<table>
<thead>
<tr>
<th>Time</th>
<th>Location</th>
<th>Sessions</th>
</tr>
</thead>
<tbody>
<tr>
<td>MONDAY</td>
<td>8:45AM</td>
<td><strong>AUDITORIUM INDEPENDENCE HALL</strong> MA. PLENARY SESSION</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TUESDAY 8:30AM</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TUESDAY 8:30AM</td>
</tr>
<tr>
<td></td>
<td></td>
<td>WEDNESDAY 8:30AM</td>
</tr>
<tr>
<td></td>
<td></td>
<td>THURSDAY 8:30AM</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FRIDAY 8:30AM</td>
</tr>
<tr>
<td></td>
<td></td>
<td><strong>ROOM 160 MATH ANNEX</strong>* TA. INFRARED/ARAMAN</td>
</tr>
<tr>
<td></td>
<td></td>
<td><strong>ROOM 170 MATH ANNEX</strong>* TB. DYNAMICS</td>
</tr>
<tr>
<td></td>
<td></td>
<td><strong>ROOM 1000 MCPHERSON LAB</strong> TC. MICROWAVE</td>
</tr>
<tr>
<td></td>
<td></td>
<td><strong>ROOM 1015 MCPHERSON LAB</strong> TD. ELECTRONIC</td>
</tr>
<tr>
<td></td>
<td></td>
<td><strong>ROOM 2015 MCPHERSON LAB</strong> TE. ATMOSPHERIC SPECIES</td>
</tr>
<tr>
<td>1:30PM</td>
<td></td>
<td>FE. MATRIX/CONDENSED PHASE</td>
</tr>
<tr>
<td></td>
<td></td>
<td>RF. MINI-SYMPOSIUM: THE THz COSMOS</td>
</tr>
<tr>
<td>ROOM 160 MATH ANNEX*</td>
<td>MF. ELECTRONIC</td>
<td>TF. ASTRONOMICAL SPECIES &amp; PROCESSES</td>
</tr>
<tr>
<td>ROOM 170 MATH ANNEX*</td>
<td>MG. INFRARED/ARAMAN</td>
<td>TG. ELECTRONIC</td>
</tr>
<tr>
<td>ROOM 1000 MCPHERSON LAB</td>
<td>MH. MICROWAVE</td>
<td>TH. MINI-SYMPOSIUM: PERTURBATIONS</td>
</tr>
<tr>
<td>ROOM 1015 MCPHERSON LAB</td>
<td>MI. RADICALS AND IONS</td>
<td>TI. INFRARED/ARAMAN</td>
</tr>
<tr>
<td>ROOM 2015 MCPHERSON LAB</td>
<td>MJ. MATRIX/CONDENSED PHASE</td>
<td>TJ. THEORY</td>
</tr>
<tr>
<td></td>
<td></td>
<td>WJ. RADICALS/IONS</td>
</tr>
<tr>
<td></td>
<td></td>
<td>RJ. RADICALS AND IONS</td>
</tr>
</tbody>
</table>

*209 W. 18th Avenue*
MA. PLENARY
MONDAY, JUNE 20, 2011 – 8:45 am
Room: AUDITORIUM, INDEPENDENCE HALL
Chair: FRANK C. DELUCIA, The Ohio State University, Columbus

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

8:45

MA01
40 min 9:00
SPECTROSCOPY AND DYNAMICS OF THE HOCO RADICAL

ROBERT E. CONTINETTI*, BERWYCK L. J. POAD, Department of Chemistry and Biochemistry, University of California San Diego, La Jolla, CA 92093; CHRISTOPHER J. JOHNSON, Department of Physics, University of California San Diego, La Jolla, CA 92093; MICHAEL E. HARDING, JOHN F. STANTON, Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, TX 78712.

*This work supported by the US Department of Energy under grant number DE-FG03-98ER14879

MA02
40 min 9:45
SPECTROSCOPIC AND THEORETICAL STUDY ON THE STRUCTURES AND DYNAMICS OF FUNCTIONAL MOLECULES - TOWARDS AN UNDERSTANDING OF THE MOLECULAR RECOGNITION FOR ENCAPSULATION COMPLEXES

TAKAYUKI EBATA, RYOJI KUSAKA, YOSHIYA INOKUCHI, Department of Chemistry, Graduate School of Science, Hiroshima University, Higashi-Hiroshima, 739-8526, Japan; SOTIRIS S. XANTHEAS, Pacific Northwest National Laboratory, 902 Battelle Boulevard, PO Box 999, MS K1-83, Richland, WA 99352.

Intermission

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

2010 Rao Award Winners
Hui-Ling Han, National Chiao Tung University
Samantha Horvath, The Ohio State University
Solveig Gaarn Olesen, University of Copenhagen

MA03
40 min 11:05
ELECTRONIC SPECTROSCOPY OF CARBON CHAINS OF ASTROPHYSICAL RELEVANCE

JOHN P. MAIER, Department of Chemistry, University of Basel, Klingelbergstrasse 80, CH-4056 Basel, Switzerland.
<table>
<thead>
<tr>
<th>Session</th>
<th>Time</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>MF01</td>
<td>1:30</td>
<td>THEORETICAL STUDIES OF OBSERVABLE TRANSITIONS TO RECOUPLED PAIR BONDED STATES OF SULFUR HALIDE COMPOUNDS: SF/SCl ($X^2\Pi \rightarrow A^2\Sigma^-$), SF$_2$/SCl$_2$ ($X^1A_1 \rightarrow 1^1B_1$, $X^1A_1 \rightarrow 1^1A_2$), AND SFCI ($X^1A' \rightarrow A^1A''$)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>JEFF LEIDING, DAVID E. WOON and THOM H. DUNNING, JR., Department of Chemistry, University of Illinois at Urbana-Champaign, Box 86-6, CLSL, 600 South Mathews, Urbana IL, 61801.</td>
</tr>
<tr>
<td>MF02</td>
<td>1:47</td>
<td>BLUE-DETECTED PHOTOASSOCIATION SPECTRUM IN Rb$_2$</td>
</tr>
<tr>
<td>MF03</td>
<td>1:59</td>
<td>AN ACCURATE NEW POTENTIAL FUNCTION FOR GROUND-STATE Xe$_2$ FROM UV AND VIRIAL COEFFICIENT DATA</td>
</tr>
<tr>
<td></td>
<td></td>
<td>ROBERT J. LE ROY, J. CAMERON MACKIE, PRAGNA CHANDRASEKHAR, Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada.</td>
</tr>
<tr>
<td>MF04</td>
<td>2:16</td>
<td>LASER-INDUCED FLUORESCENCE STUDIES OF THE JET-COOLED ALUMINUM ACETYLIDE RADICAL (Al-CCH/AICCD)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>MOHAMMED A. GHARAIBEH, DENNIS J. CLOUTHIER, Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055.</td>
</tr>
<tr>
<td>MF05</td>
<td>2:33</td>
<td>THE ELECTRONIC SPECTRUM OF H$_2$PO, THE PROTotypical PHOSPHORYL FREE RADICAL</td>
</tr>
<tr>
<td></td>
<td></td>
<td>MOHAMMED A. GHARAIBEH, DENNIS J. CLOUTHIER, Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055.</td>
</tr>
<tr>
<td>MF06</td>
<td>2:50</td>
<td>DETECTION OF THE H$_2$PS FREE RADICAL BY LASER SPECTROSCOPY</td>
</tr>
<tr>
<td></td>
<td></td>
<td>ROBERT A. GRIMMINGER, DENNIS J. CLOUTHIER, Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055, USA; RICCARDO TARRONI, Dipartimento di Chimica Fisica ed Inorganica, Università di Bologna, 40136 Bologna, Italy.</td>
</tr>
</tbody>
</table>
A SPECTROSCOPIC STUDY OF THE LINEAR-BENT ELECTRONIC TRANSITIONS OF JET-COOLED BCl₂ AND HBCI

RAMYA NAGARAJAN, JIE YANG and DENNIS J. CLOUTHIER, Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055.

Intermission

TWO-DIMENSIONAL (2+n) REMPI SPECTROSCOPY: STATE INTERACTIONS, PHOTOFRAGMENTATIONS AND ENERGETICS OF THE HYDROGEN HALIDES

JINGMING LONG, HUASHENG WANG, AGUST KVARAN, Science Institute, University of Iceland, D unstadgami 3, 107 Reykjavik, Iceland.

OPTICAL STARK SPECTROSCOPY OF THE ̃Å2Π - ̃Χ2Σ⁺ BAND OF BaOH

SARAH E. FREY AND TIMOTHY C. STEIMLE, Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287, USA.

LASER INDUCED FLUORESCENCE SPECTROSCOPY OF BORON CARBIDE

A. S-C. CHEUNG, Y.W. NG, AND H.F. PANG, Department of Chemistry, The University of Hong Kong, Pokfulam Road, Hong Kong.

IMPROVEMENT OF SPECTROSCOPIC CONSTANTS FOR THE A3Π ₁u ← X1Σg⁺ SYSTEM OF Br₂

NOBUO NISHIMIYA, TOKIO YUKIYA, and MASAO SUZUKI, Department of Electronics and Information Technology, Tokyo Polytechnic University, Iiyama 1583, Atsugi City, 243-0297 Kanagawa, Japan; ROBERT J. LE ROY, Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada.

ACCURATE ANALYTIC POTENTIALS FOR THE A3Π ₁ and X 1Σ⁺ STATES OF IBr FROM A COMBINED-ISOTOPOLOGUE DIRECT-POTENTIAL-FIT DATA ANALYSIS

TOKIO YUKIYA, NOBUO NISHIMIYA, Department of Electronics and Information Technology, Tokyo Polytechnic University, Iiyama 1583, Atsugi City, Kanagawa 243-0297, Japan; ROBERT J. LE ROY, Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada.

TRANSITION STRENGTHS IN THE VISIBLE ABSORPTION SPECTRUM OF I₂: ONE MORE PASS

J. TELLINGHUISEN, Department of Chemistry, Vanderbilt University, Nashville, TN 37235.
PHOTOELECTRON SPECTROSCOPY OF ICN$^{-}$: CHARACTERIZATION OF A CONICAL INTERSECTION IN ICN

ELISA M. MILLER, LEONID SHEPS, a YU-JU LU, JILA, Department of Chemistry and Biochemistry, University of Colorado at Boulder, Boulder, CO 80309; ANNE B. McCoy, Department of Chemistry, The Ohio State University, Columbus, OH, 43210; and W. Carl Lineberger, JILA, Department of Chemistry and Biochemistry, University of Colorado at Boulder, Boulder, CO 80309.

aPresent address: Sandia National Laboratories, Livermore, CA 94551
ARE AB INITIO QUANTUM CHEMISTRY METHODS ABLE TO PREDICT VIBRATIONAL STATES UP TO THE DISSOCIATION LIMIT FOR MULTI-ELECTRON MOLECULES CLOSE TO SPECTROSCOPIC ACCURACY?

PÉTER G. SZALAY, Eötvös Loránd University, Budapest, Hungary; FILIP HOLKA, Slovak University of Technology, Trenava, Slovak Republic; JULIEN FREMONT, MICHAEL REY, VLADIMIR G. TYUTEREV, Reims University, Reims, France.

