RADICAL

MOURAD ROUDJANE, TERRANCE J. CODD and TERRY A. MILLER, Laser Spectroscopy Facility, The Ohio State University, Columbus, Ohio 43210.

WJ07  15 min  3:12
THE RENNER-TELLER AND OHM-TELLER EFFECTS IN PROTOTYPICAL MOLECULAR CATIONS SUBJECT TO A VERY LARGE SPIN-ORBIT COUPLING

BÉRANGER GANS and MONICA GRÜTTER, Laboratorium für Physikalische Chemie, ETH Zürich, CH-8093 Zürich, Switzerland.
WJ08  15 min  3:29
OBSERVATION OF THE $\alpha_1$ CH STRETCHING MODES OF PHENYL RADICAL

CHIH-HSUAN CHANG, GRANT T. BUCKINGHAM, DAVID J. NESBITT, JILA, National Institute of Standards and Technology University of Colorado, and Department of Chemistry and Biochemistry University of Colorado at Boulder, Colorado 80309.

WJ09  15 min  3:46
HIGH RESOLUTION ROVIBRATIONAL SPECTROSCOPY OF JET-COOLED PHENYL RADICAL: THE $v_19$ OUT-OF-PHASE SYMMETRIC C-H STRETCH

GRANT T. BUCKINGHAM, CHIH-HSUAN CHANG, and DAVID J. NESBITT, JILA, National Institute of Standards and Technology and University of Colorado, Department of Chemistry and Biochemistry, Boulder, CO 80309.

Intermission

WJ10  15 min  4:20
MOLECULAR CONSTANTS OF C$_2$ IN THE $c^3\Sigma_+^-$ STATE

MASAKAZU NAKAJIMA and YASUKI ENDO, Department of Basic Science, The University of Tokyo, Tokyo 153-8902, Japan.

WJ11  15 min  4:37

WANG CHEN, JIAN TANG and KENTAROU KAWAGUCHI, Graduate School of Natural Science and Technology Okayama University, 3-1-1 Tsushima-Naka, Okayama 700-8530, Japan.

WJ12  15 min  4:54
THE ETHYL RADICAL IN SUPERFLUID HELIUM NANODROPLETS: ROVIBRATIONAL SPECTROSCOPY AND AB INITIO CALCULATIONS

PAUL L. RASTON, CHRISTOPHER P. MORADI, Department of Chemistry, University of Georgia, Athens, Georgia 30602-2556; JAY AGARWAL, JUSTIN M. TURNER, HENRY F. SCHEFFER III, Center for Computational Chemistry, University of Georgia, Athens, Georgia 30602-2556; GARY E. DOUBERY, Department of Chemistry, University of Georgia, Athens, Georgia 30602-2556.

WJ13  15 min  5:11
INFRARED SPECTROSCOPY AND TUNNELING DYNAMICS OF THE VINYL RADICAL IN $^3$He NANODROPLETS

PAUL L. RASTON, TAO LIANG, EMMANUEL L. OBI, and GARY E. DOUBERY, Department of Chemistry, University of Georgia, Athens, Georgia 30602, USA.

WJ14  15 min  5:28
STRUCTURE AND DYNAMICS OF THE CYCLOPROPENE RADICAL CATION STUDIED BY HIGH-RESOLUTION PHOTOELECTRON SPECTROSCOPY

KONSTANTINA VASILATOU, JULIE M. MICHAUD, DENTiSA BAYKU-SHEVA, GUIDO GRASSI and FREDERIC MERKT, Laboratorium für Physikalische Chemie, ETH Zürich, CH-8093 Zürich, Switzerland.

WJ15  15 min  5:45
STRUCTURE DETERMINATION OF NON-LINEAR HYDROCARBON CHAINS BY DEUTERIUM LABELING

D. ZHAO, H. LINNARTZ, Sackler Laboratory for Astrophysics, Leiden Observatory, University of Leiden, P.O. Box 9513, NL-2300 RA Leiden; M. A. HADDAD, W. UBAChS, LaserLab, VU University Amsterdam, De Boelelaan 1081, NL-1081 HV, Amsterdam, The Netherlands.

WK. ELECTRONIC

WEDNESDAY, JUNE 19, 2013 – 1:30 PM

Room: 1153 SMITH LAB

Chair: ANTHONY MERER, Academia Sinica, Taipei, Taiwan
WK01  15 min  1:30
SPECTROSCOPY OF LiCa AND RbSr MOLECULES ON HELIUM NANODROPLETS

FLORIAN LACKNER, GÜNTER KROS and WOLFGANG E. ERNST, Institute of Experimental Physics, Graz University of Technology, Pestersgasse 16, A-8010 Graz, Austria.

WK02  15 min  1:47
SPECTROSCOPY OF Li ATOMS AND Li DIMERS IN THE TRIPLET MANIFOLD ON THE SURFACE OF HELIUM NANODROPLETS

FLORIAN LACKNER, GÜNTER KROS and WOLFGANG E. ERNST, Institute of Experimental Physics, Graz University of Technology, Pestersgasse 16, A-8010 Graz, Austria.

WK03  10 min  2:04
OBSERVATION OF THE 5 1Σ_u^+ and 5 1Π_u STATES OF Rb_2 BY POLARISATION LABELLING SPECTROSCOPY

JACEK SZCZEPKOWSKI, WODZIMIERZ JASTRZEBSKI, Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warsaw, Poland; PAWEL KOWALCZYK, ANNA GROCHOLA, Institute of Experimental Physics, Department of Physics, University of Warsaw, ul. Hoża 69, 00-681 Warsaw, Poland; ABDURAHMAN ALLOUCHE, PATRICK CROZET and AMANDA J. ROSS, Institut Lumière Matière, Université Lyon 1 & CNRS UMR5306, Université de Lyon, France.

*aSupported by the PAN-CNRS exchange programme, 2011-12

WK04  5 min  2:16
DOUBLE RESONANCE EXCITATION OF THE RUBIDIUM DIMER: THE 2 1Π_g STATE

ANASTASIA DROZDOVA, Department of Chemistry, Moscow State University, 119991 Moscow, Russia; ABDURAHMAN ALLOUCHE, GHASSAN WANNOUS, PATRICK CROZET and AMANDA J. ROSS, Institut Lumière Matière, Université Lyon 1 & CNRS UMR5306, Université de Lyon, France.

WK05  15 min  2:23
EXCITATION OF ULTRACOLD MOLECULES TO "TRILOBITE-LIKE" LONG-RANGE MOLECULAR RYDBERG STATES


WK06  15 min  2:40
HIGH RESOLUTION PHOTOELECTRON SPECTROSCOPY OF Au_2 and Au_4 BY PHOTOELECTRON IMAGING

IKER LEON, ZHENG YANG, and LAL-SHENG WANG, Department of Chemistry, Brown University, Providence, RI 02912, USA.

WK07  15 min  2:57
INTRACAVITY LASER ABSORPTION SPECTROSCOPY OF PLATINUM NITRIDE IN THE NEAR INFRARED

LEAH C. O’BRIEN, KAITLIN A. WOMACK, Department of Chemistry, Southern Illinois University, Edwardsville, IL 62026-1652; JAMES J. O’BRIEN, SEAN WHITTEMORE, Department of Chemistry, University of Missouri, St Louis, MO 63121-4499.

WK08  10 min  3:14
REANALYSIS OF THE NEAR INFRARED ELECTRONIC TRANSITIONS OF NICI

LEAH C. O’BRIEN, TAYLOR DAIMS, Department of Chemistry, Southern Illinois University, Edwardsville, IL 62026-1652; JAMES J. O’BRIEN, Department of Chemistry, University of Missouri, St Louis, MO 63121-4499.

WK09  10 min  3:26
INTRACAVITY LASER ABSORPTION SPECTROSCOPY OF ZIRCONIUM FLUORIDE IN THE NEAR INFRARED

LEAH C. O’BRIEN, JACK C. HARMS, Department of Chemistry, Southern Illinois University, Edwardsville, IL 62026-1652; JAMES J. O’BRIEN, Department of Chemistry and Biochemistry, University of Missouri, St Louis, MO 63121-4499.

Intermission
WK10 

15 min 4:00 

ROTATIONAL AND HYPERFINE STRUCTURE IN THE [176]2.5−X2.5 AND [233]2.5−X2.5 TRANSITIONS OF IRIDIUM MONOXIDE

C. LINTON, D. W. TOKARYK, Physics Department and Centre for Laser, Atomic and Molecular Sciences, University of New Brunswick, Fredericton, NB, Canada E3B 5A3; A. G. ADAM, J. A. DAIGLE, L. M. ESSON, A. D. GRANGER, A. M. SMITH, Chemistry Department and Centre for Laser, Atomic and Molecular Sciences, University of New Brunswick, Fredericton, NB, Canada E3B 5A3; T. C. STEIMLE, Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287, USA.

WK11 

15 min 4:17 

ELECTRONIC TRANSITIONS OF YTTRIUM MONOXIDE

Y.W. NG, NA WANG, ANDREW B. CLARK and A. S-C. CHEUNG, Department of Chemistry, The University of Hong Kong, Pokfulam Road, Hong Kong.

WK12 

10 min 4:34 

ELECTRONIC TRANSITIONS OF PALLADIUM AND VANADIUM DIMER

YUE QIAN, Y.W. NG, and A. S-C. CHEUNG, Department of Chemistry, The University of Hong Kong, Pokfulam Road, Hong Kong.

WK13 

15 min 4:46 

ELECTRONIC TRANSITIONS OF RUTHENIUM MONOXIDE

NA WANG, Y. W. NG, and A. S-C. CHEUNG, Department of Chemistry, The University of Hong Kong, Pokfulam Road, Hong Kong.

WK14 

10 min 5:03 

PRECISION SPECTROSCOPY OF TELLURIUM

J. COKER, J.E. FURNEAUX, Department of Physics and Astronomy, University of Oklahoma, Norman, OK 73069.

WK15 

15 min 5:15 

IONIZATION MEASUREMENT AND SPECTROSCOPY OF ThS AND ThS+

J. H. BARTLETT, M. C. HEAVEN, Department of Chemistry, Emory University, Atlanta, GA 30322.

WK16 

15 min 5:32 

A STUDY OF NbCr AND NbCr+ BY ANION PHOTOELECTRON SPECTROSCOPY

MELISSA A. BAUDHUN, PRAVEENKUMAR BOOPALACHANDRAN, SHIJAY S. RAJAN, and DOREEN G. LEOPOLD, Department of Chemistry, University of Minnesota, Minneapolis, MN 55455.

RA. MINI-SYMPHOSYUM: THEORY AND SPECTROSCOPY

THURSDAY, JUNE 20, 2013 – 8:30 AM

Room: 160 MATH ANNEX

Chair: JENS-UWE GRABOW, Gottfried-Wilhelm-Leibniz-Universitaet, Hannover, Germany

RA01 INVIDTED TALK 30 min 8:30

MANIFESTATIONS OF VIBRONIC COUPLING EFFECTS IN MOLECULAR SPECTROSCOPY: FROM THE QUENCHING OF EXCITONIC ENERGY SPLITTINGS TO THE CLEMENTS BANDS OF SO2

HORST KÖPPEL, Theoretical Chemistry, Institute of Physical Chemistry, University of Heidelberg, D-69120 Heidelberg, Germany.

RA02 15 min 9:05

TUNNELING SPLITTINGS IN VIBROMIC STRUCTURE OF CHF+ (X:E): STUDIED BY HIGH RESOLUTION PHOTOELECTRON SPECTRA AND AB INITIO THEORETICAL METHOD

YUXIANG MO, SHUMING GAO, ZUYANG DAI, and HUA LI, Department of Physics and State Key Laboratory of Low-Dimensional Quantum Physics, Tsinghua University, Beijing 100084, China.
RA03 15 min 9:22
ANALYSIS OF THE ROTATIONALLY-RESOLVED SPECTRA OF THE VIBRONICALLY-ACTIVE MOLECULES

DMITRY G. MELNIK and TERRY A. MILLER,
Laser Spectroscopy Facility, Department of Chemistry, The Ohio State University, 120 W. 18th Avenue, Columbus, Ohio 43210.

RA04 15 min 9:39
A THEORETICAL PREDICTION OF ELECTRONIC TRANSITIONS IN C₆

DAVID W. SCHWENKE, GALINA M. CHABAN, NASA Ames Research Center, Moffett Field, CA 94035.

RA05 15 min 9:56
THE RENNER EFFECT IN THE × 2A″ AND Å 2A′ ELECTRONIC STATES OF HSO/HOS

ROMAN I. OVSYANNIKOV, Institute of Applied Physics, Russian Academy of Science, Uljanov Street 96, Nizhny Novgorod, Russia 603950, and Physical and Theoretical Chemistry, Faculty of Mathematics and Natural Sciences, University of Wuppertal, D-42097 Wuppertal, Germany.

PER JENSEN, Physical and Theoretical Chemistry, Faculty of Mathematics and Natural Sciences, University of Wuppertal, D-42097 Wuppertal, Germany.

TSUNEO HIRANO, Department of Chemistry, Faculty of Science, Ochanomizu University, 1-1 Otsuka, Bunkyo-ku, Tokyo 112-8610, Japan.

Intermission

RA06 15 min 10:30
PHOTODISSOCIATION SPECTROSCOPY OF BARE AND HYDRATED PERMANGANATE IONS

JORGEN HOU MOLLER, KRISTIAN STOCHIEL, STEEN BRONSTED NIELSEN, Department of Physics and Astronomy, Aarhus University, Ny Munkegade 120, 8000 Aarhus C, Denmark.

SYDNEY H. KAUFMAN, J. MATTHIAS WEBER, JILA, and Department of Chemistry and Biochemistry, University of Colorado, Boulder, Colorado 80309, USA.