ASSIGNMENT OF INFRARED AMMONIA SPECTRA

J. TENNYSON, M. J. DOWN, C. HILL and R. J. BARBER, Department of Physics and Astronomy, University College London, London, WC1E 6BT, UK; S. N. YURCHENKO, Technische Universität Dresden, Physikalische Chemie, D–01062 Dresden, Germany.

MODELING VIBRATIONAL STRUCTURE USING HARMONICALLY-COUPLED MORSE OSCILLATORS: A GLOBAL DESCRIPTION OF THE C-H STRETCHES IN METHYL RADICAL AND ITS DEUTERATED ISOTOPOMERS

MELANIE A. ROBERTS, DAVID J. NESBITT, JILA, National Institute of Standards and Technology and University of Colorado, and Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO 80309; ANNE B. McCOY, Department of Chemistry, The Ohio State University, Columbus, OH 43210.

HIGH–RESOLUTION FOURIER TRANSFORM INFRARED SPECTROSCOPY OF SMALL BORON–CONTAINING MOLECULES

G. LI and P. F. BERNATH, Department of Chemistry, University of York, Heslington, York YO10 5DD.

INFRARED LINE INTENSITIES FOR FORMALDEHYDE FROM SIMULTANEOUS MEASUREMENTS IN THE INFRARED AND FAR INFRARED SPECTRAL RANGES

L. FISSIAUX, Laboratoire Lasers et Spectroscopies, Facultés Universitaires Notre Dame de la Paix, 61 rue de Bruxelles, B-5000 Namur, Belgium; T. FÖLDES, Service de Chimie Quantique et Photophysics, Université Libre de Bruxelles, CP 16009, 50 avenue F.D. Roosevelt, B-1050 Brussels, Belgium; F. KWABIA TCHANA, Laboratoire Interuniversitaire des Systèmes Atmosphériques, CNRS, Universités de Paris Est Créteil et Paris 7, 61 avenue du Général De Gaulle, F-94010 Créteil cedex, France; L. DAUMONT, Groupe de Spectrométrie Moléculaire et Applications, UMR CNRS 6089, Université de Reims Champagne Ardenne, Campus du Moulin de la Housse, BP 1039, 51067 Reims Cedex 2, France; M. LEPÈRE, Laboratoire Lasers et Spectroscopies, Facultés Universitaires Notre Dame de la Paix, 61 rue de Bruxelles, B-5000 Namur, Belgium; J. VANDER AUWERA, Service de Chimie Quantique et Photophysics, Université Libre de Bruxelles, CP 16009, 50 avenue F.D. Roosevelt, B-1050 Brussels, Belgium.
INFRARED SPECTROSCOPY OF CARBON- AND CARBON-SILICON CLUSTERS

J. KRIEG, V. LUTTER, I. GOTTFBEHÜT, T. F. GIESEN, S. SCHLEMMER, and S. THORWIRTH.

Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany.

Intermission

HYDROGEN BOND RING OPENING AND CLOSING IN PROTONATED METHANOL CLUSTERS PROBED BY INFRARED SPECTROSCOPY WITH AND WITHOUT ART AGGING

TORU HAMASHIMA, KEN TA MIZUSE, ASUKA FUJII, Department of Chemistry, Graduate School of Science, Tohoku University, Sendai 980-8578, Japan; and JER-LAI KUO, Institute of Atomic and Molecular Sciences, Taipei10617, Taiwan.

C...H...N HYDROGEN BOND FORMATION IN TRIMETHYLAMINE DIMER UPON ONE-PHOTON IONIZATION

YUICHIRO NAKAYAMA, YOSHIYUKI MATSUDA, ASUKA FUJII, Department of Chemistry, Graduate School of Science, Tohoku University, Sendai 980-8578, Japan.

NON-CYCLIC ISOMERS OF (H₂O)₄ IN HELIUM NANODROPLETS: INFRARED SPECTROSCOPY AND AB INITIO CALCULATIONS


MATRIX ISOLATION FTIR AND AB INITIO STUDIES ON THE CONFORMATIONS OF DIMETHYL AND DIETHYL CARBONATE AND THEIR COMPLEXES WITH WATER

BISHNU PRASAD KAR, N. RAMANATHAN, K. SUNDARARAJAN and K. S. VISWANATHAN, Chemistry Group, Indira Gandhi Centre for Atomic Research, Kalpakkam, 603 102, India.

CONFORMATIONS OF TRIMETHYL PHOSPHITE: A MATRIX ISOLATION INFRARED AND AB INITIO STUDY

N. RAMANATHAN, K. SUNDARARAJAN, BISHNU PRASAD KAR and K. S. VISWANATHAN, Chemistry Group, Indira Gandhi Centre for Atomic Research, Kalpakkam 603 102, India.
INTERMOLECULAR ASSOCIATION COMPLEXES OF 1,3-CYCLOHEXANEDIONE: PROBING OF KETO-ENOL TAUTOMERIC EQUILIBRIA IN COLD INERT GAS MATRIX, SOLUTION AND VAPOR PHASE BY INFRARED SPECTROSCOPY AND QUANTUM CHEMISTRY STUDY

BIMAN BANDYOPADHYAY, PRASENJIT PANDEY, Physical Chemistry Department, Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700032, India; AMIT K. SAMANTA, Department of Chemistry, University of Southern California, Los Angeles, CA 90089, U.S.A.; ANAMIKA MUKHOPADHYAY and TAPAS CHAKRABORTY, Physical Chemistry Department, Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700032, India.

VIBRON AND PHONON HYBRIDIZATION IN DIELECTRIC NANOSTRUCTURES

T. C. PRESTON and R. SIGNORELL, Department of Chemistry, University of British Columbia, Vancouver, B.C., Canada.
MH. MICROWAVE
MONDAY, JUNE 20, 2011 – 1:30 pm
Room: 1000 McPHERSON LAB

Chair: STEVEN SHIPMAN, New College of Florida, Sarasota, Florida

MH01 15 min 1:30
MICROWAVE SPECTRA AND STRUCTURES OF H₄C₂···AgCl AND H₄C₂···CuCl

N. R. WALKER, S. L. STEPHENS, V. A. MIKHAILOV AND A. C. LEGON, School of Chemistry, University of Bristol, Bristol, BS8 1TS, U.K.

MH02 15 min 1:47
MICROWAVE SPECTRA AND STRUCTURE OF CF₃I···CO

S. L. STEPHENS, N. R. WALKER AND A. C. LEGON, School of Chemistry, University of Bristol, Bristol, BS8 1TS, U.K.

MH03 15 min 2:04
INTERMOLECULAR INTERACTION BETWEEN CO OR CO₂ AND ETHER OR THIOETHER OR PROPYLENE OXIDE IN A COMPLEX, INVESTIGATED BY FOURIER TRANSFORM MICROWAVE SPECTROSCOPY AND ABINITIO CALCULATIONS

YOSHIYUKI KAWASHIMA, YUKARI ORITA, and AKINORI SATO, Department of Applied Chemistry, Faculty of Engineering, Kanagawa Institute of Technology, Atsugi, Kanagawa 243-0292, JAPAN; EIZI HIROT A, The Graduate University for Advanced Studies, Hayama, Kanagawa 240-0193, JAPAN.

MH04 10 min 2:21
DOES WATER PREFER TO DONATE A PROTON TO AN F OR TO A CI ATOM? - A ROTATIONAL STUDY OF CH₃CHClF...H₂O

GANG FENG, LUCA EVANGE LISTI and W. CAMINATI, Dipartimento di Chimica “G. Ciamician” dell’Università, Via Selmi 2, I-40126 Bologna, Italy; LAURA B. FAVERO, Istituto per lo Studio dei Materiali Nanostrutturati (ISMN, Sezione di Bologna), CNR, Via Gobetti 101, I-40129 Bologna, Italy; JENS-UWE GRABOW, Lehrgebiet Physikalische Chemie A, Institut für Physikalische Chemie und Elektrochemie, Universität Hannover, Callinstr. 3A, D-30167 Hannover, Germany; ZHINING XIA, Chemistry and Chemistry Engineering College, Chongqing University, Chongqing, 400030, P. R. China.

MH05 15 min 2:33
DETERMINATION OF THE STRUCTURE OF THE ARGON CYCLOPENTANONE AND NEON VAN DER WAALS COMPLEXES

WEI LIN, Department of Chemistry and Environmental Sciences, University of Texas at Brownsville, 80 Fort Brown - MO1.114, Brownsville, TX 78520; DANIEL J. FROHMAN, ANDREW H. BROOKS, Department of Chemistry, Wesleyan University, Hall-Atwater Laboratories, 52 Lawn Avenue, Middletown, CT 06459-0180; ANDREA J. MINEI, Division of Natural Sciences, Chemistry Department, College of Mount Saint Vincent, 6301 Riverdale Avenue, Riverdale, NY 10471; CHINH H. DUONG, STEWART E. NOVICK, and WALLACE C. PRINGLE, Department of Chemistry, Wesleyan University, Hall-Atwater Laboratories, 52 Lawn Avenue, Middletown, CT 06459-0180.
IMPROVED DIPOLE MOMENTS FOR ACRYLONITRILE AND PROPIONITRILE

ZBIGNIEW KISIEL, ADAM KRAŚNICKI, Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warszawa, Poland.

NOTATION CONFUSION OF SYMMETRY SPECIES FOR MOLECULES WITH SEVERAL LARGE-AMPLITUDE INTERNAL MOTIONS

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

SEMI-EXPERIMENTAL \((r_s/r_e)\) STRUCTURES FOR THE HEAVY ATOM BACKBONES OF TWO MODERATELY LARGE MOLECULES OBTAINED FROM MICROWAVE SPECTROSCOPY AND QUANTUM CHEMICAL CALCULATIONS

NORMAN C. CRAIG, Department of Chemistry and Biochemistry, Oberlin College, Oberlin, OH 44074; ALBERTO LESARRI, Departamento de Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, E-47011 Valladolid, Spain; EMILIO J. COCINERO, Departamento de Química Física, Facultad de Ciencia y Tecnología, Universidad del País Vasco, Ap. 644, E-48080 Bilbao, Spain; JENS-UWE GRABOW, Institut für Physikalische Chemie und Elektrochemie, Gottfried-Wilhelm-Leibniz-Universität Hannover, Callinstrasse 3A, D30167 Hannover, Germany.

Intermission

VIBRATIONAL ENERGIES FOR ACRYLONITRILE FROM MM-WAVE TO THZ ROTATIONAL SPECTRA

ZBIGNIEW KISIEL, LECH PSZCZÓŁKOWSKI, Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warszawa, Poland; BRIAN J. DROUIN, CAROLYN S. BRAUER, SHANSHAN YU, JOHN C. PEARSON, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Drive, Pasadena, CA 91109-8099, USA; IVAN R. MEDVEDEV, Department of Physics, Wright State University, Dayton, OH 45435, USA; SARAH FORTMAN, CHRISTOPHER NEESE, Department of Physics, The Ohio State University, Columbus, OH 43210, USA.

ROOM-TEMPERATURE CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE (RT-CP-FTMW) SPECTRUM OF PYRIDINE

AUSTIN L. MCIJUNKINS, K. MICHELLE THOMAS, APRIL RUTHVEN, AND GORDON G. BROWN, Department of Science and Mathematics, Coker College, 300 E College Ave., Hartsville, SC 29550.