RA07 15 min 10:47
MANIFESTATION OF NONADIABATIC EFFECTS IN THE IR SPECTRUM OF PARA-BENzoquinone RADICAL CATION

KRZYSZTOF PIECH, THOMAS BALLY, Department of Chemistry, University of Fribourg, CH-1700 Fribourg, Switzerland.

TAKATOSHI CHINO and JOHN F. STANTON, Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, TX 78712.

RA08 15 min 11:04
NUMERICALLY EXACT DYNAMICS OF FUNCTIONAL QUANTUM SYSTEMS - APPLICATIONS TO GaAs QUANTUM DOT QUBITS AND 2-DIMENSIONAL SPECTRA OF VERY LARGE PHOTOSYNTHETIC COMPLEXES

NIKESH S. DATTAJ, Oxford University, Department of Chemistry, Oxford, OX1 3QZ, UK.

RA09 15 min 11:21
OBSERVATION AND ANALYSIS OF BOUND → FREE TRANSITION OF Sc₂⁺ PHOTOEXCITED IN THE ULTRAVIOLET

LOANN D. POMMAREL, J. DARBY HEWITT, THOMAS C. GALVIN, and J. GARY EDEN, Laboratory for Optical Physics and Engineering, Department of Electrical and Computer Engineering, University of Illinois at Urbana-Champaign, 607 East Healey Street, Champaign, IL 61820.

RA10 15 min 11:38
EXCITED STATES OF THE DIATOMIC MOLECULE CrHe

JOHANN V. POTOTSCHNIG, MARTIN RATSCHKE, ANDREAS W. HAUSER, and WOLFGANG E. ERNST, Institute of Experimental Physics, TU Graz, Petersgasse 16, 8010 Graz, Austria.

RA11 15 min 11:55
POLARIZATION EFFECTS AND IONIC BONDING IN A POLAR DIATOMIC: THE CaF⁺ X1Σ⁺ STATE


RB. RADICALS AND IONS
THURSDAY, JUNE 20, 2013 – 8:30 AM
Room: 170 MATH ANNEX
RB01  15 min  8:30
VIBRATIONAL SPECTROSCOPY OF SYMPATHETICALLY COOLED CaH⁺ MOLECULAR IONS

NCAMISO B. KHANYILE, JAMES E. GOEDERS and KENNETH R. BROWN, Department of Chemistry, Georgia Institute of Technology, Atlanta, GA 30332.

RB02  15 min  8:47
INTRA CLUSTER REACTIONS IN N₂CO₂ CLUSTERS

JONATHAN A. MANER, MATTHEW D. McDOWELL and MICHAEL A. DUNCAN, Department of Chemistry, University of Georgia, Athens, Georgia 30602.

RB03  15 min  9:04
INFRARED PHOTODISSOCIATION SPECTROSCOPY OF METAL OXIDE CARBONYL CATIONS.

ANTONIO D. BRATHWAITE
MICHAEL A. DUNCAN, Department of Chemistry, University of Georgia, Athens, GA 30602-2256; .

RB04  15 min  9:21
ACURATE POTENTIAL ENERGY CURVES FOR THE GROUND ELECTRONIC STATES OF NeH⁺ AND ArH⁺

JOHN A. COXON, Department of Chemistry, Dalhousie University, Halifax, Nova Scotia, Canada B3H 4J8; PHOTOS G. HAJGEORGIU, Department of Life and Health Sciences, University of Nicosia, Nicosia 1700, Cyprus.

RB05  15 min  9:38
EXPANSION DISCHARGE SOURCE FOR ION BEAM LASER SPECTROSCOPY OF COLD MOLECULAR IONS

MICHAEL PORAMBO, JESSICA PEARSON, CRAIG RICCARDO, Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801; BENJAMIN J. McCALL, Departments of Chemistry and Astronomy, University of Illinois at Urbana-Champaign, Urbana, IL 61801.

RB06  15 min  10:15
INFRARED PHOTODISSOCIATION SPECTROSCOPY OF METAL BENZENE CATION COMPLEXES

K. N. REISHUS, M. A. DUNCAN, Department of Chemistry, University of Georgia, Athens, GA 30602-2256.

RB07  15 min  10:32
SPECTROSCOPY OF BENZYL-TYPE RADICALS GENERATED BY ELECTRIC DISCHARGE : JET-COOLED DICHLOROBENZYL RADICALS

YOUNG WOOK YOON and SANG KUK LEE, Department of Chemistry, Pusan National University, Pusan 609-735, Republic of Korea.

RB08  15 min  10:49
ROVIBRATIONAL SPECTROSCOPY OF THE OH-Ο₂ AND C₂H₂Ο₃ COMPLEXES IN He NANODROPLETS

EMMANUEL I. ORI and GARY E. DOUBERY, Department of Chemistry, University of Georgia, Athens, Georgia 30602, USA.

RB09  15 min  11:06
SPECTROSCOPY OF THE CH₄-HCL COMPLEX IN HELIUM NANODROPLETS

CHRISTOPHER P. MORADI and GARY E. DOUBERY, Department of Chemistry, University of Georgia, Athens, Georgia 30602-2556.

RB10  15 min  11:23
BIMOLECULAR PYROLYSIS REACTIONS STUDIED BY CHIRPED-PULSE MILLIMETER-WAVE SPECTROSCOPY

KIRILL PROZUMENT, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139; ANGAYLE K. VASILIOU, Department of Chemistry and Biochemistry, University of Colorado at Boulder, Boulder, CO 80309; RACHEL G. SHAVER, G. BARRATT PARK, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139; JOHN S. MUENTNER, Department of Chemistry, University of Rochester, Rochester, NY 14627; JOHN F. STANTON, Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, TX 78712; G. BARNES ELLISON, Department of Chemistry and Biochemistry, University of Colorado at Boulder, Boulder, CO 80309; ROBERT W. FIELD, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139.

Intermission
SLOW PHOTOELECTRON SPECTROSCOPY AND STATE-SELECTED UNIMOLECULAR DECOMPOSITION OF IONIZED DNA BASES ANALOGUES

AHMED MAHJOU and MAJDI HOCHLAF, Université Paris Est, Laboratoire Modélisation et Simulation Multi Echelle, MSME UMR 8208 CNRS, 77454 Marne la Vallée (France); LIONEL POISSON, Laboratoire Francis Perrin CNR-URA 2453, CEA ÎSIRAMIS, 91192, Gif sur Yvette (France); GUSTAVO A. GARCIA and LAURENT NAHON, Synchrotron SOLEIL, L’Orme des Merisiers, Saint Aubin BP 48, 91193 (France).

INSIGHTS ON HYDROGEN LIBERATION FROM WATER USING ANIONIC TRANSITION METAL OXIDE CLUSTERS: A COMBINED COMPUTATIONAL AND SPECTROSCOPIC STUDY

RAGHUNATH O. RAMABHADRA, JENNIFER E. MANN, SARAH E. WALLER, DAVID W. ROTHGER, CAROLINE C. JARROLD, KRISHNAN RAGHAVACHARI, DEPARTMENT OF CHEMISTRY, INDIANA UNIVERSITY, BLOOMINGTON, IN-47405.

RC. MICROWAVE
THURSDAY, JUNE 20, 2013 – 8:30 AM
Room: 1000MCPEHERSON LAB

Chair: ROBERT BOHN, University of Connecticut, Storrs, CT

RO01 15 min 8:30
THE ROTATIONAL SPECTRUM OF RUTHENIUM MONOCARBIDE USING PPMODR

TIMOTHY C. STEMLE, Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287; ALLAN G. ADAM, Center for Lasers, Atomic and Molecular Sciences and Physics Department, University of New Brunswick, Fredericton, NB Canada E3B 5A3.

*Funded by DoE-BES

RO02 15 min 8:47
PURE ROTATIONAL SPECTRA OF THE REACTION PRODUCTS OF LASER ABLATED THORIUM METAL AND OXYGEN MOLECULES ENTRAINED WITHIN SUPersonic EXPANSIONS OF NOBLE GASES

B. E. LONG, Department of Chemistry, Wesleyan University, 52 Lawn Avenue, Middletown, Connecticut, 06459; S. A. COOKE, School of Natural and Social Sciences, Purchase College SUNY, 735 Anderson Hill Road, Purchase, NY 10577, USA.

RO03 15 min 9:04
DETECTION OF THE ROTATIONAL SPECTRUM OF SULFOXILIC ACID (HOSOH)

KYLE N. CRABTREE, OSCAR MARTINEZ, JR., LOU BARREA and MICHAEL C. McCARTHY, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, 02138; SVEN THORWIRTH, I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany.

*Present address: École Normale Supérieure de Cachan, 94235 Cachan Cedex, France

RO04 15 min 9:21
GLOBAL ANALYSIS OF BROADBAND ROTATION AND VIBRATION-ROTATION SPECTRA OF SULFUR DICYANIDE

ZHENIHEW KISIEL, Institute of Physics, Polish Academy of Sciences, al. Lotników 32/46, 02-668 Warsaw, Poland; MANFRED WINNEWISSER, BRENDA P. WINNEWISSER, FRANK C. DE LUCIA, Department of Physics, The Ohio State University, Columbus, OH 43210, USA; DENNIS W. TOKARYK, Department of Physics and Centre for Laser, Atomic, and Molecular Sciences, University of New Brunswick, P.O.Box 4400, New Brunswick E3B 5A3, Canada; BRANT E. BILLINGHURST, Canadian Light Source Inc., University of Saskatchewan, 101 Perimeter Road, Saskatoon, Saskatchewan S7N 0X4, Canada.
CONTINUATION OF THE PURSUIT OF THE FAR-INFRARED SPECTRUM OF NCNCS, AT THE CANADIAN LIGHT SOURCE

MANFRED WINNEWISER, BRENTA P. WINNEWISER, FRANK C. DELUCIA, Department of Physics, The Ohio State University, Columbus, Ohio 43210-1106, USA; DENNIS W. TOKARYK, STEPHEN C. ROSS, Department of Physics and Centre for Laser, Atomic, and Molecular Sciences, University of New Brunswick, P.O. Box 4400, Fredericton NB E3B 5A3, Canada; BRANT E. BILLINGHURST, Canadian Light Source Inc., University of Saskatchewan, 101 Perimeter Road, Saskatoon, Saskatchewan S7N 0X4, Canada.

TERAHERTZ SPECTROSCOPY OF CaH (X^2Σ^+), MgH (X^2Σ^+), AND ZnH (X^2Σ^+): EXTREME HYDRIDE SYNTHESIS

MATTHEW P. BUCCINO, Department of Chemistry and Biochemistry, University of Arizona, Tucson, Arizona 85721; and LUCY M. ZIURYS, Department of Chemistry and Biochemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, Arizona 85721.

Intermission

THE MILLIMETER DIRECT ABSORPTION AND FOURIER-TRANSFORM MICROWAVE SPECTRUM OF VANADIUM SULFIDE (X^4Σ^-)

GILLES ADANDE, L.M. ZIURYS, Department of Chemistry, Steward Observatory University of Arizona, Tucson, 85721.

MILLIMETER AND SUB-MILLIMETER SPECTROSCOPY OF C6H (X^3Σ^+)

JIE MIN, LUCY, M. ZIURYS, Department of Chemistry and Biochemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, AZ 85721.

CHARACTERIZATION OF SILICON SULFIDES BY CHIRPED-PULSE ROTATIONAL SPECTROSCOPY

MICHAEL C. McCARTHY, KYLIE N. CRABTREE, OSCAR MARTINEZ, JR., Harvard-Smithsonian Center for Astrophysics, Harvard University, 29 Cambridge Street, Cambridge, MA 02138, and School of Engineering and Applied Sciences, Harvard University, 29 Oxford Street, Cambridge, MA 02138.

DETECTION OF TWO HIGHLY-STABLE SILICON NITRIDES BY CHIRPED-PULSE ROTATIONAL SPECTROSCOPY: HSINSi and SiH2NSi

MICHAEL C. McCARTHY, KYLIE N. CRABTREE, OSCAR MARTINEZ, JR., Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, and School of Engineering and Applied Sciences, Harvard University, 29 Oxford Street, Cambridge, MA 02138.

FOURIER-TRANSFORM MICROWAVE SPECTROSCOPY OF HCCNSi AND NCNSi

S. THORWIRTH, I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany. R. I. KAISER, Department of Chemistry, University of Hawaii at Manoa, Honolulu, HI 96822, U.S.A.; M. C. MCCARTHY, K. N. CRABTREE, O. MARTINEZ, JR., Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, and School of Engineering and Applied Sciences, Harvard University, 29 Oxford Street, Cambridge, MA 02138, U.S.A.

SUBSTITUTION STRUCTURES OF MULTIPLE SILICON-CONTAINING SPECIES BY CHIRPED PULSE FTMW SPECTROSCOPY

NATHAN A. SEIFERT, SIMON LOBSIGER, BROOKS H. PATE, Department of Chemistry, University of Virginia, Mccormick Rd., Charlottesville, VA 22904-4319; GAMIL A. GUIRGIS, JASON S. OVERBY, Department of Chemistry & Biochemistry, College of Charleston, Charleston, SC 29424 USA; JAMES R. DURIG, Department of Chemistry, University of Missouri-Kansas City, Kansas City, MO 64110 USA.

RD. ELECTRONIC
THURSDAY, JUNE 20, 2013 – 8:30 AM
Room: 1015 MCPHERSON LAB

Chair: ALLAN S. C. CHEUNG, University of Hong Kong, Hong Kong
RD01  15 min  8:30
METHODS FOR MANIPULATING CaF USING OPTICAL POLychromatic FORCES

EDWARD E. EYLER, SCOTT E. GALICA, and LEELAND M. ALDRIDGE, Department of Physics, University of Connecticut, Storrs, CT 06269, USA.

RD02  15 min  8:47
NEW LINE LIST'S INCLUDING INTENSITIES FOR THE C2 SWAN SYSTEM (d^2II_a-^3II_a), C2 SINGLET SYSTEMS AND ROVIBRATIONAL TRANSITIONS WITHIN THE NH X^3Σ^- GROUND STATE.

J. S. A. BROOKE, Department of Chemistry, University of York, York, UK; P. F. BERNATH, Department of Chemistry & Biochemistry, Old Dominion University, Norfolk, VA, USA; C. M. WESTERN, School of Chemistry, University of Bristol, Bristol, UK; T. W. SCHMIDT and G. B. BACSKAY, School of Chemistry, The University of Sydney, New South Wales, Australia; M. C. VAN HEMERT, Department of Chemistry, Gorlaeus Laboratories, Leiden University, The Netherlands; G. C. GROENENBOOM, Theoretical Chemistry, Institute for Molecules and Materials (IMM), Radboud University Nijmegen, Nijmegen, The Netherlands.

RD03  15 min  9:04
MEASUREMENT OF ABSOLUTE HYDROXYL RADICAL CONCENTRATION IN LEAN FUEL-AIR MIXTURES EXCITED BY NANOSECOND PULSED DISCHARGEa.

Z. YIN, W. R. LEMPERT, I. V. ADAMOVICH, The Ohio State University, Dept. of Mechanical and Aerospace Engineering, Columbus, OH 43210.

RD04  15 min  9:21
LASER INDUCED FLUORESCENCE SPECTROSCOPY OF JET COOLED SiN : ROTATIONAL ANALYSIS OF THE HOT BANDS

MASARU FUKUSHIMA and TAKASHI ISHIWATA, Faculty of Information Sciences, Hiroshima City University, Asa-Minami, Hiroshima 731-3194, Japan.

RD05  15 min  9:38
THE ELECTRIC DIPOLE MOMENT OF Iridium Monosilicide, IrSi

ANH LE AND TIMOTHY C. STEIMLE, Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287; LAN CHENG AND JOHN F. STANTON, The University of Texas at Austin, Austin, TX 78712-0165.

RD06  15 min  9:55
TRIPLE-SINGLET MIXING in SiH: the 1^3A_g^+ - ^3A_2 TRANSITIONa

RUOHAN ZHANG AND TIMOTHY C. STEIMLE, Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287.

"Funded by the NSF

RD07  15 min  10:12
MULTIPLEXED MODR WITH APPLICATIONS TO THE ELECTRONIC SPECTRUM OF SO2

G. BARRATT PARK and ROBERT W. FIELD, Department of Chemistry and Biochemistry, University of York, York, UK; ANDREW R. WHITEHILL and SHUHEI ONO, Department of Earth, Atmospheric, and Planetary Sciences, Massachusetts Institute of Technology, Cambridge, MA 02139.

RD08  15 min  10:45
SPECTROSCOPY OF THE NO-Ar COMPLEX IN THE VICINITY OF THE 3p → X^2II TRANSITIONS IN Nitric OXIDE

JOE P. HARRIS, TIMOTHY G. WRIGHT, ADRIAN M. GARDNER, ANNA ANDREJEVA, NICHOLAS A. BESLEY and OLGA V. ERSHOVA, School of Chemistry, University Park, University of Nottingham, NG7 2RD, United Kingdom; JACEK KLOS, Department of Chemistry, University of Maryland, College Park, MD 20742.

RD09  15 min  11:02
AN INTRODUCTION TO HIGH RESOLUTION COHERENT MULTIDIMENSIONAL SPECTROSCOPY

PETER C. CHEN, THRESA A. WELLS, and ZURI R. HOUSE, Spelman College Chemistry Department, 350 Spelman Lane, Atlanta, GA 30314; and BENJAMIN R. STRANGFELD, Department of Chemistry and Chemical Biology, Georgia Institute of Technology, Atlanta, GA 30332.

RD10  15 min  11:19
STRATEGIES FOR INTERPRETING HIGH RESOLUTION COHERENT MULTIDIMENSIONAL SPECTRA

THRESA A. WELLS, ZURI R. HOUSE, and PETER C. CHEN, Spelman College Chemistry Department, 350 Spelman Lane, Atlanta, GA 30314; BENJAMIN R. STRANGFELD, Department of Chemistry and Chemical Biology, Georgia Institute of Technology, Atlanta, GA 30332.
RE. MINI-SYMPOSIUM: SPECTROSCOPY OF PLANETARY ATMOSPHERES
THURSDAY, JUNE 20, 2013 – 8:30 AM
Room: 2015 MCPHERSON LAB

Chair: VINCENT BOUDON, CNRS/Université de Bourgogne, Dijon, France

RE01  INVITED TALK  30 min  8:30
SATELLITE REMOTE SENSING OF THE REACTIVE LOWER ATMOSPHERE USING MEDIUM RESOLUTION INFRARED MEASUREMENTS: HIGHLIGHTS FROM IASI MISSION
P.F. COEUR, Atmospheric Spectroscopy / Quantum Chemistry and Photophysics, Université Libre de Bruxelles CP160/09, Brussels, Belgium.

RE02  15 min  9:05
THE REVISED METHANE DATABASE IN HITRAN 2012
LINDA R. BROWN, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr., Pasadena, CA 91109.

RE03  15 min  9:22
HITRAN2012 AND REMOTE SENSING OF PLANETARY ATMOSPHERES
J.E. GORDON, L. S. ROTHMAN, G. LI, Harvard-Smithsonian Center for Astrophysics, Atomic and Molecular Physics Division, Cambridge MA 02138-1516, USA.

RE04  15 min  9:39
COSMIC-RAY IONIZATION AND HAZES ON HOT JUPITERS
PAUL B RIMMER, CHRISTIANE HELLING, SUPA, School of Physics and Astronomy, University of St Andrews, KY16 9SS, CATHERINE WALSH, Leiden Observatory, P.O. Box 9513, NL-2300 RA Leiden, The Netherlands.

RE05  15 min  9:56
SPECTROSCOPY FOR HOT SUPER-EARTH EXOPLANETS
P.F. BERNATH and M. DULICK, Department of Chemistry & Biochemistry, Old Dominion University, 4541 Hampton Boulevard, Norfolk, VA, 23529-0126, USA.

Intermission

RE06  10 min  10:30
SPECTROSCOPIC STUDY OF CYANOACETYLENE CATION: SLOW PHOTO-ELECTRON SPECTROSCOPY AND AB-INITIO INVESTIGATIONS
AHMED MAHJOUB, MARTIN SCHWELL, YVES BENILAN, NICOLAS FRAY and MARIE-CLAUDE GAZEAU, LISA UMR CNRS 7583, Univ. Paris Est Creteil & Univ. Paris Diderot, Institut Pierre Simon Laplace, 61 Ave du General de Gaulle, 94010, Creteil, France; GUSTAVO A. GARCIA and FRANCOIS GAIE-LEVERL, Synchrotron SOLEIL, LaAZOrme des Merisiers, St.Aubin, B.P. 48, 91192, Gif-sur-Yvette Cedex, France; NORBERT CHAMPION and SYDNEY LEACH, LERMA UMR CNRS 8112, Observatoire de Paris-Meudon, 5 place Jules-Jansen, 92195, Meudon, France.
THE $\nu_{12} + \nu_6 - \nu_5$ AND $\nu_{11} - \nu_{12}$ BANDS OF $^{12}$CH$_3$$^1$CH$_3$: A FREQUENCY ANALYSIS INCLUDING DATA FROM THE FOUR LOWEST VIBRATIONAL STATES

N. MOAZZEN-AHMADI, J. NOROOZOLIAEIE, Department of Physics and Astronomy, University of Calgary, 2500 University Dr., N.W., Calgary, Alberta T2N 1N4, Canada; V.-M. HÖRNEMAN, Department of Physical Sciences, University of Oulu, P.O. Box 3000, FI-90014 Oulu, Finland.

IDENTIFICATION OF PROTONATED PYRENE (1-C$_{16}$H$_{11}^+$) AND ITS NEUTRAL COUNTERPART ISOLATED IN SOLID PARA-HYDROGEN

MOHAMED BAHOU, Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu 30010, Taiwan; YU-JONG WU, National Synchrotron Radiation Research Center, 101 Hsin-Ann Road, Hsinchu Science Park, Hsinchu 30076, Taiwan; YUN-PERN LEE, Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu 30010, Taiwan and Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan.

VIBRONIC SPECTROSCOPY OF A STRUCTURAL ISOMER OF QUINOLINE: (2)-PHENYLVINYLNNITRILE

DEEPAK N. MEHTA-HURT, JOSEPH A. KORN, and TIMOTHY S. ZWIER, Department of Chemistry, Purdue University, West Lafayette, IN 47907-2084 U.S.A.

HIGH RESOLUTION INFRARED SPECTRA OF PLASMA JET-COOLED DI- AND TRIACETYLENE IN THE C-H STRETCH REGION BY CW CAVITY RING-DOWN SPECTROSCOPY

D. ZHAO, J. GUSS, A. WALSH, K. DONEY, H. LINNARTZ, Sackler Laboratory for Astrophysics, Leiden Observatory, University of Leiden, P.O. Box 9513, NL-2300 RA Leiden, the Netherlands.

RF. ASTRONOMICAL SPECIES AND PROCESSES
THURSDAY, JUNE 20, 2013 – 1:30 PM
Room: 160 MATH ANNEX

Chair: NICK INDRILOLO, Johns Hopkins University, Baltimore, MD

DISTRIBUTION OF SO$_2$ AND SO IN THE ENVELOPE OF VY-CANIS MAJORIS: INSIGHT INTO CIRCUM-STELLAR SULFUR CHEMISTRY

GILLES ADANDE, L.M. ZIURYS, Department of Chemistry, Steward Observatory University of Arizona, Tucson, 85721.

S. BRÜNKEN, H.S.P. MÜLLER, I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany; T. KAMIŃSKI, K.M. MENTEN, Max-Planck Institut für Radioastronomie, 53121 Bonn, Germany; C.A. GOTT-LIEB, N.A. PATEL, K.H. YOUNG, M.C. McCARTHY, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 02138, USA; J.M. WINTERS, Institut de Radioastronomie Millimétrique, 38406 Saint-Martin d’Hères, France; L. DECIN, Instituut voor Sterrenkunde, Katholieke Universiteit Leuven, 3001 Leuven, Belgium, and Sterrenkundig Instituut Anton Pannekoek, University of Amsterdam, 1098 Amsterdam, The Netherlands.
RF03  15 min  2:04
TRANSITION-METAL OXIDES IN WARM CIRCUM-STELLAR ENVIRONMENTS

MIROSŁAW R. SCHMIDT, N. Copernicus Astronomical Center, Department of Astrophysics, PL-87-100 Toruń, ul. Rabańską 8, Poland; TOMASZ KAMIŃSKI, Max Planck Institut für Radioastronomie, Auf dem Hügel 69, 53121 Bonn, Germany; and ROMUALD TYLENDLA, N. Copernicus Astronomical Center, Department of Astrophysics, PL-87-100 Toruń, ul. Rabańską 8, Poland.

RF04  15 min  2:21
OBSERVATIONS AND ANALYSIS OF EXTENDED TAIL TOWARD RED IN THE DIFFUSE INTERSTELLAR BANDS OF HERSCHEL 36

TAKESHI OKA, Department of Astronomy and Astrophysics, University of Chicago, Chicago, IL 60637; DANIEL E. WELTY, SEAN JOHN-SON, DONALD G. YORK, LEW M. HOBBS, Department of Physics and Astronomy, Carthage College, Kenosha, WI 53140; and JULIE DAHLSTROM.

RF05  15 min  2:38
MULTI-RESOLUTION STUDIES OF COMPLEX MOLECULES IN HIGH MASS STAR FORMING REGIONS

DOUGLAS N. FREDEL, Department of Astronomy, University of Illinois, 1002 W. Green St., Urbana, IL 61801.

RF06  15 min  2:55
IONIZATION OF H₂ BY X-RAYS IN THE CENTRAL MOLECULAR ZONE OF THE GALACTIC CENTER

MASAHIRO NOTANI and TAKESHI OKA, Department of Astronomy and Astrophysics and Department of Chemistry, the Enrico Fermi Institute, the University of Chicago, Chicago, Illinois, 60637, USA.

RF07  15 min  3:12
CARMA OBSERVATIONS OF PAH RICH SOURCES: NGC 2023, L134N AND GGD 27

P. BRANDON CARROLL, BRETT A. MCguire, Department of Chemistry, California Institute of Technology, Pasadena CA, 91125; GEOFFREY A. BLAKE, Divisions of Geological and Planetary Sciences and Chemistry and Chemical Engineering, California Institute of Technology, Pasadena CA, 91125.

RF08  15 min  3:29
A SEARCH FOR HCO⁺ AND HCN EMISSION IN PLANETARY NEBULAE

DEBORAH R. SCHMIDT, Department of Astronomy, Steward Observatory, The University of Arizona, Tucson, AZ 85721; and LUCY M. ZHU, Department of Chemistry and Biochemistry, Department of Astronomy, Steward Observatory, The University of Arizona, Tucson, AZ 85721.

Intermission

RF09  15 min  4:00
IDENTIFICATION AND ASSIGNMENT OF THE FIRST_excITED TORSIONAL STATE OF CH₂DOH WITHIN THE a₂, e₂, AND a₃ TORSIONAL LEVELS

JOHN C. PEARSON, SHANSHAN YU, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr., Pasadena, CA 91109, USA; L. H. COUDERT, LISA, CNRS/Universités Paris Est et Paris Diderot, 61 Avenue du Général de Gaulle, 94010 Créteil, France; L. MARGULÉS, R. A. MOTYENKO, Laboratoire PhLAM, UMR 8523 CNRS, Bât. P5, Université des Sciences et Technologies de Lille 1, 59655 Villeneuve d’Ascq Cedex, France; and S. KLEE, Physikalisch-Chemisches Institut, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany.