THE ROTATIONAL SPECTRUM OF BIOMOLECULAR RELATED COMPOUNDS.¹

VANESA VAQUERO, and DAVID W. PRATT, Department of Chemistry, University of Pittsburgh, Pittsburgh, PA 15260.

¹Work supported by NSF(CHE-0911117)
MH12 15 min 4:51
FLUORINE SUBSTITUTION IN NEUROTRANSMITTERS: MICROWAVE SPECTROSCOPY AND MODELLING OF THE CONFORMATIONAL SPACE AND NON BONDING INTERACTIONS

S. MELANDRI, A. MARIS and A. MERLONI, Dipartimento di Chimica Ciamician, Università di Bologna, via Selmi 2, 40126 Bologna, Italy.

MH13 15 min 5:08
NEUROTRANSMITTERS IN THE GAS PHASE: LA-MB-FTMW STUDIES


MH14 15 min 5:25
LA-MB-FTMW STUDIES OF SUGARS

MI01 10 min 1:30
ISOTOPIC EFFECTS IN CHEMICAL REACTIONS OF SINGLE IONS

JAMES E. GOEDERS, CRAIG R. CLARK, and KENNETH R. BROWN, Georgia Institute of Technology.

MI02 15 min 1:42
MODELING THE INFLUENCE OF NUCLEAR SPIN IN THE REACTION OF H$_3^+$ WITH H$_2$

KYLE N. CRABTREE, BRIAN A. TOM, a BENJAMIN J. McCALL, Department of Chemistry, University of Illinois, Urbana, IL 61801, USA.

a Present Address: Department of Chemistry, United States Air Force Academy, Air Force Academy, CO 80840, USA

MI03 15 min 1:59
SPECTROSCOPIC MEASUREMENTS OF THE REACTION H$_3^+$ + H$_2$ → H$_2$ + H$_3^+$

KYLE N. CRABTREE, CAROL A. KAUFFMAN, BRIAN A. TOM, a EFTALDA BEČKA, BRETT A. McGUIRE, b BENJAMIN J. McCALL, Department of Chemistry, University of Illinois, Urbana, IL 61801, USA.

a Present Address: Department of Chemistry, United States Air Force Academy, Air Force Academy, CO 80840, USA
b Present Address: Department of Chemistry, Emory University, Atlanta, GA 30322, USA

MI04 15 min 2:16
INFRARED PHOTODISSOCIATION SPECTROSCOPY OF FIRST ROW TRANSITION METAL-CARBONYL CATIONS

ANTONIO D. BRAITHWAITE, ALLEN M. RICKS, ZACH D. REED, MICHAEL A. DUNCAN, Department of Chemistry, University of Georgia, Athens, GA 30602-2256.

MI05 15 min 2:33
INFRARED PHOTODISSOCIATION SPECTROSCOPY OF METAL ION WATER COMPLEXES

B. BANDYOPADHYAY, P. D. CARNEGIE and M. A. DUNCAN, University of Georgia, Athens, Georgia-30605, USA.

MI06 15 min 2:50
VIBRATIONALLY DRIVEN ELECTRON TRANSFER IN CH$_3$NO$_2$·CH$_3$I CLUSTERS

BENJAMIN J. KNURR, CHRISTOPHER L. ADAMS and J. MATTHIAS WEBER, JILA, NIST and Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO 80309.
PHOTOELECTRON IMAGING OF NITROETHANE, NITROPROPANE AND NITROBUTANE

CHRISTOPHER L. ADAMS, BENJAMIN J. KNURR and J. MATHIAS WEBER, JILA, NIST and Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO 80309.

Intermission

ROTATIONAL SPECTRA OF N$_2$OH$^+$ AND CH$_2$CHCNH$^+$ MOLECULAR IONS

OSCAR MARTINEZ, JR., VALERIO LATTANZI, and MICHAEL C. McCARTHY, Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, and School of Engineering and Applied Science, Harvard University, Cambridge, MA 02138; SVEN THORWITH, Max-Planck-Institut für Radioastronomie, Bonn, Germany, and I. Physikalisches Institut, Universität zu Köln, Germany.

NOISE IMMUNE CAVITY ENHANCED OPTICAL HETERODYNE VELOCITY MODULATION SPECTROSCOPY

BRIAN SILLER, ANDREW MILLS, MICHAEL PORAMBO, Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801; BENJAMIN McCALL, Departments of Chemistry and Astronomy, University of Illinois at Urbana-Champaign, Urbana, IL 61801.

LINESHAPE AND SENSITIVITY OF SPECTROSCOPIC SIGNALS OF N$_2^+$ IN A POSITIVE COLUMN COLLECTED USING NOISE IMMUNE CAVITY ENHANCED OPTICAL HETERODYNE VELOCITY MODULATION SPECTROSCOPY

ANDREW MILLS, BRIAN SILLER, MICHAEL PORAMBO, 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.

PROGRESS AND RECENT DEVELOPMENTS IN SENSITIVE, COOLED, RESOLVED ION BEAM SPECTROSCOPY (SCRIBES)

MICHAEL PORAMBO, ANDREW MILLS, BRIAN SILLER, HOLGER KRECKEL, MANORI PERERA, Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801; BENJAMIN McCALL, Departments of Chemistry and Astronomy, University of Illinois at Urbana-Champaign, Urbana, IL 61801.

PHOTODISSOCIATION SPECTROSCOPY OF Ca$^+$-H$_2$O IN THE TEMPERATURE-VARIABLE ION TRAP

HARUKI ISHIKAWA, TORU EGUCHI, TAKUMI NAKANO, AKIMASA FUJIHARA$^a$, KIYOKAZU FUKE, Department of Chemistry, Graduate School of Science, Kobe University, Nada-ku, Kobe 657-8501, Japan.

$^a$Present address: Osaka Prefecture University, Japan
HIGH-RESOLUTION IR ACTION SPECTRUM OF C$_2$H$_2^+$

SABRINA GÄRTNER, JÜRGEN KRIEG, OSKAR ASVANY and STEPHAN SCHLEMMER, I. Physikalisches Institut, Universität zu Köln.
MJ01 15 min  1:30

**FLUORESCENCE OF MATRIX-ISOLATED BIACYTIL**

Erin E. Gatrone, Nathan G. Kuchmas and C. A. Baumann, Department of Chemistry, The University of Scranton, Scranton, PA 18510-4626.

---

MJ02 15 min  1:47

**EXPERIMENTAL THERMOCHEMISTRY OF GAS PHASE CYTOSINE TAUTOMERS**

A. M. Morrison and G. E. Douberty, Department of Chemistry, University of Georgia, Athens, Georgia 30602-2556.

---

MJ03 10 min  2:04

**TAUTOMERS OF CYTOSINE AND THEIR EXCITED ELECTRONIC STATES: A MATRIX ISOLATION SPECTROSCOPIC AND QUANTUM CHEMICAL STUDY**

Gábor Bazsó, György Tarczay, Laboratory of Molecular Spectroscopy, Institute of Chemistry, Eötvös Loránd University, Pf. 32, Budapest, H-1518, Hungary; Geza Fogarasi, Péter G. Szalay, Laboratory of Theoretical Chemistry, Institute of Chemistry, Eötvös Loránd University, Pf. 32, Budapest, H-1518, Hungary.

---

MJ04 15 min  2:16

**PULSED JET DISCHARGE MATRIX ISOLATION AND COMPUTATIONAL STUDY OF HALOGEN ATOM COMPLEXES: Br–BrCH₂X (X=H,Cl,Br)**

Aimable Kalume, Lisa George and Scott A. Reid, Department of Chemistry, Marquette University, Milwaukee, WI 53233.

---

MJ05 15 min  2:33

**PHOTOINDUCED ELECTRON TRANSFER IN THE C₂H₄–Br₂ COMPLEX**

Aimable Kalume, Lisa George and Scott A. Reid, Department of Chemistry, Marquette University, Milwaukee, WI 53233.

---

MJ06 15 min  2:50

**INFRARED SPECTRA OF THE 2-CHLOROETHYL RADICAL IN SOLID PARA-HYDROGEN**

Jay C. Amicangelo, School of Science, Penn State Erie, Erie, PA 16563; Mohammed Bahou, Barbara Golec, 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, Taiwan.
Intermission

MJ07 15 min 3:30
FTIR ISOTOPIC AND DFT STUDIES OF SiC$_5$ TRAPPED IN SOLID Ar

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

MJ08 15 min 3:47
FTIR AND DFT STUDIES OF THE MgC$_3^-$ ANION IN SOLID Ar

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

MJ09 15 min 4:04
DIMINISHED CAGE EFFECT IN $p$-H$_2$: IR IDENTIFICATION OF INTERMEDIATES IN ADDITION REACTIONS OF Cl ATOM WITH UNSATURATED HYDROCARBONS

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; MOHAMMED BAHOU, BARBARA GOLEC, Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu 30010, Taiwan.

MJ10 15 min 4:21
MOLECULAR HYDROGEN INTERACTIONS WITHIN METAL-ORGANIC FRAMEWORKS

S. FITZGERALD, C. PIERCE, J. SCHLOSS, B. THOMPSON, Department of Physics and Astronomy, Oberlin College, Oberlin, OH 44074; J. ROWSELL, Department of Chemistry and Biochemistry, Oberlin College, Oberlin, OH 44074.

MJ11 15 min 4:38
ELECTRON SPIN RESONANCE INVESTIGATION OF FORMATION MECHANISMS OF MATRIX ISOLATED $H_4^+$

M. CORRENTI, J. BANISAIKAS, L. B. KNIGHT, JR., Department of Chemistry, Furman University, Greenville, SC.
TA01  10 min  8:30
TIME RESOLVED FTIR ANALYSIS OF COMBUSTION OF ETHANOL AND GASOLINE COMBUSTION IN AN INTERNAL COMBUSTION ENGINE

ALLEN R. WHITE, STEPHEN SAKAI, Department of Mechanical Engineering, Rose-Hulman Institute of Technology, 5500 Wabash Ave., Terre Haute, IN 47803; REBECCA B. DEVASHER, Department of Chemistry, Rose-Hulman Institute of Technology, 5500 Wabash Ave., Terre Haute, IN 47803.

TA02  10 min  8:42
TIME RESOLVED FTIR ANALYSIS OF TAILPIPE EXHAUST FOR SEVERAL AUTOMOBILES

ALLEN R. WHITE, JAMES ALLEN, Department of Mechanical Engineering, Rose-Hulman Institute of Technology, 5500 Wabash Ave., Terre Haute, IN 47803; REBECCA B. DEVASHER, Department of Chemistry, Rose-Hulman Institute of Technology, 5500 Wabash Ave., Terre Haute, IN 47803.

TA03  15 min  8:54
HIGH-RESOLUTION MID-INFRARED SPECTROSCOPY OF DEUTERATED WATER CLUSTERS USING A QUANTUM CASCADE LASER-BASED CAVITY RINGDOWN SPECTROMETER

JACOB T. STEWART, BRIAN E. BRUMFIELD, 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.

TA04  15 min  9:11
MID-IR CAVITY RING-DOWN SPECTROMETER FOR BIOLOGICAL TRACE NITRIC OXIDE DETECTION

VINCENT KAN, AHEMD RAGAB, VITALI STSIAPURA, KEVIN K. LEHMANN, Department of Chemistry and School of Medicine, University of Virginia, Charlottesville VA, 22904-4319; BENJAMIN M. GASTON, School of Medicine, University of Virginia, Charlottesville VA, 22904-4319.