RF10  15 min  4:17
ANALYSIS OF THE ROTATION-TORSION SPECTRUM OF CH₂DOH WITHIN THE e₀, e₁, AND a₁ TORSIONAL LEVELS

L. H. COUDERT, LISA, CNRS/Universités Paris Est et Paris Diderot, 61 Avenue du Général de Gaulle, 94010 Créteil, France; JOHN C. PEARSON, SHANSHAN YU, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr., Pasadena, CA 91109, USA; L. MARGULÉS, R. A. MOTYENKO, Laboratoire PhLAM, UMR 8523 CNRS, Bât. P5, Université des Sciences et Technologies de Lille 1, 59655 Villeneuve d’Ascq Cedex, France; and S. KLEE, Physikalisch-Chemisches Institut, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany.

RF11  15 min  4:34
A GLOBAL FIT OF THE X⁺II, A⁺²Σ⁺, B⁺²Σ⁺ AND C⁺²Σ⁺ STATES OF SIX OH ISOTOPOLOGUES

SHANSHAN YU, JOHN C. PEARSON AND BRIAN J. DROUIN, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109.
RF12  15 min  4:51
MICROWAVE SPECTROSCOPY OF TRANS-ETHYL METHYL ETHER IN THE GROUND STATE
KAORI KOBAYASHI, YUSUKE SAKAI, SHOZO TSUNEKAWA, Department of Physics, University of Toyama, 3190 Gofuku, Toyama, 930-8555 Japan; TAIHEI MIYAMOTO, MASAHARU FUJITAKE and NOBUKIMI OHASHI, Kanazawa University, Japan.

RF13  15 min  5:08
JET-COOLED EXCITATION SPECTRA OF LARGE BENZANNULATED BENZYL RADICALS: 9-ANTHRACYL METHYL (C_{12}H_{11}) and 1-PYRENYL METHYL (C_{17}H_{11})
GERARD D. O’CONNOR, GEORGE B. BACSKAY, GABRIELLE V.G. WOODHOUSE, TYLER P. TROY, KLAAS NAUTA, SCOTT H. KABLE and TIMOTHY W. SCHMIDT, School of Chemistry, The University of Sydney, NSW 2006, Australia.

RF14  15 min  5:25
ROTATIONAL STRUCTURE OF THE IR/FIR BANDS OF SMALL PAHS
O. PIRALIa, S. GRUETa, M. VERVLOET, Ligne AILES, Synchrotron SOLEIL, L’Orme des Merisiers Saint-Aubin, 91192 Gif sur Yvette Cedex - France; M. GOUDET, T. R. HUET, Laboratoire de Physique des Lasers, Atomes et Molécules, UMR 8523 CNRS - Université Lille 1, Bâtiment P5, F-59655 Villeneuve d’Ascq Cedex, France; R. GEORGES, Université de Rennes 1, Institut de Physique de Rennes, CNRS, UMR 6251, F-35042 Rennes Cedex, France; P. SOULARD, P. ASSelin, UPMC Université Paris 06, UMR 7075 CNRS, Laboratoire de Dynamique, Interactions et Réactivité (LADIR), F-75005, Paris, France.

aAlso at: Institut des Sciences Moléculaires d’Orsay, UMR 8214 CNRS-Université Paris-Sud, Bât. 210, 91405 Orsay cedex, France.

RF15  15 min  5:42
SYNCHROTRON-BASED HIGHEST RESOLUTION FTIR SPECTROSCOPY OF AZULENE, NAPHTHALENE (C_{10}H_{16}), INDOLE (C_{9}H_{11}N) AND BIPHENYL (C_{12}H_{10})
S. ALBERT, M. QUACK, PHYSICAL CHEMISTRY, ETH ZURICH, CH-8093 ZURICH, SWITZERLAND; PH. LERCH, SWISS LIGHT SOURCE, PAUL-SCHERRER-INSTITUTE, CH-5232 VILLENEN, SWITZERLAND.

RF16  15 min  5:59
PHOTOGENERATION OF, AND EFFICIENT COLLISIONAL ENERGY TRANSFER FROM, VIBRATIONALLY EXCITED HYDROGEN ISOCYANIDE (HNC)
MICHAEL J. WILHELM, Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104; and HAI-LUNG DAI, Department of Chemistry, Temple University, Philadelphia, PA 19122.

"Present Address: Department of Chemistry, Temple University, Philadelphia, PA 19122

RG. THEORY
THURSDAY, JUNE 20, 2013 – 1:30 PM
Room: 170 MATH ANNEX

Chair: SO HIRATA, University of Illinois, Urbana, IL

RG01  15 min  1:30
SYMMETRY, DEGENERACY, AND STATISTICAL WEIGHTS OF H_{2}^{+}
KYLE N. CRABTREE, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, 02138; BENJAMIN J. MCCALL, Departments of Chemistry, Astronomy, and Physics, University of Illinois, Urbana, IL, 61801.
RG02 15 min 1:47
INVESTIGATION OF LARGE-AMPLITUDE MOTIONS OF H₂⁺ AND THE DYNAMICS OF THE PROTON TRANSFER BETWEEN H₂⁺ AND H₂

ZHOU LIN and ANNE B. McCOY, Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH 43210.

RG03 10 min 2:04
EINSTEIN A COEFFICIENTS FOR VIBRATION-ROTATIONAL TRANSITIONS OF NO

M. GUTIÉRREZ, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA 30332, USA; J. F. OGISLIE, Escuela de Química and CELEQ, Universidad de Costa Rica, San José 2060, Costa Rica.

RG04 15 min 2:16
OZONE PHOTOLYSIS: STRONG ISOTOPOMER SELECTIVITY IN THE STRATOSPHERE

FABIEN GATTI, CTMM Institut Charles Gerhardt UMR-CNRS 5253 University of Montpellier, France; STEVE NDENGUE, REMY JOST, Univ. Grenoble 1 / CNRS, LIPhy UMR 5588, Grenoble, F-38041, France; GABOR HALASZ, AGNES VIBOK, Department of Information Technology, University of Debrecen, P.O. Box 12, H-4010 Debrecen, Hungary.

RG05 15 min 2:33
LINE SHAPE PARAMETERS FOR CO₂ TRANSITIONS: ACCURATE PREDICTIONS FROM COMPLEX ROBERT-BONAMY CALCULATIONS

JULIEN LAMOURoux AND ROBERT R. GAMACHE, Department of Environmental, Earth, and Atmospheric Sciences, University of Massachusetts Lowell, Lowell, MA 01854, USA.

RG06 15 min 2:50
AB INITIO CLASSICAL DYNAMICS SIMULATIONS OF CO₂ LINE-MIXING EFFECTS IN INFRARED BANDS

JULIEN LAMOURoux*, JEAN-MICHEL HARTMANN, HA TRAN, Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA, CNRS UMR 7583), Université Paris-est Créteil, Université Paris Diderot, Institut Pierre-Simon Laplace, 94010 Créteil Cedex, France; MARCEL SNELS, ISAC-CNRS, Via del Fosso del Cavaliere, 100 00153 Rome, Italy; STEFANIA STEFANI and GIUSEPPE PICCIONI, IAPS-JASF, Via del Fosso del Cavaliere, 100 00153 Rome, Italy.

*Support by the French Agence Nationale de la Recherche (ANR) is gratefully acknowledged.

RG07 15 min 3:07
TOWARDS EXPERIMENTAL ACCURACY FROM THE FIRST PRINCIPLES

O.L. POLYANSKY, L. LODI, J. TENNYSON, Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK; N.F. ZOBOV, Institute of Applied Physics, Russian Academy of Sciences, 46 Uljanov St., 603950, Nizhny Novgorod, Russia.

RG08 15 min 3:24
HOW MANY VIBRATIONAL LEVELS DOES THE GROUND ELECTRONIC STATE OF THE SODIUM DIMER SUPPORT?

PHOTOS G. HAJI-GEORGIOU, Department of Life and Health Sciences, University of Nicosia, Nicosia 1080, Cyprus.

Intermission

RG09 15 min 4:00
RESONANCE AND REVOLVS IN QUANTUM ROTORS: COMPARING HALF-INTEGER SPIN AND INTEGER SPIN

ALVASON ZHENHUA LI and WILLIAM G. HARter, Microelectronics-Photonics Program, Department of Physics, University of Arkansas, Fayetteville, AR 72701.

RG10 15 min 4:17
EFFECTS OF SUPERFINE STRUCTURE LEVEL-CLUSTER CROSSING ON AMPLITUDE AND PHASE REVIVAL DYNAMICS: COMPARING TETRAHEDRAL AND OCTAHEDRAL SPHERICAL ROTORS WITH ICOSAHEDRAL ROTORS

WILLIAM G. HARTER and ALVASON ZHENHUA LI, Department of Physics, University of Arkansas, Fayetteville, AR 72701.

RG11 15 min 4:34
EXACT QUANTUM DYNAMICS CALCULATIONS USING PHASE SPACE WAVELETS

THOMAS HALVERSON, BILL POIRIER, Department of Chemistry and Biochemistry, and Department of Physics, Texas Tech University, P.O. Box 41061, Lubbock TX, USA.

RG12 15 min 4:51
ACHIEVING THE COMPLETE-BASIS LIMIT IN LARGE MOLECULAR CLUSTERS: COMputationally EFFICIENT PROCEDURES TO ELIMINATE BASIS-SET SUPERPOSITION ERROR

RYAN M. RICHARD, JOHN M. HERBERT, Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH 43210.
RG13
15 min 5:08
VIBRATIONAL ANALYSIS ON I(H₂O)⁻ AND I(D₂O)⁻ SPECTRA

MENG HUANG and ANNE B. McCLOY, Department of Chemistry, The Ohio State University, Columbus, Ohio 43210.

RG14
10 min 5:25
AB-INITIO STUDY OF THE GROUP 2 HYDRIDE ANIONS

JOE P. HARRIS, TIMOTHY G. WRIGHT and DANIEL R. MANSHP, School of Chemistry, University Park, University of Nottingham, NG7 2RD, United Kingdom.

RH. DYNAMICS
THURSDAY, JUNE 20, 2013 – 1:30 PM
Room: 1000 MCPHERSON LAB

Chair: GEOFFREY DUXBURY, University of Strathclyde, Bearsden, United Kingdom

RH01 15 min 1:30
TORSION-INVERSION TUNNELING PATTERNS IN THE CH-STRETCH VIBRationally EXCITED STATES OF THE G₁₂ MOLECULES

MAHESH B. DAWADI, RAM S. BHATTA and DAVID S. PERRY, Department of Chemistry, The University of Akron, Akron OH, 44325.

RH02 15 min 1:47
COUPLING OF THE C-H STRETCH TO LARGE-AMPLITUDE TORSION AND INVERSION MOTIONS: COMPARISON OF CH₂CH₂, CH₃OH⁺ AND CH₂NH₂

RAM S. BHATTA, Department of Polymer Science and Department of Chemistry, The University of Akron; DAVID S. PERRY, Department of Chemistry, The University of Akron, OH 44325.

RH03 15 min 2:04
HYDROGEN ABSTRACTION FROM METHANE BY BROMINE AND CHLORINE RADICALS: A DYNAMICS COMPARISON

ANDREW E. BERKE, ETHAN H. VOLPA, F. FLEMING CRIM, Chemistry Department, University of Wisconsin - Madison, Madison, Wisconsin 53706.

RH04 15 min 2:21
A NEW APPROACH TOWARD TRANSITION STATE SPECTROSCOPY

KIRILL PROZUMENT, RACHEL G. SHAVER, MONIKA A. CIUBA, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139; JOHN S. MUENTER, Department of Chemistry, University of Rochester, Rochester, NY 14627; G. BARRATT PARK, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139; JOHN F. STANTON, Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, TX 78712; HUA GUO, Department of Chemistry, University of New Mexico, Albuquerque, NM 87131; BRYAN M. WONG, Materials Chemistry Department, Sandia National Laboratories, Livermore, CA 94550; DAVID S. PERRY, Department of Chemistry, The University of Akron, Akron, OH 44325; ROBERT W. FIELD, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139.
RH05  15 min  2:38
PHOTODISSOCIATION DYNAMICS OF VINYL CYANIDE STUDIED BY CHIRPED-PULSE MILLIMETER-WAVE SPECTROSCOPY OF HCN AND HNC PRODUCTS

KIRILL PROZUMENT, RACHEL G. SHAVER, JOSHUA H. BARABAN, G. BARRATT PARK, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139; ARTHUR G. SUITS, Department of Chemistry, Wayne State University, Detroit, MI 48202; JOHN S. MUENTER, Department of Chemistry, University of Rochester, Rochester, NY 14627; ROBERT W. FIELD, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139.

RH06  15 min  2:55
ENERGY TRANSFER AND LASING OF THE LOWER Ar(3p^3/2) STATES IN Ar AND He

JIANGE HAN and MICHAEL C. HEAVEN, Department of Chemistry, Emory University, Atlanta, GA 30322.

RH07  15 min  3:12
GRAVITATION WAVE AND GRAVITATIONAL-PHOTON INTERACTION

KHOLMURAD KHASANOVA, Lomonosov Moscow State University, Gas and Wave Dynamics Department, Moscow, Russia, 119991, GSP-1, 1 Leninskie Gory Str. Email: khohlkh@bk.ru.

Interruption

RH08  15 min  3:45
PROBING CHEMICAL DYNAMICS WITH HIGH RESOLUTION SPECTROSCOPY: CHIRPED-PULSE FOURIER-TRANSFORM MICROWAVE SPECTROSCOPY COUPLED WITH A HYPERTHERMAL SOURCE

NATHANIEL M. KIDWELL, VANESA VAQUERO VARGAS, DEEPAK N. MEHTA-HURT, JOSEPH A. CORN, BRIAN C. DIAMOND, and TIMOTHY S. ZWIER, Department of Chemistry, Purdue University, West Lafayette, IN 47907-2084.