TA05  15 min  9:28
OFF-AXIS CAVITY RING DOWN SPECTROSCOPY BASED ON A CONTINUOUS-WAVE OPTICAL PARAMETRIC OSCILLATOR

JARI PELTOLA, MIKAEL SILTANEN and LAURI HALONEN, Laboratory of Physical Chemistry, Department of Chemistry, P.O. BOX 55 (A.I. Virtasen aukio 1), FI-00014 University of Helsinki, Finland; MARKKU VAINIO, Laboratory of Physical Chemistry, Department of Chemistry, P.O. BOX 55 (A.I. Virtasen aukio 1), FI-00014 University of Helsinki, Finland and Centre for Metrology and Accreditation, P.O. Box 9, FIN-02151 Espoo, Finland.
OH DETECTION USING OFF-AXIS INTEGRATED CAVITY OUTPUT SPECTROSCOPY (OA-ICOS)

CHRISTOPHE LENGIGNON, WEIXIONG ZHAO, WEIDONG CHEN, ERIC FERTEIN, CECILE COEUR, Laboratoire de Physico-Chimie de l’Atmosphere, Universite du littoral Cote d’Opale, Dunkerque - France; DENIS PETITPREZ, Laboratoire de Physicochimie des Processus de Combustion et de l’Atmosphere, Universite des Sciences et Technologies de Lille, 59655 Villeneuve d’Ascq Cedex - France.

This work is supported by the IRENI program of the Region Nord-Pas de Calais. The support of the Groupement de Recherche International SAMIA between CNRS (France), RFBR (Russia) and CAS (China) is acknowledged.

TA07 15 min 10:15
CAVITY RINGDOWN LASER ABSORPTION SPECTROSCOPY (CRLAS) of ISOTOPICALLY LABELED ACETYLENE BETWEEN 12,500 - 13,600 cm⁻¹

CHRISTOPHER J. LUE, MICHAEL N. SULLIVAN, MARK E. DRAGANJAC, and SCOTT W. REEVE, Arkansas Center for Laser Applications and Science and Department of Chemistry and Physics, Arkansas State University, P.O. Box 419, State University, AR 72467.

Intermission

TA08 15 min 10:32
AUTOMATIC TUNING OF AN ACULIGHT OPTICAL PARAMETRIC OSCILLATOR


TA09 15 min 10:49
PRECISION MEASUREMENT OF CARBON DIOXIDE HOTBAND TRANSITION AT 4.3 MICRON USING A HOT CELL

PEI-LING LUO, JYUN-YU TIAN, HSHAN-CHEN CHEN, Institute of Photonics Technologies, National Tsing Hua University, Hsinchu, Taiwan 30013; YU-HUNG LIEN, JOW-TSONG SHY, Department of Physics, National Tsing Hua University, Hsinchu, Taiwan 30013.

TA10 15 min 11:06
HIGH PRECISION MID-IR SPECTROSCOPY OF $^{14}\text{N}_2^{16}\text{O}$ NEAR 4.5 μm

WEI-JO TING, JOW-TSONG SHY, Department of Physics, National Tsing Hua University, Hsinchu, Taiwan 30013, R.O.C.

TA11 15 min 11:23
MIR-IR SATURATION SPECTROSCOPY OF HeH⁺ MOLECULAR ION

HSUAN-CHEN CHEN, Institute of Photonics Technologies, National Tsing Hua University, Hsinchu, Taiwan 30013, R.O.C; WEI-JO TING, Department of Physics, National Tsing Hua University, Hsinchu, Taiwan 30013, R.O.C; JOW-TSONG SHY, Department of Physics, National Tsing Hua University, Hsinchu, Taiwan 30013, R.O.C; Institute of Photonics Technologies, National Tsing Hua University, Hsinchu, Taiwan 30013, R.O.C.
STATE OF WATER MOLECULES AND SILANOL GROUPS IN OPAL MINERALS: A NEAR INFRARED SPECTROSCOPIC STUDY OF OPALS FROM SLOVAKIA

MIROSLAV BOBON, Department of Physics, Faculty of Natural Sciences, Constantine the Philosopher University in Nitra, Slovakia; ALFRED A. CHRISTY, Department of Science, Faculty of Engineering and Science, University of Agder, Serviceboks 422, 4604 Kristiansand, Norway; DANIEL KLUVANEČ and L’UDMILA ILLASOVÁ, Gemological Institute, Faculty of Natural Sciences, Constantine The Philosopher University in Nitra, Slovakia.
TB. DYNAMICS
TUESDAY, JUNE 21, 2011 – 8:30 am
Room: 170 MATH ANNEX

Chair: DAVID PERRY, University of Akron, Akron, Ohio

TB01 10 min 8:30
FREE-INDUCTION DECAY SIGNALS USING A VOLTAGE MODULATED QUANTUM CASCADE LASER

G. DUXBURY and N. LANGFORD, Department of Physics, SUPA, John Anderson Building, University of Strathclyde, 107 Rottenrow, Glas gow G4 0NG, Scotland, UK.

TB02 15 min 8:42
OBSERVATION OF INFRARED FREE INDUCTION DECAY AND OPTICAL NUTATION SIGNALS FROM NITROUS OXIDE USING A VOLTAGE MODULATED QUANTUM CASCADE LASER

G. DUXBURY and N. LANGFORD, Department of Physics, SUPA, John Anderson Building, University of Strathclyde, 107 Rottenrow, Glasgow G4 0NG, Scotland, UK; J. F. KELLY and T. F. BLAKE, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, PO Box 999, MS K-88, Richland, Washington 99352.

TB03 15 min 8:59
SUB-DOPPLER SPECTRA OF INFRARED HYPERFINE TRANSITIONS OF NITRIC OXIDE USING A PULSE MODULATED QUANTUM CASCADE LASER

G. DUXBURY and N. LANGFORD, Department of Physics, SUPA, John Anderson Building, University of Strathclyde, 107 Rottenrow, Glasgow G4 0NG, Scotland, UK; J. F. KELLY and T. F. BLAKE, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, PO Box 999, MS K-88, Richland, Washington 99352.

TB04 15 min 9:16
KINETIC INVESTIGATION OF COLLISION INDUCED EXCITATION TRANSFER IN Kr*(4p^55p^1) + Kr (4p^6) AND Kr*(4p^55p^1) + He (1s^2) MIXTURES

MD. HUMAYUN KABIR and MICHAEL C. HEAVEN, Department of Chemistry, Emory University, Atlanta, GA 30322.

TB05 15 min 9:33
IR/THZ DOUBLE RESONANCE SPECTROSCOPY ENERGY DYNAMICS AT ATMOSPHERIC Pressures

DANE J. PHILLIPS, ELIZABETH A. TANNER, Kratos Defense and Security Solutions Digital Fusion Solutions Advanced Technologies Division, 5030 Bradford Dr., Building I, Suite 210, Huntsville, AL 35805; HENRY O. EVERITT, Army Aviation and Missile RD&E Center, Weapon Sciences Directorate, Redstone Arsenal, AL 35898; IVAN R. MEDVEDEV, Department of Physics, 3640 Colonel Glenn Hwy, Wright State University, Dayton, OH 45435; JENNIFER HOLT, CHRISTOPHER F. NEES, and FRANK C. DE LUCIA, Department of Physics, 191 Woodruff Ave. Ohio State University, Columbus, OH 43210.
ULTRAFAST STRUCTURAL DYNAMICS OF TERTIARY AMINES UPON ELECTRONIC EXCITATION

XINXIN CHENG, MICHAEL P. MINITTI, SANGHAMITRA DEB, YAO ZHANG, JAMES BUDARZ, PETER M. WEBER, Department of Chemistry, Brown University, Providence, Rhode Island 02912.

ULTRAFAST STRUCTURAL DYNAMICS OF 1,3-CYCLOHEXADIENE: ELECTRONIC STATE DEPENDENCE

CHRISTINE C. BÜHLER, MICHAEL P. MINITTI, SANGHAMITRA DEB, PETER M. WEBER, Department of Chemistry, Brown University, Providence, Rhode Island 02912; JIE BAO, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139.

Intermission

PHOTOCHEMISTRY OF BENZYLALLENE: PHOTOCHEMICAL PATHWAYS TO NAPHTHALENE

JOSHUA A. SEBREE, NATHAN KIDWELL, TIMOTHY S. ZWIER, Department of Chemistry, Purdue University, West Lafayette, IN 47907; ALEX NOLAN, ROBERT McMahan, Department of Chemistry, University of Wisconsin, Madison WI 53706; TALITHA SELBY, Department of Chemistry, University of Wisconsin Washington County, West Bend, WI 53095; MAREK ZGIERSKI, National Research Council Canada, Ottawa, ON.

BIMOLECULAR REACTIONS OF A DIFFERENT COLOR: CH$_3$D + CHLORINE WITH VARIED PHOTOLYSIS WAVELENGTHS

ANDREW E. BERKE, CHRISTOPHER J. ANNESLEY, and F. FLEMING CRIM, Chemistry Department, University of Wisconsin - Madison, Madison, Wisconsin 53706.

COMPARATIVE TORSION-INVERSION DYNAMICS FOR CH$_3$CH$_2^+$, CH$_3$OH$_2^+$ AND CH$_3$NH$_2$

RAM S. BHATTA and DAVID S. PERRY, Department of Chemistry, The University of Akron, OH 44325-3601.

STATE-TO-STATE ROTATIONAL AND VIBRATIONAL ENERGY TRANSFERS FOLLOWING VIBRATIONAL EXCITATION OF (1010$^0$$^0$) AND (0112$^0$$^0$) IN THE GROUND ELECTRONIC STATE OF ACETYLENE

JIANDE HAN, KEITH FREEL, and MICHAEL C. HEAVEN, Department of Chemistry, Emory University, Atlanta, GA 30322.

VIBRATIONAL PREDISSOCIATION DYNAMICS OF THE (H$_2$O)$_2$ DIMER

L. C. CH’NG, B. E. ROCHE, A. K. MOLLNER, and H. REISLER, Department of Chemistry, University of Southern California, Los Angeles, CA, 90089.
DETERMINATION OF THE DISSOCIATION ENERGY OF AMMONIA DIMER: A VIBRATIONAL PREDISSOCIATION STUDY

AMANDA S. CASE, CORNELIA G. HEID, SCOTT. H. KABLE, and F. FLEMING CRIM, Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706.
TC. MICROWAVE
TUESDAY, JUNE 21, 2011 – 8:30 am
Room: 1000 McPHERSON LAB

Chair: STEPHEN COOKE, University of North Texas, Denton, Texas

TC01 10 min 8:30
EASY-GOING ON-SPECTROMETER OPTIMISATION OF PHASE MODULATED HOMONUCLEAR DECOUPLING SEQUENCES IN SOLID-STATE NMR


TC02 15 min 8:42
QUANTUM-CHEMICAL CALCULATIONS OF SPECTROSCOPIC PARAMETERS FOR ROTATIONAL SPECTROSCOPY: THE NEED OF THE INTERPLAY BETWEEN EXPERIMENT AND THEORY

CRISTINA PUZZARINI, Dipartimento di Chimica “G. Ciamician”, Università di Bologna, I-40126 Bologna, Italy.