RH09  15 min  4:02
J-SPECIFIC DYNAMICS IN AN OPTICAL CEN- TRIFUGE USING TRANSIENT IR SPECTROSCOPY

MATTHEW J. MURRAY, QINGNAN LIU, CARLOS TORO and AMY S. MULLIN, Department of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742.

RH10  15 min  4:19
OBSERVATION OF NEW DYNAMICS IN THE STATE-RESOLVED COLLISIONAL RELAXATION OF HIGHLY EXCITED MOLECULES

GERALDINE O. ECHERI, MATTHEW SMARTE, WENDELL W. WALTERS, JILL M. CLEVELAND, CHRISTINE MCCARTY, ALICE KUNIN and AMY S. MULLIN, Department of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742.

RH11  10 min  4:36
TIME RESOLVED INFRARED EMISSION FROM VIBRATIONAL EXCITED ACETYLENE FOLLOWING SUPER ENERGY TRANSFER COLLISIONS WITH HOT HYDROGEN

J. M. SMITH, M. NIKOW, J. MA and H. L. DAI, Department of Chemistry, Temple University, Philadelphia, Pennsylvania 19122, USA.

RH12  15 min  4:48
TIME-RESOLVED IR-IR DOUBLE RESONANCE FOR THE $\nu_4$ AND $2\nu_4 - \nu_4$ VIBRATION-ROTATION TRANSITIONS OF CHF

YUSUKE OKABAYASHI, JIAN TANG, YUKI MIYAMOTO, KENTAROU KAWAGUCHI, Graduate School of Natural Science and Technology, Okayama University, 3-1-1 Tsushima-Naka, Okayama 700-8530, Japan.

RH13  15 min  5:05
VIBRATIONAL ENERGY RELAXATION OF CHLOOROIODOMETHANE IN COLD ARGON

AMBER JAIN and EDWIN L. SIBERT III, Department of Chemistry and Theoretical Chemistry Institute, University of Wisconsin-Madison, WI 53706.

RH14  15 min  5:22
DETERMINATION OF DIFFERENTIAL CROSS SECTIONS OF THE STATE-TO-STATE INELASTIC COLLISIONS IN BULBS. A THREE-DIMENSIONAL SLICED FLUORESCENCE IMAGING STUDY

KUO-MEI CHEN, Department of Chemistry, National Sun Yat-sen University, Kaohsiung, Taiwan, Republic of China.

RH15  15 min  5:39
ION IMAGING STUDIES OF CH$_4$$_2$ PHOTODISSOCIATION AT 248 NM

JULIA H. LEHMAN, HONGWEI LI and MARSHA I. LESTER, Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323.
RI. ATMOSPHERIC SPECIES
THURSDAY, JUNE 20, 2013 – 1:30 PM
Room: 1015 MCPHERSON LAB

Chair: YEN-CHU HSU, Academia Sinica, Taipei, Taiwan

RI01 15 min 1:30
HITRAN2012: DOWN TO EARTH

L E GORDON, L. S. ROTHMAN, G. LI,
Harvard-Smithsonian Center for Astrophysics,
Atomic and Molecular Physics Division, Cambridge MA 02138-1516, USA.

RI02 15 min 1:47
CAVITY-ENHANCED, FREQUENCY-AGILE RAPID
SCANNING (FARS) SPECTROSCOPY: MEASURE-
MENT PRINCIPLES

JOSEPH T. HODGES, DAVID A. LONG, GAR-
WING TRUONG, KEVIN O. DOUGLASS,
STEPHEN E. MAXWELL, ROGER VAN ZEE,
and DAVID F. PLUSQUELLIC, National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, MD 20899, USA.

RI03 15 min 2:04
CAVITY-ENHANCED, FREQUENCY-AGILE RAPID
SCANNING (FARS) SPECTROSCOPY: EXPERIMENTAL REALIZATIONS AND MEASUREMENT RESULTS

DAVID A. LONG, GAR-WING TRUONG,
ROGER VAN ZEE, DAVID F. PLUSQUELLIC,
and JOSEPH T. HODGES, National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, MD 20899, USA.

RI04 15 min 2:21
PERFORMANCE OF A CRYOGENIC 21 METER-PATH COPPER HERIOTT CELL VACUUM COUPLED TO A BRUKER 125HR SYSTEM

ARLAN W. MANTZ, Dept. of Physics,
Connecticut College, New London, CT 06320;
KEEYOON SUNG, TIMOTHY J. CRAWFORD,
SHANSHAN YU, LINDA R. BROWN, Jet
Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr., Pasadena, CA 91109; MARY ANN H. SMITH, Science Direc-
torate, NASA Langley Research Center, Hampton, VA 23681; V. MALATHY DEVI, D. CHRIS
BENNER, Dept. of Physics, The College of William and Mary, Williamsburg, VA 23187.

RI05 15 min 2:38
FREQUENCY-COMB REFERENCED, SUB-DOPPLER SPECTROSCOPY OF HOT BANDS OF ACETYLENE IN THE REGION OF THE ν1 + ν3 COMBINATION BAND

CHRISTOPHER P. MCRAVEN, Chemistry De-
partment, Brookhaven National Laboratory, Up-
ton, New York 11973; MATTHEW J. CICH,
SALVATORE M. CAIOLA, Department of Chem-
istry, Stony Brook University, Stony Brook,
New York 11794; TREvor J. SEARS, Chem-
istry Department, Brookhaven National Labora-
tory, Upton, New York 11973; GREGORY E.
HALL, Chemistry Department, Brookhaven Na-
tional Laboratory, Upton, New York 11973.

RI06 15 min 2:55
DIAGNOSTIC CHEMICAL ANALYSIS OF EX-
HALED HUMAN BREATH USING A NOVEL SUB-
MILLIMETER/TERAHERTZ SPECTROSCOPIC AP-
PROACH

ALYSSA M. FOSNIGHT, BENJAMIN L.
MORAN, DANIELA R. BRANCO, JESSICA R.
THOMAS, IVAN R. MEDVEDEV, Department of Physics, Wright State University, 3640 Colonel Glenn Highway, Dayton, OH 45435, USA.

RI07 15 min 3:12
TERAHERTZ CHEMICAL ANALYSIS OF EXHALED HUMAN BREATH - BROAD ESSAY OF CHEMICALS

DANIELA R. BRANCO, ALYSSA M. FOS-
NIGHT, JESSICA R. THOMAS, IVAN R.
MEDVEDEV, Department of Physics, Wright State University, 3640 Colonel Glenn Highway,
Dayton, OH 45435, USA.

Intermission
RI08  15 min  3:45
SF6: THE FORBIDDEN BAND UNVEILED

V. Boudon, Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR 6303 CNRS-Université de Bourgogne, 9 Av. A. Savary, BP 47870, F-21078 Dijon Cedex, France; L. Manceron, Laboratoire de Dynamique, Interactions et Réactivité, CNRS UMR 7075, 4 Place Jussieu, F-75252 Paris Cedex, France; F. Kwabia-Tchana, Laboratoire Interuniversitaire des Systèmes Atmosphériques, UMR CNRS 7653, Université Paris-Est Créteil et Université Paris-Diderot, 61 Avenue du Général de Gaulle, 94010 Créteil Cedex, France; P. Roy, Ligne AILES - Synchrotron SOLEIL, L’Orme des Merisiers, F-91120 Gif-sur-Yvette, France.

RI09  15 min  4:02
FREQUENCY ANALYSIS OF THE 10 μm REGION OF THE ETHYLENE SPECTRUM USING THE D2h TOP DATA SYSTEM.

M.-T. Bourgeois, M. Rotger, Groupe de Spectrométrie Moléculaire et Atmosphérique, CNRS UMR 7391, Université de Reims Champagne-Ardenne, Moulin de la Housse, B.P. 1039, Cases 16-17, F-51687 Reims Cedex, France; M. Tudorie, J. Vander Auwera, Service de Chimie Quantique et Photophysique, C.P. 160/09, Université Libre de Bruxelles, 50, avenue F. D. Roosevelt, B-1050 Brussels, Belgium; V. Boudon, Laboratoire Interdisciplinaire Carnot de Bourgogne, CNRS UMR 6303, Université de Bourgogne, 9, Avenue Alain Savary, BP 47870, F-21078 Dijon Cedex, France.

RI10  15 min  4:19
INFRARED ABSORPTION SPECTRUM OF THE SIMPLEST CRIEGEE INTERMEDIATE CH3OO

Yu-Te Su, Yu-Hsuan Huang, Henryk Witek, Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu 30010, Taiwan; Yuan-Pern Lee, Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu 30010, Taiwan and Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan.

RI11  15 min  4:36
POSSIBLE OBSERVATION OF THE 3A’ - 1A’ ELECTRONIC TRANSITION OF THE METHYLENE PEROXY CRIEGEE INTERMEDIATE

Neal D. Kline and Terry A. Miller, Laser Spectroscopy Facility, Department of Chemistry, The Ohio State University, 120 W. 18th Avenue, Columbus, Ohio 43210; Marc Coons and John Herbert, Department of Chemistry, The Ohio State University, Columbus, Ohio 43210.

RI12  15 min  4:53
UV SPECTRUM AND PHOTOCHEMISTRY OF THE SIMPLEST CRIEGEE INTERMEDIATE CH3OO

Joseph M. Beames, Fang Liu, Lu Lu, and Marsha I. Lester, Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323.

RI13  15 min  5:10
SPECTROSCOPIC CHARACTERIZATION OF AN ALKYL-SUBSTITUTED CRIEGEE INTERMEDIATE CH3CHO AND ITS OH RADICAL PRODUCTS

Joseph M. Beames, Fang Liu, Lu Lu and Marsha I. Lester, Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323.

RI14  15 min  5:27
RATE CONSTANTS AND DEUTERIUM ISO-ToPE EFFECTS FOR METHOXY RADICAL REACTING WITH NO2 AND O2


RI15  15 min  5:44
ABSOLUTE VUV PHOTOIONIZATION SPECTRA FOR HCHO, HO2, AND H2O2 FROM 10.5-120 eV

Leah G. Dodson*, Linhan Shen, Nathan C. Edgington*, Kana Take-Matsu, California Institute of Technology, Division of Chemistry and Chemical Engineering, Pasadena, CA; John D. Savee, Oliver Welz, Craig A. Taatjes, David L. Osborn, Sandia National Lab, Livermore, CA; Stanley P. Sander, Jet Propulsion Laboratory, Pasadena, CA; Mit-Chio Okumura, California Institute of Technology, Division of Chemistry and Chemical Engineering, Pasadena, CA.

*Support from the EPA STAR fellowship and NSF grant CHE-095749 are gratefully acknowledged.
*Present address: Rochester Institute of Technology, Rochester, NY

RI16  15 min  6:01
LABORATORY INVESTIGATION OF THE AIRGLOW BANDS

Brian Drovin, Shanshan Yu, Timothy J. Crawford, Charles E. Miller, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr., Pasadena, CA 91109; Jeng-Hwa Yee, Applied Physics Laboratory, The Johns Hopkins University, 11100, Johns Hopkins Rd, Laurel, MD 20723-6099.
RJ. INFRARED/RAMAN
THURSDAY, JUNE 20, 2013 – 1:30 PM
Room: 2015 MCPHERSON LAB

Chair: LAURA MCCUNN, Marshall University, Huntington, WV

**RJ01**
15 min 1:30

EXPERIMENTAL FT-IR, DISPERSIVE RAMAN AND THEORETICAL DFT CALCULATIONS ON Cu(II) CHLORIDE COMPLEX OF P-TOLUIDINE

TAYYIBE BARDAKCI, MUSTAFA KUMRU,
Department of Physics, Faculty of Arts and Sciences, Fatih University, 34500 Buğazceköy, İstanbul, Turkey.

**RJ02**
15 min 1:47

INFRARED SPECTROSCOPY OF PHENOL-TRIETHYLSILANE DIHYDROGEN-BONDED CLUSTER

HARUKI ISHIKAWA, TAKAYUKI KAWASAKI, Department of Chemistry, School of Science, Kitsato University, Minami-ku, Sagamihara 252-0373, Japan.

**RJ03**
10 min 2:04

A NEW, LOW TEMPERATURE LONG PATH CELL FOR MID-IR TO THz SPECTROSCOPY WITH SYNCHROTRON RADIATION AT SOLEIL

F. KWABIA TCHANA, F. WILLAERT, X. LAND-SHEERE, J.M. FLAUD, Laboratoire Interuniversitaire des Systèmes Atmosphérique (LISA), UMR CNRS 7583, Université Paris-Est Créteil (UPEC) et Université Paris-Diderot (UPD), 61 Avenue du Général de Gaulle, 94000 Créteil Cedex, France; L. LAGO, M. CHA-PUIS, P. ROY, Synchrotron SOLEIL, L’Orme des Merisiers Saint-Aubin, 91192 Gif-sur-Yvette, France; L. MANCERON, Laboratoire LADIR, UMR7073 CNRS, Université Pierre et Marie Curie, 75252 Paris Cedex, France.

**RJ04**
10 min 2:16

SYNCHROTRON BASED HIGH RESOLUTION FAR-IR SPECTROSCOPY OF 1,1-DICHLOROETHYLENE

REBECCA A. PEEBLES, LENA F. ELMUTI, and SEAN A. PEEBLES, Department of Chemistry, Eastern Illinois University, 600 Lincoln Ave., Charleston, IL 61920; DANIEL A. OBENCHAIN, Department of Chemistry, Wesleyan University, 52 Lawn Avenue, Middletown, CT 06459-0180.

**RJ05**
15 min 2:28

SYNCHROTRON-BASED STUDY OF THE FAR IR SPECTRUM OF SILACYCLOBUTANE: THE ν29 AND ν30 BANDS

ZIQU CHEN, CODY W. VAN DUK, SAMANTHA HARDER AND JENNIFER VAN Wijngaarden, Department of Chemistry, University of Manitoba, Winnipeg MB R3T 2N2 Canada.

**RJ06**
15 min 2:45

GAS PHASE VIBRATIONAL SPECTROSCOPY OF WEAKLY VOLATIL SAFETY TAGGANTS USING A SYNCHROTRON SOURCE

ARNAUD CUISSET, FRANCIS HINDLE, GAEI MOURET, Laboratoire de Physico-Chimie de l’Atmosphère, 189A Ave. Maurice Schumann, 59140 Dunkerque, France; SEBASTIEN GRUET, OLIVIER PIRALI, PASCALE ROY, Ligne AILES, synchrotron SOLEIL, L’Orme des Merisiers, Saint Aubin, BP 48, 91192 Gif-sur-Yvette, France.

**RJ07**
15 min 3:02

SYNCHROTRON BASED FOURIER TRANSFORM FAR-INFRARED SPECTROSCOPY OF CHNO2

SYLVESTRE TWAGIRAYEZU, BRANT E. BILLINGHURST AND TIM MAY, Canadian Light Source Inc., University of Saskatchewan, 44 Innovation Blvd, Saskatoon, SK S7N 2V3; MAHESH B. DAWADI, DAVID S. PERRY, Department of Chemistry, The University of Akron, Akron OH 44325.

**RJ08**
15 min 3:40

ISOLATION AND CHARACTERIZATION OF FORMATE/NI(CYCLAM)2+ COMPLEXES WITH CRYOGENIC ION VIBRATIONAL PREDISSOCIATION

ARRON B. WOLK, JOSEPH A. FOURNIER, CONRAD T. WOLKE, and MARK A. JOHN-SON, DEPARTMENT OF CHEMISTRY, YALE UNIVERSITY, NEW HAVEN, CT 06520.

Intermission
CHARACTERIZATION OF STRUCTURAL MOTIFS FOR CO₂ ACCOMMODATION BY IONIC SPECIES RELEVANT TO PHOTOELECTROCatalysis USING CRYOGENIC VIBRATIONAL PREDISSOCIATION SPECTROSCOPY

JOSEPH A. Fournier, Christopher J. Johnson, Conrad T. Wolke, Arron B. Wolk, Christopher M. Leavitt, Kristen J. Breen, and Mark A. Johnson, Department of Chemistry, Yale University, New Haven, CT 06520.

THZ SPECTROSCOPY AND DFT MODELING OF INTERMOLECULAR VIBRATIONS IN HYDROPHOBIC AMINO ACIDS

Michael R. C. Williams, Daniel J. Aschaffenburg, Charles A. Schmuttenmaer, Yale University, Department of Chemistry, P.O. Box 208107, 225 Prospect St., New Haven, CT 06520-8107. USA.

STRUCTURES AND THE HYDROGEN BONDING ABILITIES OF ESTROGENS STUDIED BY SUPERSONIC JET/LASER SPECTROSCOPY

Fumiya Morishima, Yoshiya Inokuchi, and Takayuki Ebata, Graduate School of Science, Hiroshima University 1-3-1, Kagamiyama, Higashi-Hiroshima 739-8526, JAPAN.

DEUTERATION EFFECT ON THE NH/ND STRETCH BAND OF THE JET-COOLED 7-AMINO-1-3-METHYLCYCLOPENTANONE CONFORMERS: A COMPUTATIONAL INVESTIGATION

Watheq Al-Basheer, Physics Department, King Fahd University of Petroleum and Minerals, Dhahran 31261 Saudi Arabia.

SPECTROSCOPY OF THE GROUND, FIRST AND SECOND EXCITED TORSIONAL STATES OF ACETALDEHYDE FROM 0.05 TO 1.6 THz.

Vadim V. Il’yushin, Ivan Smirnov, Eugene A. Alekseev, Institute of Radio Astronomy of NASU, Cheronograrna 4, 61002 Kharkov, Ukraine; Laurent Margulès, Roman A. Motiyenko, Laboratoire de Physique des Lasers, Atomes et Molécules, UMR 5233 CNRS-Université Lille 1, Bâtiment P5, F-59655 Villeneuve d’Ascq Cedex, France; Brian Droin, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Drive, Pasadena, CA 91109-8099, USA.

DEUTERATION EFFECT ON THE NH/ND STRETCH BAND OF THE JET-COOLED 7-AMINO-1-3-METHYLCYCLOPENTANONE CONFORMERS: A COMPUTATIONAL INVESTIGATION

Watheq Al-Basheer, Physics Department, King Fahd University of Petroleum and Minerals, Dhahran 31261 Saudi Arabia.

SPECTROSCOPY OF THE GROUND, FIRST AND SECOND EXCITED TORSIONAL STATES OF ACETALDEHYDE FROM 0.05 TO 1.6 THz.

Vadim V. Il’yushin, Ivan Smirnov, Eugene A. Alekseev, Institute of Radio Astronomy of NASU, Cheronograrna 4, 61002 Kharkov, Ukraine; Laurent Margulès, Roman A. Motiyenko, Laboratoire de Physique des Lasers, Atomes et Molécules, UMR 5233 CNRS-Université Lille 1, Bâtiment P5, F-59655 Villeneuve d’Ascq Cedex, France; Brian Droin, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Drive, Pasadena, CA 91109-8099, USA.

*Part of this work was done within the Ukranian-French CNRS-PICS 6051 project.
RK02
A SEMIEXPERIMENTAL EQUILIBRIUM STRUCTURE OF cis-HEXATRIENE FROM MICROWAVE SPECTROSCOPY
NORMAN C. CRAIG, YIHUI CHEN, HANNAH A. FUSON, HENGFENG TIAN, and HERMAN VAN BESIEN, Department of Chemistry and Biochemistry, Oberlin College, Oberlin, Ohio 44074; H. D. RUDOLPH, Department of Chemistry, University of Ulm, D-89069 Ulm, Germany. JEAN DEMAIN, Laboratoire de Physique des Lasers, Atomes et Molécules, Université de Lille I, 59655 Villeneuve d’Ascq Cedex, France.

RK03
ANALYSIS OF THE ROTATIONAL STRUCTURE IN THE HIGH-RESOLUTION INFRARED SPECTRA OF cis, cis- AND trans, trans-1,4-DIFLUOROBUTADIENE-1,4-d1 AND trans, trans-1,4-DIFLUOROBUTADIENE-1,4-d2
NORMAN C. CRAIG, YIHUI CHEN, YUHUA LU, CHRISTOPHER F. NEESE, and DEA-CON J. NEMCHICK, Department of Chemistry and Biochemistry, Oberlin College, Oberlin, OH 44074; THOMAS A. BLAKE, Pacific Northwest National Laboratory, Richland, WA 99352.

RK04
THE DELICATE BALANCE OF HYDROGEN BOND FORCES IN D-THREONINOL
D. ZHANG, VANESA VAQUERO VARA, BRIAN C. DIAM and TIMOTHY S. ZWIER, Department of Chemistry, Purdue University, West Lafayette, IN 47907; DAVID W. PRATT, Department of Chemistry, University of Vermont, Burlington VT 05405.

RK05
WAVEGUIDE CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF 2-ETHOXYETHANOL
MARIA A. PHILLIPS and STEVEN T. SHIPMAN, Division of Natural Sciences, New College of Florida, Sarasota, FL 34243.

RK06
WAVEGUIDE CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF 1-PROPAHETHOL
BRITTANY P. GORDON and STEVEN T. SHIPMAN, Division of Natural Sciences, New College of Florida, Sarasota, FL 34243.

RK07
ENERGY TRANSFER COLLISIONAL PROCESS INVOLVING HETEROMOLECULAR COLLISIONS BETWEEN METHYL FLUORIDE AND N2, Ar, He, CO2, AND AIR
DANE J. PHILLIPS, IERUS Technologies, 2904 Westcorp Blvd Ste 210, Huntsville, AL 35805; HENRY O. EVERITT, Army Aviation and Missle RD&E Center, Redstone Arsenal, AL 35898.

RK08
MILLIMETER WAVE TUNNELING-ROTATIONAL SPECTRUM OF PHENOL
L. KOLESNIKOVÁ, A. M. DAILY, J. L. ALONSO, Grupo de Espectroscopía Molecular (GEM), Edificio Química, Laboratorios de Espectroscopía y Bioespectroscopía, Parque Científico, Universidad de Valladolid, 47011 Valladolid, Spain; B. TERCERO, J. CERNICHARO, Departamento de Astrofísica, Centro de Astrobiología CAB, CSIC-INTA, Ctra. de Torrejón a Ajalvir km 4, 28850 Madrid, Spain.

Intermission

RK09
ROTATIONAL SPECTROSCOPY UNVEILS ELEVEN CONFORMERS OF ADRENALINE
C. CABEZAS, V. CORTÍJO, S. MATA, J. C. LÓPEZ, J. L. ALONSO Grupo de Espectroscopía Molecular (GEM), Edificio Química, Laboratorios de Espectroscopía y Bioespectroscopía, Parque Científico, Universidad de Valladolid, 47011 Valladolid, Spain.

RK10
PROBING THE TAUTOMERISM OF HISTIDINE
C. BERMÚDEZ, C. CABEZAS, S. MATA, J. L. ALONSO, Grupo de Espectroscopía Molecular (GEM), Edificio Química, Laboratorios de Espectroscopía y Bioespectroscopía, Parque Científico, Universidad de Valladolid, 47011 Valladolid, Spain.

RK11
DEUTERIUM QUADRUPOLE COUPLING IN PROPOLIC ACID AND FLUOROBENZENES MEASURED WITH FTMW SPECTROMETER USING MULTIPLE FIDS
MING SUN, BRYAN M. SAR-GUS, SPENCER J. CAREY and STEPHEN G. KUKOLICH, Department of Chemistry and Biochemistry, The University of Arizona, Tucson, Arizona 85721..

*Supported by THE NATIONAL SCIENCE FOUNDATION
RK12
15 min 4:26
MICROWAVE SPECTRA OF FLUORINATED PROPYLONIC ACIDS AND THEIR HYDRATES

DANIEL A. OBENCHAIN, G. S. GRUBBS II, STEWART E. NOVICK, Department of Chemistry, Wesleyan University, Middletown, CT 06459; STEPHEN A. COOKE, School of Natural and Social Sciences, Purchase College, SUNY, 735 Anderson Hill Road, Purchase, NY 10577; AGAPITO SERRATO III and WELIN, Department of Chemistry and Environmental Science, University of Texas at Brownsville, Brownsville, TX 78520.

RK13
10 min 4:43
MW SPECTROSCOPY COUPLED WITH ULTRAFAST UV LASER VAPORIZATION: SUCCINIC ACID IN THE GAS PHASE

ESTibaliz MendeZ, PatriCia eciJa, emilIo J. CoCinero, fernando castano, francisco J. BaSterretxema, Departamento de Quimica Física, Facultad de Ciencia y Tecnología, Universidad del País Vasco (UPV/EHU), Ap.614, E-48940, Bilbao, Spain; Peter D. Godfrey, don McNaughton, School of Chemistry, Box 23 Victoria 3800 Monash University, Australia; Michaela K. Jahn, K.P. RajAPPan NaIr, JenS-ueW grabow, Institut für Physikalische Chemie und Elektrochemie, Gottfried-Wilhelm-Leibniz-Universität, 30167 Hannover, Germany.

RK14
15 min 4:55
CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF 3-VINYL BENZALDEHYDE

Miranda Smith and Gordon G. brown, Department of Science and Mathematics, Coker College, 300 E College Ave., Hartsville, SC 29550.

RK15
10 min 5:12
CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF META-CHLOROBENZALDEHYDE

Sean T. Arnold, Jessica A. Garrett, and Gordon G. Brown, Department of Science and Mathematics, Coker College, 300 E College Ave., Hartsville, SC 29550.

RK16
15 min 5:24
ROTATIONAL SPECTRUM OF HEXAFLUOROISO-PROPANOL AND COMPARISON TO HEXAFLUOROISOBUTENE

Abhishek shahi, and E. Arunan, Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore, India-560012.

FA. ASTRONOMICAL SPECIES AND PROCESSES
FRIDAY, JUNE 21, 2013 – 8:30 AM
Room: 160 Math Annex

Chair: Kyle Crabtree, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA

PA01
15 min 8:30
THE PUBLICLY AVAILABLE PREBiotic INTER-STELLAR MOLECULAR SURVEY (PRIMOS): EXPANDING SPECTROSCOPIC CHARACTERIZATIONS, EXTENDING TO NEW SOURCES, AND ADDING TO THE KNOWN MOLECULAR INVENTORY

Brett A. mcguire, P. Brandon carroll, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125; Joanna F. corby, Department of Astronomy, University of Virginia, Charlottesville, VA 22904; Ryan A. loomis, Department of Chemistry, University of Virginia, Charlottesville, VA 22904; Geoffrey A. Blake, Division of Chemistry and Chemical Engineering and Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, CA 91125; Jan M. Hollis, NASA Goddard Space Flight Center, Greenbelt, MD 20771; Frank J. Lovas, National Institute of Standards and Technology, Gaithersburg, MD 20899; philip R. Jewel, and Anthony J.
FA02 15 min 8:47
THE IONIZATION TOWARD THE HIGH-MASS STAR-FORMING REGION NGC 6334 I

J. MORALES, University of Puerto Rico, Río Piedras Campus, Physics Department, San Juan, Puerto Rico 00931; C. CECCARELLI, Institut de Planétologie et d’Astrophysique de Grenoble (IPAG) UMR 5274, Grenoble, F-38041, France; L. OLMI, Osservatorio Astrofisico di Arcetri - INAF, Largo E. Fermi 5, I-50125, Firenze, Italy; D. LJS, California Institute of Technology, Pasadena, CA 91125, USA; R. PLUME, Department of Physics and Astronomy, University of Calgary, Calgary, AB T2N 1N4, Canada; P. SCHILKE, I. Physikalisches Institut der Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany.