TC03 15 min 8:59
ROTATIONAL SPECTRUM OF CH$_2$F FROM 5 GHZ UP TO 1 THZ: ACCURATE SPECTROSCOPIC AND HYPERFINE PARAMETERS

CRISTINA PUZZARINI, GABRIELE CAZZOLI, Dipartimento di Chimica ”G. Ciamician”, Università di Bologna, I-40126 Bologna, Italy; JUAN CARLOS LÓPEZ, JOSÉ LUIS ALONSO, Departamento de Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, E-47005, Valladolid, Spain; AGOSTINO BALDACCI, ALESSANDRO BALDAN, Dipartimento di Chimica Fisica, Università “Ca’ Foscari” Venezia, D.D. 2137, I-30123 Venezia, Italy; STELLA STOPKOWICZ, LAN CHENG, JÜRGEN GAUSS, Institut für Physikalische Chemie, Universität Mainz, D-55099 Mainz, Germany.

TC04 15 min 9:16
ANALYSIS OF THE ROTATIONAL SPECTRUM OF HDO IN ITS $v_2 = 0$ AND 1 VIBRATIONAL STATES UP TO 2.8 THz

HOLGER S. P. MÜLLER, S. BRÜNKEN, C. P. ENDRES, F. LEWEN, I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany; J. C. PEARSON, S. YU, B. J. DROUIN, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109, USA; H. MÄDER, Institut für Physikalische Chemie, Christian-Albrechts-Universität, 24098 Kiel, Germany.

TC05 15 min 9:33
ROTATIONAL SPECTROSCOPY OF HD$^{18}$O

JOHN C. PEARSON*, SHANSHAN YU, HARSHAL GUPTA and BRIAN J. DROUIN, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr., Pasadena, CA 91109.

*A part of this work was performed at the Jet Propulsion Laboratory, California Institute of Technology under contract with the National Aeronautics and Space Administration. Copyright 2010 © California Institute of Technology. All rights reserved.
CHIRPED-PULSE TERAHERTZ SPECTROSCOPY FOR BROADBAND TRACE GAS SENSING

EYAL GERECHT, KEVIN O. DOUGLASS, DAVID F. PLUSQUELLIC, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY, OPTICAL TECHNOLOGY DIVISION, GAITHERSBURG, MD 20899.

Intermission

VIBRATIONAL POPULATION DISTRIBUTION IN FORMALDEHYDE EXPANDING FROM CHEN PYROLYSIS NOZZLE MEASURED BY CHIRPED PULSE MILLIMETER WAVE SPECTROSCOPY

KIRILL KUYANOV-PROZUMENT, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139; ANGAYLE VASILIOU, Department of Chemistry and Biochemistry, University of Colorado at Boulder, Boulder, CO 80309; G. BARRATT PARK, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139; JOHN S. MUENTER, Department of Chemistry, University of Rochester, Rochester, NY 14627; JOHN F. STANTON, Department of Chemistry, University of Texas, Austin, TX 78712; G. BARNEY 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.

THE MILLIMETER/SUBMILLIMETER SPECTRUM OF METHYLPHOSPHINE, CH$_3$PH$_2$ ($\tilde{X}^1$A)

D. T. HALFEN, Department of Chemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, AZ 85721; D. J. CLOUTHIER, Department of Chemistry, University of Kentucky, Lexington, KY 40506; and L. M. ZIURYS, Department of Chemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, AZ 85721.

FOURIER TRANSFORM MICROWAVE SPECTRUM OF THE FeCN RADICAL ($\tilde{X}^3\Delta_i$) AND CONFIRMATION OF THE GROUND ELECTRONIC STATE

D. T. HALFEN, Department of Chemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, AZ 85721; M. A. FLORY, CNA, Frankfort, KY; B. J. HARRIS, and L. M. ZIURYS, Department of Chemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, AZ 85721.

THE PURE ROTATIONAL SPECTRUM OF THE ZnSH RADICAL ($\tilde{X}^2\Delta'$)

MATTHEW P. BUCCHINO, GILLES R. ADANDE and LUCY M. ZIURYS, Department of Chemistry and Biochemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, Arizona 85721.

HYPERFINE SPLITTING AND ROTATIONAL ANALYSIS OF THE DIATOMIC MOLECULE ZINC MONOSULFIDE, ZnS.

DANIEL J. FROHMAN, G. S. GRUBBS II, and STEWART E. NOVICK, Department of Chemistry, Wesleyan University, Hall-Atwater Laboratories, 52 Lawn Avenue, Middletown, CT 06459-0180.

*Support from CHE-1011214
CAVITY AND CHIRPED PULSE ROTATIONAL SPECTRUM OF THE LASER ABLATION SYNTHESIZED, OPEN-SHELL MOLECULE TIN MONOCHLORIDE, SnCl\textsuperscript{a}

G. S. GRUBBS II, DANIEL J. FROHMAN, STEWART E. NOVICK, Department of Chemistry, Wesleyan University, Hall-Atwater Laboratories, 52 Lawn Avenue, Middletown, CT 06459-0180; and S. A. COOKE, Department of Chemistry, University of North Texas, 1155 Union Circle # 305070, Denton, TX 76203-5017.

\textsuperscript{a}Support from CHE-1011214
SPECTROSCOPIC CHARACTERIZATION OF $\text{Be}_2^+ X^2 \Sigma_u^+ AND THE IONIZATION ENERGY OF \text{Be}_2$

I. O. ANTONOV, B. J. BARKER, V. E. BONDYBEY, M. C. HEAVEN, Department of Chemistry, Emory University, Atlanta, GA 30322.

FOURIER TRANSFORM EMISSION SPECTROSCOPY OF THE $B^2 \Sigma^+ - X^2 \Sigma^+$ (VIOLET) SYSTEM OF $^{13}\text{C}^{14}\text{N}$

R. S. RAM and P. F. BERNA TH, Department of Chemistry, University of York, Heslington, York YO10 5DD.

FOURIER TRANSFORM EMISSION SPECTROSCOPY OF THE $E^2 \Pi - X^2 \Sigma^+$ TRANSITION OF CaH AND CaD

R. S. RAM, K. TERESZCHUK and P. F. BERNA TH, Department of Chemistry, University of York, Heslington, York YO10 5DD, UK; I. E. GORDON, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 02138, USA; K. A.W ALKER, Department of Physics, University of Toronto, Toronto, Ont., M5S 1A7, Canada.

JET-COOLED LASER-INDUCED FLUORESCENCE SPECTROSCOPY OF LARGE SECONDARY ALKOXY RADICALS

JINJUN LIU, MING-WEI CHEN, TERRY A. MILLER, Laser Spectroscopy Facility, Department of Chemistry, the Ohio State University, 120 W. 18th Ave., Columbus, Ohio 43210; W. L. MEERTS, Radboud University, Institute for Molecules and Materials, Heyendaalseweg 135, NL-6525 AJ Nijmegen, The Netherlands.

HIGH RESOLUTION LASER SPECTROSCOPY OF SrOCH$_3$

D. FORTHOMME, C. LINTON, D. W. TOKARYK, Centre for Laser, Atomic, and Molecular Sciences and Physics Department, 8 Bailey Dr., University of New Brunswick, P.O. Box 4400, Fredericton, NB, Canada E3B 5A3; A. G. ADAM, A. D. GRANGER, L. E. DOWNIE, W. S. HOPKINS, Centre for Laser, Atomic, and Molecular Sciences and Chemistry Department, 30 Dineen Dr., University of New Brunswick, P.O. Box 4400, Fredericton, NB, Canada E3B 5A3.

DEVELOPMENT OF BROAD RANGE SCAN CAPABILITIES WITH JET COOLED CAVITY RINGDOWN SPECTROSCOPY

TERRANCE J. CODD, MING-WEI CHEN and TERRY A. MILLER, Laser Spectroscopy Facility, The Ohio State University, Columbus, Ohio 43210.
THE JET-COOLED HIGH RESOLUTION $\tilde{A}^2E'' - \tilde{X}^2A'_2$ VIBRONIC BANDS OF NO$_3$

MING-WEI CHEN, TERRANCE J. CODD, GABRIEL M. P. JUST, and TERRY A. MILLER, Laser Spectroscopy Facility, Department of Chemistry, The Ohio State University, 120 W. 18th Avenue, Columbus, Ohio 43210.

*present address: Lawrence Berkeley National Laboratory, Berkeley, CA 94720

CAVITY RINGDOWN SPECTROSCOPY AND KINETICS OF HO$_2$+HCHO: DETECTION OF THE $\nu_1$ AND $\tilde{A}$-$\tilde{X}$ BANDS OF HOCH$_2$OO

MATTHEW K. SPRAGUE, MITCHIO OKUMURA, California Institute of Technology, Division of Chemistry, MC 127-72, Pasadena, CA 91125; and STANLEY P. SANDER, Jet Propulsion Laboratory, California Institute of Technology, MS 183-901, Pasadena, CA 91109.

*Support from the NDSEG Fellowship, California Air Resources Board Contracts 03-333 and 07-730, and NASA Upper Atmosphere Research Program Grants NAG5-11657, NNG06GD88G and NNX09AE21G are gratefully acknowledged

CAVITY RINGDOWN SPECTROSCOPY AND KINETICS OF BUTOXY ISOMERIZATION: DETECTION OF THE $\tilde{A}$-$\tilde{X}$ BAND OF HOC$_4$H$_8$OO

MATTHEW K. SPRAGUE, MITCHIO OKUMURA, California Institute of Technology, Division of Chemistry, MC 127-72, Pasadena, CA 91125; and STANLEY P. SANDER, Jet Propulsion Laboratory, California Institute of Technology, MS 183-901, Pasadena, CA 91109.

*Support from the NDSEG Fellowship, California Air Resources Board Contracts 03-333 and 07-730, and NASA Upper Atmosphere Research Program Grants NAG5-11657, NNG06GD88G and NNX09AE21G are gratefully acknowledged

STUDY OF PHENYLACETYLENE BY CAVITY RING-DOWN SPECTROSCOPY

GARY V. LOPEZ, PHILIP M. JOHNSON, TREvor J. SEARS, Department of Chemistry, Stony Brook University, Stony Brook, New York 11794; and CHIH-HSUAN CHANG, Department of Chemistry, Brookhaven National Laboratory, Upton, New York 11973.

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

SPECTROSCOPY AND IONIZATION THRESHOLDS OF ISOELECTRONIC 1-PHENYLALLYL AND BENZYLALLENYL RESONANCE STABILIZED RADICALS

JOSHUA A. SEBREE, NATHAN KIDWELL, EVAN BUCHANAN, TIMOTHY S. ZWIER, Department of Chemistry, Purdue University, West Lafayette, IN 47907; MAREK ZGIERSKI, National Research Council Canada, Ottawa, ON.
TE. ATMOSPHERIC SPECIES
TUESDAY, JUNE 21, 2011 – 8:30 am
Room: 2015 McPHERSON LAB

Chair: VINCENT BOUDON, CNRS - Universite de Bourgogne, Dijon, France

TE01 15 min 8:30
LINE PARAMETERS OF CARBON DIOXIDE IN THE 4850 CM$^{-1}$ REGION

D. CHRIS BENNER, V. MALATHY DEVI, EMILY NUGENT, Department of Physics, College of William and Mary, Williamsburg, VA 23187-8795; KEEYOUNG SUNG, LINDA R. BROWN, CHARLES E. MILLER, ROBERT A. TOTH, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr., Pasadena, CA 91109, U.S.A..