FA03 15 min 9:04
ROTATIONAL SPECTRA OF ISOTOPIC CH$_3$CN IN THEIR $v_8 = 1$ EXCITED VIBRATIONAL STATES

HOLGER S. P. MÜLLER, I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany; B. J. DROUIN, J. C. PEARSON, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109, USA; A. BELLOCHE, K. M. MENTEN, Max-Planck Institut für Radioastronomie, 53121 Bonn, Germany.

FA04 15 min 9:21
THE FIRST EXTENSIVE MOLECULAR STUDY OF AN OXYGEN-RICH PLANETARY NEBULA: OBSERVATIONS OF SiO, SO$_2$, AND SO

JESSICA L EDWARDS, LUCY M. ZIURYS, Department of Chemistry and Biochemistry, Department of Astronomy, Steward Observatory, The University of Arizona, Tucson, AZ 85721.

FA05 15 min 9:38
MAPPING THE MOLECULAR OUTFLOWS OF THE HIGH EXCITATION RED SPIDER NEBULA (NGC 6537)

JESSICA L EDWARDS, LUCY M. ZIURYS, Department of Chemistry and Biochemistry, Department of Astronomy, Steward Observatory, The University of Arizona, Tucson, AZ 85721.

FA06 15 min 9:55
STRUCTURE OF THE DENSE MOLECULAR GAS IN THE HELIX NEBULA: LARGE SCALE MAPPING OF HCO$^+$

N. R. ZEIGLER, L. M. ZIURYS, Department of Chemistry, University of Arizona, PO Box 210041, 1306 East University Blvd, Tucson, AZ, 85721, USA; L. N. ZACK, Department of Chemistry, University of Basel, Klingelbergstrasse 80, CH-4066 Basel, Switzerland.

FA07 15 min 10:30
THE CM-, MM- AND SUBMM-WAVE SPECTRUM OF ALLYL ISOCYANIDE AND RADIOASTRONOMICAL OBSERVATIONS IN ORION KL AND THE PRIMOS LINE SURVEY

I. HAYAKAL, R. A. MOTIYENKO, L. MARIGÜLES, and T. R. HUET, Laboratoire PhLAM, UMR5233 CNRS-Université Lille 1, F-59655 Villeneuve d’Ascq Cedex, France; P. ECIJA, E. J. COCINERO, F. BASTERRTEXEA, J. A. FERNÁNDEZ, F. CASTANO, Departamento de Química Física, Facultad de Ciencia y Tecnología, Universidad del País Vasco, Barrio Sarriena s/n, 48940 Leioa (Spain); B. TERCERO, J. CERNICHARO, Centro de Astrobiología (CSIC-INTA). Ctra de Ajalvir, Km 4, 28850 Torrejón de Ardoz, Madrid, Spain; A. LESARRI, Departamento de Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, 47011 Valladolid (Spain); J. C. GUILLEMIN, Sciences Chimiques de Rennes -Ecole Nationale Supérieure de Chimie de Rennes-CNRS -35700 Rennes, France.

FA08 15 min 10:47
MILLIMETER-WAVE SPECTROSCOPY OF AMINO-MALONONITRILE

ROMANA MOTIYENKO, LAURENT MARIGÜLES, Laboratoire PhLAM, UMR 5233 CNRS - Université Lille 1, 59655 Villeneuve d’Ascq Cedex, France; JEAN-CLAUDE GUILLEMIN, Institut des Sciences Chimiques de Rennes, UMR 6226 CNRS - ENSCR, 35708 Rennes Cedex 7, France.

FA09 15 min 11:04
TORSION-ROTATION-VIBRATION EFFECTS IN THE $\nu_{20}$, $2\nu_{21}$, $2\nu_{13}$ AND $\nu_{21} + \nu_{13}$ STATES OF CH$_3$C$_2$N

ADAM M. DALY, JOHN C. PEARSON, SHANSHAN YU, BRIAN J. DROUIN, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr., Pasadena, CA 91109; C. BERMÚDEZ, J. L. ALONSO, Grupo de Espectroscopia Molecular (GEM), Edificio Químina, Laboratorios de Espectroscopia y Bi-espectroscopia, Parque Científico, Universidad de Valladolid, 47011 Valladolid, Spain.
FA10 15 min 11:21

MILLIMETER-WAVE SPECTRUM OF CARBONYL DIAZIDE IN PURSUIT OF DIAZIRINONE

BRENT K. AMBERGER, BRIAN J. ESSELMAN, R. CLAUDE WOODS and ROBERT J. McMAHON. The University of Wisconsin - Madison Department of Chemistry, 1101 University Avenue, Madison, WI 53705.

FA11 15 min 11:38

MILLIMETER-WAVE SPECTRUM OF PYRIDAZINE

BRENT K. AMBERGER, BRIAN J. ESSELMAN, JOSH D. SHUTTER, R. CLAUDE WOODS and ROBERT J. McMAHON, The University of Wisconsin - Madison Department of Chemistry, 1101 University Avenue, Madison, WI 53705.

FB. MINI-SYMPOSIUM: THEORY AND SPECTROSCOPY
FRIDAY, JUNE 21, 2013 – 8:30 AM

Room: 170 MATH ANNEX

Chair: STEPHEN COY, Massachusetts Institute of Technology, Cambridge, MA

FB01 INVITED TALK 30 min 8:30

ROTATIONAL SPECTROSCOPY MEETS THEORY

CRISTINA PUZZARINI, Dipartimento di Chimica "G. Ciamiciin" Università di Bologna, I-40126 Bologna, Italy.

FB02 15 min 9:05

ANALYSIS OF THE MICROWAVE SPECTRUM OF THE THREE-TOP MOLECULE TRIMETHOXYL METHANE

L. H. COUDEBERT, LISA, CNRS/Universit Ars Est et Paris Diderot, 61 Avenue du Général de Gaulle, 94010 Créteil, France; G. FENG, AND W. CAMINATI, Dipartimento di Chimica "G. Ciamician," Università di Bologna, Via F. Selmi, 40126 Bologna, Italy.

FB03 15 min 9:22

EXTENSION OF THE MEASUREMENT, ASSIGNMENT, AND FIT IN THE GROUND STATE OF THE TWO-TOP MOLECULE METHYL ACETATE

H. V. L. NGUYEN, I. KLEINER, Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA), UMR 7583 (CNRS/Univ. Paris Est et Paris Diderot), Université de Paris Est, 61 avenue du Général de Gaulle, F-94010 Créteil cedex, France; S. SHIPMAN, Division of Natural Sciences, New College of Florida, 5800 Bay Shore Road, Sarasota, FL 34243-2109, USA; and K. KOBAYASHI, Department of Physics, Faculty of Science, Toyama University, 3190 Go fuku Toyama, Toyama, 930-8555, Japan.

FB04 15 min 9:39

A FITTING PROGRAM FOR MOLECULES WITH TWO EQUIVALENT TOPS AND C2V POINT-GROUP SYMMETRY AT EQUILIBRIUM: APPLICATION TO EXISTING MICROWAVE, MILLIMETER, AND SUB-MILLIMETER SPECTROSCOPIC DATA OF ACETONE

VADIM V. ILYUSHIN, Institute of Radio Astronomy of NASU, Chernovoproporna 4, 61002 Kharkov, Ukraine. NIST Guest Worker June - August 2009.; JON T. HOUGEN, Sensor Science Division, National Institute of Standards and Technology, Gaithersburg, MD 20899-8441, USA.
FB05  15 min  9:56
GAS PHASE ROVIBRATIONAL SPECTROSCOPY OF DMSO. PART I: WHEN A SYNCHROTRON SOURCE REVEALS AN UNUSUAL ROTATIONAL BEHAVIOUR

ARNAUD CUISET, DMITRI A. SADOVSKII, Laboratoire de Physico-Chimie de l’Atmosphère, 189A Ave. Maurice Schumann, 59140 Dunkerque, France; OLIVIER PIRALI, Laboratoire de Physico-Chimie de l’Atmosphère, SOLEIL, L’Orne des Merisiers, Saint Aubin, BP 48, 91192 Gif-sur-Yvette, France.

FB06  15 min  10:13
GAS PHASE ROVIBRATIONAL SPECTROSCOPY OF DMSO. PART II: TOWARDS THE TERAHERTZ OBSERVATION OF 4-FOLD CLUSTERS

ARNAUD CUISET, MARIE-ALINE MARTIN-DRUMEL, FRANCIS HINDLE, GAEL MOURET, DMITRI A. SADOVSKII, Laboratoire de Physico-Chimie de l’Atmosphère, 189A Ave. Maurice Schumann, 59140 Dunkerque, France.

Intermission

FB07  15 min  10:45
WHAT IS THE NATURE OF THE DOUBLETS IN THE E-METHANOL LAMB-DIP SPECTRA?


FB08  15 min  11:02
ROTATIONAL SPECTROSCOPY AND QUANTUM CHEMICAL CALCULATIONS OF A FRUIT ESTER: THE MICROWAVE SPECTRUM OF n-BUTYL ACETATE


FB09  15 min  11:19
HIGH RESOLUTION THZ AND FIR SPECTROSCOPY OF SOCl₂

M. A. MARTIN-DRUMEL, A. CUISET, D. A. SADOVSKII, G. MOURET, F. HINDLE, Laboratoire de Physico-Chimie de l’Atmosphère, EA 4493, Université du Littoral Côte d’Opale, 59140 Dunkerque, France; O. PIRALI, Laboratoire de Sciences Moléculaires d’Orsay-CNRS, UMR 8214, Université Paris XI, bât. 310, 91405 Orsay Cedex, France; SOLEIL Synchrotron, AILES beamline, L’Orne des Merisiers, Saint-Aubin, 91192 Gif-Sur-Yvette, France.

FB10  15 min  11:36
STRUCTURE OF THE BENZENE DIMER—GOVERNED BY DYNAMICS

MELANIE SCHNELL, Center for Free-Electron Laser Science, 22761 Hamburg, Germany; Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany. UNDINE ERLEKAM, GERT VON HELDEN, GERARD MEIJER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany. PHILIP R. BUNKER, National Research Council of Canada, Ottawa, Ontario K1A 0R6, Canada; JENS-UWE GRABOW, Institut für Physikalische Chemie und Elektrochemie, Gottfried-Wilhelm-Leibniz-Universität, 30167 Hannover, Germany. AD VAN DER AVOIRD, Institute for Molecules and Materials, Radboud University, 6525 AJ Nijmegen, The Netherlands.

FB11  15 min  11:53
HOW TO CALCULATE SPIN-SPIN COUPLING AND SPIN-ROTATION COUPLING STRENGTHS AND THEIR UNCERTAINTIES FROM SPECTROSCOPIC DATA: APPLICATION TO THE (1Σ⁺(g)) STATE OF DIATOMIC LITHIUM

NIKESH S. DATTANI, Department of Chemistry, Oxford University, Oxford, OX1 3QZ, UK; XUAN LI, Chemical Science Division, Lawrence Berkeley National Laboratory, Berkeley, 94720-8176, USA.

FB12  Post-deadline 10 min  12:10
Abstract

VIBRATIONAL VS ELECTRONIC POLARIZABILITY AND FIRST HYPERPOLARIZABILITY OF SOME PUSH-PULL METAL PORPHYRINS

M. H. BEN ALI, Laboratoire de Chimie Théorique et Quantique, USTHB University, Algiers 16111, Algeria; A. SAAL, Department of Chemistry, USTHB University, Tizi-Ouzou 15000, Algeria; O. OUAMERI, Laboratoire de Chimie Théorique et Quantique, USTHB University, Algiers 16111, Algeria.
FC. MICROWAVE
FRIDAY, JUNE 21, 2013 – 8:30 AM
Room: 1000 MCPHERSON LAB

Chair: STEPHEN COOKE, Purchase College SUNY, Purchase, NY

FC01  15 min  8:30
FLUORINE SUBSTITUTION AND COMPLEXATION EFFECTS ON FLEXIBILITY AND TUNNELING PATHWAYS: THE ROTATIONAL SPECTRUM 2-FLUOROBENZYLAMINE AND BENZYLAMINE-WATER

S. MELANDRI, A. MARIS, C. CALABRESE, L EVANGELISTI AND W. CAMINATI, Dipartimento di Chimica Ciamiciac, Università di Bologna, via Selmi 2,40126 Bologna, Italy.

FC02  15 min  8:47
FTMW OBSERVATION AND ANALYSIS OF THE p-H2−AgCl AND ω-H2−AgCl COMPLEX

G. S. GRUBBS II, DANIEL A. OBENCHAIN, HERBERT M. PICKETT and STEWART E. NOVICK, Department of Chemistry, Wesleyan University, 52 Lawn Avenue, Middletown, CT, 06459-0180, USA (email to GSG2: ggrubbs@wesleyan.edu).

FC03  15 min  9:04
HYDROGEN INTERACTION WITH METAL HALIDES: THE NUCLEAR QUADRUPOLE COUPLING CONSTANT OF GOLD IN THE p-H2−AuCl COMPLEX AND TRENDS IN THE OTHER HYDROGEN-COINAGE METAL HALIDE INTERACTIONS

DANIEL A. OBENCHAIN, G. S. GRUBBS II, HERBERT M. PICKETT, and STEWART E. NOVICK, Department of Chemistry, Wesleyan University, 52 Lawn Avenue, Middletown, CT, 06459-0180, USA.