TE02 15 min 8:47
TOWARDS AN ACCURATE INFRARED LINELIST FOR CO$_2$ AND ISOTOPOLOGUES

TIMOTHY J. LEE, MS 245-1, NASA Ames Research Center, Moffett Field, CA, 94035; XINCHUAN HUANG, SETI Institute, 189 Bernardo Ave, Suite 100, Mountain View, CA, 94043; DAVID W. SCHWENKE, MS T27B-1, NASA Ames Research Center, Moffett Field, CA, 94035; and SERGEY TASHKUN, Laboratory of Theoretical Spectroscopy, V.E. Zuev Institute of Atmospheric Optics, SB, Russian Academy of Science, 634055, Tomsk, Russia.

TE03 15 min 9:04
SELF- AND AIR-BROADENING OF $^{12}$C$^{16}$O, $^{13}$C$^{16}$O AND $^{12}$C$^{18}$O AT 2.3 µm


TE04 15 min 9:21
MEASUREMENTS OF LINE POSITIONS AND INTENSITIES OF $^{14}$NH$_3$ IN THE 1.5 µm REGION


TE05 15 min 9:38
THE 5-0 OVERTONE BAND OF HCl BY INTRACAVITY LASER ABSORPTION SPECTROSCOPY

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

Intermission
FREQUENCY COMB-REFERENCE MEASUREMENTS OF SELF- AND NITROGEN-PERTURBED LINE SHAPES IN THE $\nu_1 + \nu_3$ BAND OF ACETYLENE

MATTHEW J. CICH, GARY V. LOPEZ, TREVOR J. SEARS*, Department of Chemistry, Stony Brook University, Stony Brook, New York 11794; C. P. MCRAVEN, 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; and DANIEL HURTMAND, Service de Chimie Quantique et de Photophysique(Atoms, Molecules et Atmospheres), Universite Libre de Bruxelles, Bruxelles, Belgium B-10050.

TEMPERATURE DEPENDENCE OF SELF- and NITROGEN-GAS LINE SHAPE PERTURBATIONS IN THE $\nu_1 + \nu_3$ BAND OF ACETYLENE

MATTHEW J. CICH, GARY V. LOPEZ, TREVOR J. SEARS*, Department of Chemistry, Stony Brook University, Stony Brook, New York 11794; C. P. MCRAVEN, 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; and DANIEL HURTMAND, Service de Chimie Quantique et de Photophysique(Atoms, Molecules et Atmospheres), Universite Libre de Bruxelles, Bruxelles, Belgium B-10050.

REVISION OF SPECTRAL PARAMETERS FOR THE B- AND $\gamma$-BANDS OF OXYGEN AND THEIR VALIDATION USING ATMOSPHERIC SPECTRA WITH THE SUN AS SOURCE

I. E. GORDON, L. S. ROTHMAN, Harvard-Smithsonian Center for Astrophysics, Atomic and Molecular Physics Division, Cambridge MA 02138, USA; G. C. TOON, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Drive, Pasadena, CA 91109, USA.

ROTATIONAL AND HYPERFINE ANALYSIS OF THE $a^1 \Delta_g - X^3 \Sigma_g^-$ BAND OF $^{17}$O-CONTAINING ISOTOPOLOGUES OF OXYGEN MEASURED BY CRDS AT ROOM AND LIQUID NITROGEN TEMPERATURES

O. M. LESHCISHINA, S. KASSI, Université de Grenoble, CNRS UMR 5588, LIPHY, 38041 Grenoble, France; I. E. GORDON, Harvard-Smithsonian Center for Astrophysics, Atomic and Molecular Physics Division, Cambridge MA 02138-1516, USA; S. YU, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Drive, Pasadena, CA 91109, USA; A. CAMPARGUE, Université de Grenoble, CNRS UMR 5588, LIPHY, 38041 Grenoble, France.

A GLOBAL FIT OF THE $X^3 \Sigma_g^-, a^1 \Delta_g, b^1 \Sigma_g^+$ AND $B^3 \Sigma_u^-$ STATES OF THE SIX ISOTOPOLOGUES OF OXYGEN

SHANSHAN YU, CHARLES E. MILLER AND BRIAN J. DROUIN, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109; HOLGER S.P. MÜLLER, I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany.
NEW HIGH RESOLUTION OZONE ABSORPTION CROSS SECTIONS

ANNA SERDYUCHENKO, VICTOR GORSHELEV, MARK WEBER, and JOHN P. BURROWS, Institute for Environmental Physics, University of Bremen, Otto-Hahn Allee 1, D-28359 Bremen, Germany.

LINE MIXING IN ATMOSPHERIC OZONE

COREY CASTO AND FRANK C. DE LUCIA, Department of Physics, The Ohio State University, Columbus, OH 43210-1106.
TF ASTRONOMICAL SPECIES AND PROCESSES
TUESDAY, JUNE 21, 2011 – 1:30 pm
Room: 160 MATH ANNEX

Chair: NATHAN CROCKETT, University of Michigan, Ann Arbor, Michigan

TF01 15 min 1:30
GISBERT WINNEWISSER: AN APPRECIATION
ERIC HERBST, Departments of Physics, Chemistry, and Astronomy, The Ohio State University, Columbus OH.

TF02 15 min 1:47
SCRUTINY OF THE CORE OF THE GALACTIC CENTER BY H$_3^+$ AND CO: GCIRS 3 AND GCIRS 1W
M. GOTO, Max-Planck-Institute for Astronomy, Heidelberg, D-69117, Germany; T. USUDA, Subaru Telescope, Hilo, HI 96720; T. R. GEBALLE, Gemini Observatory, Hilo, HI 96720; N. INDRIOLO, B. J. MCCALL, Department of Astronomy and Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801; T. OKA, Department of Astronomy and Astrophysics and Department of Chemistry, University of Chicago, Chicago, IL 60637.

TF03 15 min 2:04
INVESTIGATING THE COSMIC-RAY IONIZATION RATE IN THE GALACTIC ISM WITH H$_3^+$ OBSERVATIONS
NICK INDRIOLO, Department of Astronomy, University of Illinois at Urbana-Champaign, Urbana, IL 61801; THOMAS R. GEBALLE, Gemini Observatory, Hilo, HI 96720; TAKEHI OKA, Department of Astronomy & Astrophysics and Department of Chemistry, University of Chicago, Chicago, IL 60637; BENJAMIN J. McCALL, Departments of Astronomy and Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801.

TF04 10 min 2:21
CAVITY RING DOWN SPECTROSCOPY OF MOLECULAR IONS IN THE 3 µm REGION
JOSEPH S. GUSS, HARALD VERBRAAK and HAROLD LINNARTZ, Leiden Observatory, University of Leiden, 2300 RA Leiden, The Netherlands.

TF05 15 min 2:33
SUBMILLIMETER-WAVE ROTATIONAL SPECTROSCOPY OF H$_2$F$^+$
R. FUJIMORI, K. KAWAGUCHI, Department of Chemistry, Faculty of Science, Okayama University, 3-1-1, Tsushima-Naka, Okayama 700-8530, Japan; T. AMANO, Department of Chemistry and Department of Physics and Astronomy, University of Waterloo, 200 University Avenue West, Waterloo, ON N2L 3G1, Canada.

TF06 15 min 2:50
DETECTION OF FeCN (X$^2\Delta_u$) IN THE CIRCUMSTELLAR ENVELOPE OF IRC+10216
L. N. ZACK, D. T. HALFEN, and L. M. ZIURYS, Department of Chemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, AZ, 85721.
THE QUEST FOR COMPLEX MOLECULES IN SPACE. SEARCHES FOR CYANIDES RELATED TO \textit{n-}\textit{PROPYL CYANIDE IN SGR B2(N)}


\textbf{Intermission}

WHAT MOLECULAR LINES CAN TELL ABOUT EARLY STAGES OF MASSIVE STARS

\textbf{TATIANA VASYUNINA, ERIC HERBST}, \textit{Ohio State University, 191 W. Woodruff Ave., 43210, Columbus, OH, USA}; \textbf{HENDRIK LINZ, THOMAS HENNING, HENRIK BEUTHER}, \textit{Max Planck Institute for Astronomy (MPIA), Königstuhl 17, D-69117 Heidelberg, Germany}; \textbf{IGOR ZINCHENKO}, \textit{Institute of Applied Physics of the Russian Academy of Sciences, Ulyanova 46, 603950 Nizhny Novgorod, Russia}; \textbf{MAXIM VORONKOV}, \textit{Australia Telescope National Facility, CSIRO Astronomy and Space Science, PO Box 76, Epping, NSW 1710, Australia}.

NUCLEAR SPIN OF H$_3^+$ IN DIFFUSE MOLECULAR CLOUDS

\textbf{KYLE N. CRABTREE, NICK INDRIOLO, HOLGER KRECKEL, BRIAN A. TOM}, \textbf{BENJAMIN J. Mc-CALL}, \textit{Department of Chemistry, University of Illinois, Urbana, IL 61801, USA}.

MOLECULAR ABUNDANCES IN THE DISK OF AN ACTIVE GALACTIC NUCLEUS

\textbf{N. HARADA}, \textit{Department of Physics, The Ohio State University, Columbus, OH, U.S.A., 43210}; \textbf{T. A. THOMPSON}, \textit{Department of Astronomy and Center for Cosmology and Astro-Particle Physics (CCAPP), The Ohio State University, Columbus, OH, U.S.A., 43210}; \textbf{E. HERBST}, \textit{Departments of Physics, Astronomy, and Chemistry, The Ohio State University, Columbus, OH, U.S.A., 43210}.

A STUDY OF HCO$^+$ AND CS IN PLANETARY NEBULAE

\textbf{JESSICA L. DODD, L. M. ZIURYS, N. J. WOOLF}, \textit{Department of Chemistry and Biochemistry, Department of Astronomy, Steward Observatory, The University of Arizona, Tucson, AZ 85721}.

THE ARO 1 mm SURVEY OF THE OXYGEN-RICH ENVELOPE OF SUPERGIANT STAR NML CYGNUS

\textbf{JESSICA L. DODD, L. M. ZIURYS, N. J. WOOLF}, \textit{Department of Chemistry and Biochemistry, Department of Astronomy, Steward Observatory, The University of Arizona, Tucson, AZ 85721}. 
WATER COLLISIONS WITH NORMAL AND PARAHYDROGEN

**BRIAN J. DROUIN, JOHN C. PEARSON, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109-8099; LAURENT WIESENFELD, ALEXANDRE FAURE, UJF-Grenoble 1/CNRS, Institut de Planétologie et d’Astrophysique de Grenoble (IPAG) UMR 5274, Grenoble, F-38041, France.**

LOW TEMPERATURE LINESHAPE OF HYDROGEN DEUTERIDE

**BRIAN J. DROUIN, HARSHAL GUPTA, JOHN C. PEARSON, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109-8099.**

A QUANTUM CHEMICAL INVESTIGATION OF THE STABILITY AND CHEMISTRY OF THE ANIONS OF CO AND H₂CO IN ASTROPHYSICAL ICES

**L. CHEN and D. E. WOON, Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana IL 61801.**

WARM AND DIFFUSE GAS AND HIGH IONIZATION RATE NEAR THE GALACTIC CENTER

**T. OKA, C. P. MORONG, Department of Astronomy and Astrophysics and Department of Chemistry, University of Chicago, Chicago, IL 60637; T. R. GEBALLE, Gemini Observatory, Hilo, HI 96720; N. INDRIOLO, B. J. MCCALL, Department of Astronomy and Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801; M. GOTO, Max-Planck-Institute for Astronomy, Heidelberg, D-69117, Germany; T. USUDA, Subaru Telescope, Hilo, HI 96720.**
TG. ELECTRONIC
TUESDAY, JUNE 21, 2011 – 1:30 pm
Room: 170 MATH ANNEX

Chair: DAVID PRATT, University of Pittsburgh, Pittsburgh, Pennsylvania

TG01 15 min 1:30
FREQUENCY AND TIME DOMAIN STUDIES OF TOLUENE

ADRIAN M. GARDNER, ALISTAIR M. GREEN, JULIA A. DAVIS, KATHARINE L. REID and TIMOTHY G. WRIGHT, School of Chemistry, University of Nottingham, University Park, Nottingham, NG7 2RD, United Kingdom.

TG02 15 min 1:47
HYDROGEN-BOUND COMPLEXES OF TROPOLONE: GATEWAYS FOR THE INTERROGATION OF MULTIPLE PROTON-TRANSFER EVENTS

DEACON J. NEMCHICK, KATHRYN CHEW, JOHN E. WOLFF, and PATRICK H. VACCARO, Department of Chemistry, Yale University, P.O. Box 208017, New Haven, CT 06520-8107 USA.

TG03 15 min 2:04
ROTATION-TUNNELING ANALYSIS OF EXCITED-STATE PROTON TRANSFER IN DEUTERATED TROPOLONE

KATHRYN CHEW, DEACON J. NEMCHICK, JOHN E. WOLFF, and PATRICK H. VACCARO, Department of Chemistry, Yale University, P.O. Box 208107, New Haven, CT 06520-8107 USA.

TG04 15 min 2:21
LASER SPECTROSCOPIC STUDY ON STRUCTURES OF 3n-CROWN-n (n = 4, 5, 6) COMPLEXES WITH PHENOL

RYOJI KUSAKA and TAKAYUKI EBATA, Department of Chemistry, Graduate School of Science, Hiroshima University, Higashi-Hiroshima, 739-8526, Japan.

TG05 15 min 2:38
HIGH RESOLUTION STARK SPECTROSCOPY OF MODEL DONOR-ACCEPTOR AMINOBENZONITRILES IN THE GAS PHASE.*

ADAM J. FLEISHER, CASEY L. CLEMENTS, RYAN G. BIRD, DAVID W. PRATT, Department of Chemistry, University of Pittsburgh, Pittsburgh, PA 15260; LEONARDO ALVAREZ-VALTIERRA, División de Ciencias e Ingenierías, Universidad de Guanajuato, Campus León, León, Gto. 37150, Mexico.

*Work supported by the NSF (CHE-0911117).

TG06 15 min 2:55
ROTATIONALLY RESOLVED ELECTRONIC SPECTROSCOPY OF BIOMOLECULES IN THE GAS PHASE. MELATONIN.

JOHN T. YI, and DAVID W. PRATT, University of Pittsburgh, Department of Chemistry, Pittsburgh, PA 15260, USA; CHRISTIAN BRAND, MIRIAM WOLLENHAPU, and MICHAEL SCHMITT, Heinrich-Heine-Universität, Institut für Physikalische Chemie I, 40225 Düsseldorf, Germany; W. LEO MEERTS, Radboud University Nijmegen, Institute for Molecules and Materials, Heyendaalseweg 135, NL-6525 AJ Nijmegen, The Netherlands.
TG07 15 min 3:12
VIBRONIC SPECTROSCOPY OF JET-COOLED 1,4-PHENYLENE DIISOCYANIDE

DEEPAK N. MEHTA, ANNA K. GUTBERLET, and TIMOTHY S. ZWER, Department of Chemistry, Purdue University, West Lafayette, IN 47907.

Intermission

TG08 15 min 3:45
EXCITED STATE DYNAMICS OF 7-AZAINDOLE HOMODIMER IN FROZEN NITROGEN MATRIX

MOITRAYEE MUKHERJEE, BIMAN BANDYOPADHYAY, SHRUTAMA KARMAKAR and TAPAS CHAKRABORTY, Physical Chemistry Department, Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700032, India.

TG09 15 min 4:02
EXCITED STATE PERTURBATIONS OF 7-AZAINDOLE MEDIATED THROUGH MICRO-SOLVATION.a

JUSTIN W. YOUNG, and DAVID W. PRATT, Department of Chemistry, University of Pittsburgh, Pittsburgh, PA 15260.

aWork supported by NSF(CHE-0911117)

TG10 15 min 4:19
CHIROPTICAL SPECTROSCOPY IN THE VAPOR PHASE

PRIYANKA LAHIRI, BENJAMIN D. LONG, KENNETH B. WIBERG, and PATRICK H. VACCARO, Department of Chemistry, Yale University, P.O. Box 208107, New Haven, CT 06520-8107 USA.

TG11 15 min 4:36
SINGLE MOLECULE SPECTROSCOPIC STUDY OF TWO ORGANIC RECTIFIERS

DEBRA JO SCARDINO, RAJESH KOTA, DANIEL L. MATTERN, and NATHAN I. HAMMER, University of Mississippi, Department of Chemistry & Biochemistry, Oxford, MS 38677.

TG12 15 min 4:53
THE ROLE OF $\pi\sigma^*$ STATE IN INTRAMOLECULAR CHARGE TRANSFER OF 4-(DIMETHYLAMINO)-BENZONITRILE AND RELATED MOLECULES

TAKASHIGE FUJIWARA, Department of Physics, The Ohio State University, Columbus OH 43210; MAREK Z. ZGIESKI, Steacie Institute for Molecular Science, National Research Council of Canada, Ottawa, K1A 0R6 CANADA; EDWARD C. LIM, Department of Chemistry and The Center for Laser and Optical Spectroscopy, The University of Akron, Akron OH 44325-3601.

TG13 15 min 5:10
ULTRAFAST DYNAMICS IN NITRO- AND (ORGANOPHOSPHINE)GOLD(I)-POLYCYCLIC AROMATIC HYDROCARBONS

R. AARON VOGT, CHRISTIAN REICHARDT, CARLOS E. CRESPO-HERNÁNDEZ, THOMAS G. GRAY, Department of Chemistry and Center for Chemical Dynamics, Case Western Reserve University, Cleveland, Ohio 44106, USA.
EXCITED STATE DYNAMICS IN 2-AMINOPURINE RIBONUCLEOSIDE: FROM FEMTOSECOND TO MICROSECOND TIME SCALE

CHENGWEI WEN, CHRISTIAN REICHARDT, CARLOS E. CRESPO-HERNÁNDEZ. Department of Chemistry and Center for Chemical Dynamics, Case Western Reserve University, 10900 Euclid Ave., Cleveland, Ohio 44106.
TH. MINI-SYMPOSIUM: SPECTROSCOPIC PERTURBATIONS
TUESDAY, JUNE 21, 2011 – 1:30 pm
Room: 1000 McPHERSON LAB

Chair: CAROLINE CHICK JARROLD, Indiana University, Bloomington, Indiana

TH01 30 min 1:30
Journal of Molecular Spectroscopy Review Lecture
PERTURBATIONS I HAVE KNOWN AND LOVED
ROBERT W. FIELD, Department of Chemistry, MIT, Cambridge, MA.

TH02 15 min 2:05
VIBRONIC PERTURBATIONS IN THE ELECTRONIC SPECTRUM OF BeC
BEAU J. BARKER, IVAN O. ANTONOV, MICHAEL C. HEAVEN, Department of Chemistry, Emory University, Atlanta, GA 30322; RICHARD DAWES, Department of Chemistry, Missouri University of Science and Technology, Rolla, MO 65409.

TH03 15 min 2:22
PERTURBATIONS IN THE SPECTRA OF HIGH RYDBERG STATES: CHANNEL INTERACTIONS, STARK AND ZEEMAN EFFECTS
CHRISTA HAASE, MARTIN SCHÄFER, STEPHEN D. HOGAN and FRÉDÉRIC MERKT, Laboratorium für Physikalische Chemie, ETH-Zürich, 8093 Zürich, Switzerland.

TH04 15 min 2:39
DATA AND ANALYSIS OF SPIN-ORBIT COUPLED $A^1\Sigma_u^+$ AND $b^3\Pi_u$ STATES OF Cs$_2$
ANDREY V. STOLYAROV, Department of Chemistry, Moscow State University, GSP-2 Leninskiie gory 1/3, Moscow 119992, Russia; THOMAS H. BERGEMAN, Department of Physics and Astronomy, State University of New York, Stony Brook, New York 11794-3800.

TH05 15 min 2:56
SPECTROSCOPIC SIGNATURES OF ISOMERIZATION IN THE S$_1$ STATE OF C$_2$H$_2$
J. H. BARABAN, A. H. STEEVES, 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.

TH06 15 min 3:13
EVIDENCE OF PERTURBATIONS ON THE S$_1$ SURFACE OF ACETYLENE FROM PATTERNS IN STIMULATED EMISSION PUMPING SPECTRA
G. BARRATT PARK, JOSHUA H. BARABAN, ADAM H. STEEVES, and ROBERT W. FIELD, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139.
Intermission

TH07 15 min 3:45
THE GERADE RYDBERG STATES OF MOLECULAR HYDROGEN

DANIEL SPRECHER and FRÉDÉRIC MERKT, ETH Zürich, Laboratorium für Physikalische Chemie, Wolfgang-Pauli-Strasse 10, 8093 Zürich, Switzerland; CHRISTIAN JUNGEN, Laboratoire Aimé Cotton, CNRS II, Bâtiment 505, Campus d’Orsay, 91405 Orsay Cedex, France.

TH08 15 min 4:02
ROTATIONALLY RESOLVED SPECTROSCOPY OF THE ELECTRONICALLY EXCITED C AND D STATES OF ArXe AND KrXe

LORENA PITICCO, MARTIN SCHÄFER, and FRÉDÉRIC MERKT, ETH Zürich, Laboratorium für Physikalische Chemie, Wolfgang-Pauli-Strasse 10, 8093 Zürich, Switzerland.

TH09 15 min 4:19
ANALYSIS OF STRONGLY PERTURBED $^{1}_1\Pi - 2^{3}\Sigma^+ - b^{3}\Pi$ STATES OF THE KRb MOLECULE

J. T. KIM, Department of Photonic Engineering, Chosun University, Gwangju, 501-759, Korea; Y. LEE, Department of Chemistry, Mokpo National University, Jeonnam 534-729, Korea; B. KIM, Department of Chemistry, KAIST, Daejeon, 305-701, Korea; D. WANG, Department of Physics, The Chinese University of Hong Kong, Shatin, Hong Kong; W. C. STWALLEY, P. L. GOULD, and E. E. EYLER, Department of Physics, University of Connecticut, Storrs, CT 06269, USA.

TH10 15 min 4:36
OBSERVATION OF THE SYSTEM $(1)^1\Sigma_u^+ - (1)^3\Pi_u$ of SR$_2$ BY FOURIER TRANSFORM SPECTROSCOPY AND ITS ANALYSIS

A. STEIN, H. KNÖCKEL, and E. TIEMANN, Institut für Quantenoptik, Leibniz Universität Hannover, Welfengarten 1, 30167 Hannover, Germany.