FC04  15 min  9:21
THE SUBMILLIMETER SPECTRUM OF NeO

JENNIFER A. HOLT, CHRISTOPHER F. NEESE, FRANK C. DE LUCIA, Microwave Laboratory, The Ohio State University, Columbus, Ohio 43210.

Intermission

FC05  15 min  10:00
THE ROTATIONAL SPECTRUM OF H2S: THE H2\textsuperscript{13}S ISOTOPOLOGUE AND THE SUB-DOPPLER RESOLUTION IN THE THz REGIME

GABRIELE CAZZOLI, CRISTINA PUZZARINI, Dipartimento di Chimica “G. Ciamiciac”, Università di Bologna, I-40126 Bologna, Italy.

FC06  15 min  10:17
EXAMINING PREBIOTIC CHEMISTRY USING O(31) INSERTION REACTIONS

BRIAN M. HAYS, JACOB C. LAAS, SUSANNA L. WIDICUS WEAVER, Emory University, Department of Chemistry, Atlanta, GA 30322.

FC07  15 min  10:34
LABORATORY DETECTION OF IZnCH\textsubscript{3} (X\textsuperscript{1}A\textsubscript{1}) : FURTHER EVIDENCE FOR ZINC INSERTION

MATTHEW P. BUCCHINO, Department of Chemistry and Biochemistry, University of Arizona, Tucson, Arizona 85721; JUSTIN P. YOUNG, Department of Chemistry, Canisius College, Buffalo, New York 14208; PHIL M. SHERIDAN, Department of Chemistry, Canisius College, Buffalo, New York 14208; and LUCY M. ZIURYS, Department of Chemistry and Biochemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, Arizona 85721.

FC08  15 min  10:51
FURTHER STUDIES OF POTASSIUM-BEARING MOLECULES: THE MILLIMETER-WAVE SPECTRUM OF KSH (X\textsuperscript{1}A\textsuperscript{′})

MATTHEW P. BUCCHINO, Department of Chemistry and Biochemistry, University of Arizona, Tucson, Arizona 85721; JUSTIN P. YOUNG, PHIL M. SHERIDAN and DAVID EWING, Department of Chemistry, Canisius College, Buffalo, New York 14208; LUCY M. ZIURYS, Department of Chemistry and Biochemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, Arizona 85721.

FC09  Post-deadline  15 min  11:08
Abstract

ROTATIONAL SPECTRUM OF PROPARGYL ALCOHOL DIMER

DEVENDRA MANI and E. ARUN, Department of Inorganic and Physical Chemistry, Indian Institute of Science Bangalore, India-560012.
FD. ELECTRONIC
FRIDAY, JUNE 21, 2013 – 8:30 AM
Room: 1015 MCPHERSON LAB

Chair: MOURAD ROUDJANE, The Ohio State University, Columbus, OH

FD01 15 min  8:30
A THEORETICAL STUDY OF CN SPECTROSCOPY FROM THE IR TO THE VUV

DAVID W. SCHWENKE, NASA Ames Research Center, Moffett Field, CA 94035.

FD02 15 min  8:47
LINE STRENGTHS IN THE FORM OF EINSTEIN A COEFFICIENTS AND OSCILLATOR STRENGTHS OF THE $\tilde{\nu} \Pi - \tilde{\chi} \Sigma^+$ (RED) AND $\tilde{\beta} \Sigma^+ - \tilde{\chi} \Sigma^+$ (VIOLET) SYSTEMS OF CN

R. S. RAM and J. S. A. BROOK, Department of Chemistry, University of York, York, Y010 5DD, UK; G. LI, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 02138, USA; D. W. SCHWENKE, NASA Ames Research Center, Moffett Field, CA 94035-1000, USA; P. F. BERNATH, Department of Chemistry and Biochemistry, Old Dominion University, Norfolk, VA 23529, USA.

FD03 15 min  9:04
ARGON-INDUCED PRESSURE BROADENING, SHIFTING, AND NARROWING IN THE CN $\tilde{\Lambda} \Pi - \tilde{\chi} \Sigma^+$ (1-0) BAND

D. FORTHOMMER, C. P. MCRAVEN, T. J. SEARS, G. E. HALL, Chemistry Department, Brookhaven National Laboratory, Bldg. 555A, P. O. Box 5000, Upton, NY 11973, USA.

FD04 10 min  9:21
LIFETIMES OF THE $\tilde{A}$ STATES OF Cs

YI-JEN WANG, CHIAO-WEI CHEN, LI-UZHU ZHOU, ANTHONY J. MERRER, YEN-CHU HSU, Institute of Atomic and Molecular Sciences, Academia Sinica, P. O. Box 23-166, Taipei 10617, Taiwan, R. O. C.

FD05 10 min  9:33
LIFETIMES OF THE $\tilde{A}$ STATES OF THE C$_2$-NE AND C$_2$-AR COMPLEXES

YI-JEN WANG, CHIAO-WEI CHEN, ANTHONY J. MERRER, YEN-CHU HSU, Institute of Atomic and Molecular Sciences, Academia Sinica, P. O. Box 23-166, Taipei 10617, Taiwan, R. O. C.

Intermission

FD06 15 min  10:00
QUASILINEAR EVIDENCE FOR THE EQUILIBRIUM STRUCTURE OF B$_2$OH

KYLE MASCARITIOLO, JEREMY M. MERIT, MICHAEL C. HEAVEN, Emory University, Department of Chemistry, Atlanta, GA 30322.

FD07 15 min  10:17
A MODEL OF ELECTRONICALLY-EXCITED STATES OF N$_2$ AND ITS EXTREME-ULTRAVIOLET SPECTRUM.

A. N. HEAYS, Leiden Observatory, Leiden University, P.O. Box 9513, 2300 RA Leiden, The Netherlands; B. R. LEWIS and S. T. GIBSON, Research School of Physics and Engineering, The Australian National University, Canberra, ACT 0200, Australia.

FD08 10 min  10:34
TWO-DIMENSIONAL SUBCICoseCOND TIME-RESOLVED FLUORESCENCE ANISOTROPY: OPTICAL KERR-GATING WITH A DYNAMIC POLARIZATION EXCITATION

TAKASHIGE FUJIMURA, Department of Chemistry and Biochemistry, The Ohio State University, Columbus OH 43210; NATALIE C. ROMANO, DAVID A. MODARELLI, and EDWARD C. LIM, Department of Chemistry and The Center for Laser and Optical Spectroscopy, The University of Akron, Akron OH 44325-3601.

FD09 15 min  10:46
THE ORIGIN OF ANOMALOUS ELECTRONIC CIRCULAR DICHROISM SPECTRA OF [RuP$_2$Cl$_2$(tpz)$_2Cl_2$]+ IN ACETONITRILE

H.-G. YU, Department of Chemistry, Brookhaven National Laboratory, Upton, NY 11973-5000, USA.

*This work was performed at the Brookhaven National Laboratory under Contract No. DE-AC02-98CH10886 with the U.S. Department of Energy and supported by its Division of Chemical Sciences, Office of Basic Energy Sciences, and also used the resource at NERSC.*
FD10  15 min  11:03

AB INITIO STUDY OF ION-PAIR STATES OF THE IODINE MOLECULE

VADIM A. ALEKSEEV. Institute of Physics, St. Petersburg State University, Uljanovskaja St. 1, Peterhof, 198504 St. Petersburg, Russia.

FD11  Post-deadline  15 min  11:20

Abstract

MEASURING THE ELECTRON ELECTRIC DIPOLE MOMENT USING YTERBIUM FLUORIDE MOLECULES


FD12  Post-deadline  15 min  11:37

Abstract

LASERCOOLED RaF AS A LABORATORY FOR TESTING FUNDAMENTAL SYMMETRIES

TIMUR ISAEV and ROBERT BERGER, Clemens-Schöpf Institute, Technical University of Darmstadt, 64287 Darmstadt, Germany.

FD13  Post-deadline  15 min  11:54

Abstract

PROSPECTS FOR FUNDAMENTAL SYMMETRY TESTS WITH POLYATOMIC MOLECULES

ROBERT BERGER and TIMUR ISAEV, Clemens-Schöpf Institute, Technical University of Darmstadt, 64287 Darmstadt, Germany.

FD14  Post-deadline  15 min  12:11

Abstract

ELECTRIC QUADRUPOLE TRANSITION MEASUREMENTS OF HYDROGEN MOLECULE WITH HIGH PRECISION

CUN-FENG CHENG, JIN WANG, YAN TAN, AN-WEN LIU, SHUI-MING HU, Hefei National Laboratory for Physical Science at Microscale, University of Science and Technology of China, Hefei 230026, China.

FD15  Post-deadline  15 min  12:28

Abstract

QCL- AND CO2 LASER-BASED MID-IR SPECTROMETERS FOR HIGH ACCURACY MOLECULAR SPECTROSCOPY


FD16  Post-deadline  15 min  12:45

Abstract

ACCURATE DETERMINATION OF THE BOLTZMANN CONSTANT BY DOPPLER SPECTROSCOPY TOWARDS A NEW DEFINITION OF THE KELVIN


FE. DYNAMICS

FRIDAY, JUNE 21, 2013 – 8:30 AM
Room: 2015 MCPPHERSON LAB

Chair: TERRY GUSTAFSON, The Ohio State University, Columbus, OH

FE01  15 min  8:30

CRYOGENIC ION VIBRATIONAL SPECTROSCOPY OF PT(II)-METHANE CH ACTIVATION INTERMEDIATES

BRETT MARSH, ETIENNE GARAND, Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706.

FE02  15 min  8:47

EXPERIMENTAL CHARACTERIZATION OF IDEALIZED METAL-CENTERED REACTIONS

DARRIN BELLERT, ADAM MANSELL, and ZACHARY THEIS, Department of Chemistry, Baylor University, Waco, TX 76798.
FE03  15 min  9:04
UTILIZING METAL TO LIGAND CHARGE TRANSFER STATES OF MM QUADRUPLY BONDED COMPLEXES FOR PHOTOVOLTAIC APPLICATIONS

SHARLENE A. LEWIS, SAMANTHA E. BROWN-XU, MALCOLM H. CHISHOLM, The Ohio State University, Department of Chemistry and Biochemistry, Columbus, Ohio 43210; ARTHUR J. EPSTEIN, The Ohio State University, Department of Chemistry and Biochemistry and Department of Physics, Columbus, Ohio 43210.

FE04  15 min  9:21
VIBRATIONALLY DRIVEN HYDROGEN ABSTRACTION REACTION BY BROMINE RADICAL IN SOLUTION

JAE YOON SHIN, MICHAEL A. SHALOWSKI, and F. FLEMING CRIM, Department of Chemistry, University of Wisconsin-Madison, WI 53706.

FE05  15 min  9:38
STRUCTURAL MOTIONS AND CHARGE DELOCALIZATION IN ELECTRONICALLY EXCITED N,N'-DIMETHYLPIPERAZINE

XINXIN CHENG, Department of Chemistry, Brown University, Providence, RI 02912; SANG-HAMITRA DEB, Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104; and PETER M. WEBER, Department of Chemistry, Brown University, Providence, RI 02912.

Intermission

FE06  15 min  10:10
THEORETICAL STUDIES OF PHOTODISSOCIATION DYNAMICS OF BRCN-

BERNICE OPOKU-AGYEMAN and ANNE B. McCoiY, Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH 43210.

FE07  15 min  10:27
USING TRYPTOPHAN AS A PROBE FOR STUDYING PROTEIN HYDRATION DYNAMICS


FE08  15 min  10:44
FEMTOSECOND CONICAL INTERSECTION DYNAMICS OF TRYPTOPHAN IN PROTEINS AND VALIDATION OF SLOWDOWN OF HYDRATION LAYER DYNAMICS

J. YANG, Department of Physics, The Ohio State University, Columbus, OH 43210; L. ZHANG, Department of Chemistry, Columbia University, New York, NY 10027; L. WANG, and D. ZHONG, Department of Physics, Department of Chemistry and Biochemistry, and Programs of Biophysics, Chemical Physics, and Biochemistry, The Ohio State University, Columbus, OH 43210.

FE09  15 min  11:01
PHOTOISOMERIZATION DYNAMICS OF THE SCREEN MOLECULE AVOBENZONE

ADAM D. DUNKELBERGER, RYAN D. KIEFA, and F. FLEMING CRIM, Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706.

FE10  15 min  11:18
STUDY OF PROTON TRANSFER IN E. COLI PHOTOLYASE

MENG ZHANG, ZHEYUN LIU, JIANG LI, LIJUAN WANG and DONGPING ZHONG, 191 W. Woodruff Ave., Columbus, Ohio 43210.

FE11  Post-deadline  15 min  11:35
Abstract

DETECTION AND INTERPRETATION OF COLLISIONAL TRANSFER AND ROTATIONAL ANISOTROPY FINGERPRINTS IN RESONANT FOUR-WAVE MIXING SPECTRA.

A. KOZOV, Department of Physics, Saint-Petersburg State University, Peterhof, Saint-Petersburg 198504, Russia; P. RADI, P. MAKSYUTENKO, Department General Energy, Paul Scherrer Institute, CH-5232 Villigen, Switzerland; and D. KOZLOV, A.M. Prokhorov General Physics Institute, Russian Academy of Sciences, Vavilov str. 38, 119991 Moscow, Russia.

FE12  Post-deadline  15 min  11:52
Abstract

USING TERAHERTZ SPECTROSCOPY TO STUDY SYSTEMS WITH SOLAR ENERGY APPLICATIONS

REBECCA L. MILOT, GARY F. MOORE, LAUREN A. MARTINI, GARY W. BRUDVIG, ROBERT H. CRABTREE, and CHARLES A. SCHNUITENMAER, Department of Chemistry, Yale University, New Haven, CT 06520-8107.
AUTHOR INDEX

A
ABBOTT, H. L. – MG16
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