TH11 15 min 4:53
A NEW ANALYSIS OF A VERY OLD SPECTRUM: THE HIGHLY PERTURBED $A^2\Pi_i - X^2\Pi$, BAND SYSTEM OF THE CHLORINE CATION (Cl$_2^+$)

MOHAMMED A. GHARAIBEH, DENNIS J. CLOUTHIER, Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055.

TH12 15 min 5:10
PROBING THE ELECTRONIC STRUCTURE OF THE NICKEL MONOHALIDES: SPECTROSCOPY OF THE LOW-LYING ELECTRONIC STATES OF NiX (X=Cl,Br,I)

LLOYD MUZANGWA, VICTORIA AYLES, SILVER NYAMBO AND SCOTT A. REID, Department of Chemistry, Marquette University, Milwaukee, WI 53233.
TH13 15 min 5:27  
LASER-INDUCED FLUORESCENCE SPECTROSCOPY ON ROTATIONAL DISTRIBUTION OF HF PHOTIONS

MATT GRAU, HUANQIAN LOH, TYLER YAHN, RUSSELL STUTZ, JILA, NIST and University of Colorado, and Department of Physics, University of Colorado, Boulder, Colorado 80309-0440; ROBERT W. FIELD, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139; and ERIC A. CORNELL, JILA, NIST and University of Colorado, and Department of Physics, University of Colorado, Boulder, Colorado 80309-0440.

TH14 15 min 5:44
PERTURBATIONS IN THE GROUND ELECTRONIC STATE ROTATIONAL SPECTRUM OF TRANSITION-METAL CONTAINING MOLECULES

D. T. HALFEN, Department of Chemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, AZ 85721; R. W. FIELD, Department of Chemistry, MIT, Cambridge, MA 02139; and L. M. ZIURYS, Department of Chemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, AZ 85721.
TI. INFRARED/RAMAN
TUESDAY, JUNE 21, 2011 – 1:30 pm
Room: 1015 McPHERSON LAB

Chair: GEOFFREY DUXBURY, University of Strathclyde, Glasgow, Scotland, UK

T01 15 min 1:30
INFRARED SPECTRA OF COMPLEXES CONTAINING ACETYLENE-d2

CLÉMENT LAUZIN, J. NOROOZ OLIAEE, N. MOAZZEN-AHMADI, Department of Physics and Astronomy, University of Calgary, 2500 University Dr., N.W., Calgary, AB T2N 1N4, Canada; A.R.W. MCKELLAR, Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, ON K1A 0R6, Canada.

T02 15 min 1:47
HIGH RESOLUTION OVERTONE SPECTROSCOPY OF ACETYLENE VAN DER WAALS COMPLEXES


T03 10 min 2:04
HIGH RESOLUTION OVERTONE SPECTROSCOPY OF THE ACETYLENE VAN DER WAALS DIMER, 12(C2H2)2


T04 15 min 2:16
THE WEAKLY–BOUND CO2–ACETYLENE COMPLEX: FUNDAMENTAL AND TORSIONAL COMBINATION BAND IN THE CO2 ν3 REGION

C. LAUZIN, Laboratoire de Chimie quantique et Photophysique, CP160/09 Faculté des Sciences, Université Libre de Bruxelles (U.L.B.), Ave. Roosevelt, 50 B-1050 Brussels, Belgium; J. NOROOZ OLIAEE, M. REZAEI, N. MOAZZEN-AHMADI, Department of Physics and Astronomy, University of Calgary, Calgary, AB T2N 1N4, Canada.

T05 15 min 2:33
HIGH RESOLUTION INFRARED AND MICROWAVE SPECTRA OF NH3-HCCH AND NH3-OCS COMPLEXES: STUDIES OF WEAK C-H···N HYDROGEN BOND AND ELECTRIC MULTIPOLe INTERACTIONS

XUNCHEN LIU, YUNJIE XU, Department of Chemistry, University of Alberta, Edmonton, Canada, T6G 2G2.

T06 15 min 2:50
INFRARED SPECTRA OF WATER BENDING BANDS OF PROPYLENE OXIDE-WATER COMPLEXES: SEQUENTIAL SOLVATION OF A CHIRAL MOLECULE IN WATER

XUNCHEN LIU, YUNJIE XU, Department of Chemistry, University of Alberta, Edmonton, Canada, T6G 2G2.
Intermission

TI07
FIRST INFRARED SPECTRA OF CN-RARE GAS AND CN-H₂/D₂ COMPLEXES VIA IR-UV FLUORESCENCE DEPLETION SPECTROSCOPY

BRIDGET A. O’DONNELL, MELODIE TING, JOSEPH M. BEAMES, and MARSHA I. LESTER,Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323.

*Research is supported by the Chemistry Division of the National Science Foundation

TI08
CARBON DIOXIDE CLUSTERS: (CO₂)₆ TO (CO₂)₁₃

A.R.W. MCKELLAR, Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, ON K1A 0R6, Canada; J. NOROOZ OLIAE, M. DEHGHANY, and N. MOAZZEN-AHMADI, Department of Physics and Astronomy, University of Calgary, 2500 University Dr., N.W., Calgary, AB T2N 1N4, Canada.

TI09
THEORETICAL AND EXPERIMENTAL STUDY OF THE ROVIBRATIONAL SPECTRA OF CO₂-(para-H₂)-He TRIMERS

HU LIN, Institute of Theoretical Chemistry, State Key Lab. of Theoretical & Computational Chemistry, Jilin Univ., 2519 Jiefang Rd, Changchun 130023, P.R.China; Chemistry Dept., Univ. of Waterloo, Waterloo, Ontario N2L 3G1, Canada; ROBERT J. LE ROY, PIERRE-NICHOLAS ROY, Chemistry Dept., Univ. of Waterloo, Waterloo, Ontario N2L 3G1, Canada; A. R. W. McKELLAR, Steacie Institute for Molecular Sciences, NRCC, Ottawa, Ontario K1A 0R6, Canada.

TI10
SPECTROSCOPIC OBSERVATION OF CS₂ DIMER

M. REZAEI, J. NOROOZ OLIAE, N. MOAZZEN-AHMADI, Department of Physics and Astronomy, University of Calgary, Calgary, AB T2N 1N4, Canada; A.R.W. MCKELLAR, Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, ON K1A 0R6, Canada.

TI11
INFRARED SPECTRA OF CS₂ TRIMER: OBSERVATION OF AN ISOMER WITH D₃ SYMMETRY

M. REZAEI, J. NOROOZ OLIAE, N. MOAZZEN-AHMADI, Department of Physics and Astronomy, University of Calgary, Calgary, AB T2N 1N4, Canada; A.R.W. MCKELLAR, Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, ON K1A 0R6, Canada.

TI12
INFRARED SPECTRA OF He–CS₂, Ne–CS₂, AND Ar–CS₂

F. MIVEHVAR, J. NOROOZ OLIAE, N. MOAZZEN-AHMADI, Department of Physics and Astronomy, University of Calgary, Calgary, AB T2N 1N4, Canada.
TJ. THEORY
TUESDAY, JUNE 21, 2011 – 1:30 pm
Room: 2015 McPHERSON LAB

Chair: JUANA VAZQUEZ, University of Texas at Austin, Austin, Texas

TJ01
A SEMICLASSICAL DIRECT POTENTIAL FITTING SCHEME FOR DIATOMICS

J. TELLINGHUISEN, Department of Chemistry, Vanderbilt University, Nashville, TN 37235.

TJ02
UNEXPECTED PROPERTIES OF THE MORSE OSCILLATOR

ANNE B. McCOY, Department of Chemistry, The Ohio State University, Columbus, OH 43210.

TJ03
IMPROVED DIABATIC MODEL FOR VIBRONIC COUPLING IN THE GROUND ELECTRONIC STATE OF NO₃

J.F. STANTON, Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, TX 78712.

TJ04
EFFECT OF JAHN-TELLER AND SPIN-ORBIT COUPLING ON $\tilde{X}^{2}E$ INFRARED SPECTRUM OF CH₃O

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

TJ05
VIBRATIONAL DYNAMICS AROUND THE CONICAL INTERSECTION RESULTING FROM THE $\tilde{A} \rightarrow \tilde{X}$ LASER INDUCED FLUORESCENCE OF THE METHOXY (CH₃O) RADICAL

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

TJ06
BREAKING THE SYMMETRY IN JAHN-TELLER ACTIVE MOLECULES BY ASYMMETRIC ISOTOPIIC SUBSTITUTION: SPLITTING THE ZERO-POINT VIBRONIC LEVEL.

DMITRY G. MELNIK, JINJUN LIU, TERRY A. MILLER, Laser Spectroscopy Facility, Department of Chemistry, The Ohio State University, 120 W. 18th Avenue, Columbus, Ohio 43210; ROBERT F. CURL, Department of Chemistry and Rice Quantum Institute, Rice University, Houston, Texas 77005.

TJ07
AN ALGEBRAIC METHOD FOR EXPLORING QUANTUM MONODROMY AND QUANTUM PHASE TRANSITIONS IN NON-RIGID MOLECULES

D. LARESE, Department of Chemistry, Yale University, New Haven CT 06520-8107, USA; F. IACHELLO, Center for Theoretical Physics, Yale University, New Haven CT 06520-8120, USA.
VIBRATIONALLY AVERAGED LONG-RANGE MOLECULE-MOLECULE DISPERSION COEFFICIENTS FROM COUPLED-CLUSTER CALCULATIONS

MATTHEW SCHMIDT and MARCEL NOOIJEN, Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada.

Intermission

EXOMOL: MOLECULAR LINE LISTS FOR EXOPLANET AND OTHER ATMOSPHERES

J. TENNYSON, R. J. BARBER, A. AZZAM, M. DOWN, and C. HILL, Department of Physics and Astronomy, University College London, London, WC1E 6BT, UK; S. N. YURCHENKO, Technische Universität Dresden, Physikalische Chemie, D–01062 Dresden, Germany.

USING DIFFUSION MONTE CARLO TO PROBE THE ROTATIONALLY EXCITED STATES OF H$_3^+$ AND ITS ISOTOPOLOGUES

BETHANY A. WELLEN, ANDREW S. PETIT, and ANNE B. McCOY, Department of Chemistry, The Ohio State University, Columbus, OH 43210.

COMPUTATIONAL HIGH-FREQUENCY OVERTONE SPECTRA OF THE WATER AMMONIA COMPLEX

ELINA SÄLLI and LAURI HALONEN, Laboratory of Physical Chemistry, University of Helsinki, Finland (email to elina.salli@helsinki.fi).


TEEMU SALMI, LAURI HALONEN, Laboratory of Physical Chemistry, P.O. Box 55 (A.I. Virtasen aukio 1), FIN-00014 University of Helsinki, Finland.

COLLISION INDUCED VELOCITY CHANGES FROM MOLECULAR DYNAMIC SIMULATIONS. APPLICATION TO THE SPECTRAL SHAPE OF THE Q(1) RAMAN LINES OF H$_2$/H$_2$.H.TRAN and J.M. HARTMANN, Laboratoire Interuniversitaire des Systemes Atmospheriques, Université Paris Est Creteil et Université Paris Diderot, 94010 Creteil Cedex, France.

EFFECTIVE POTENTIAL APPROACH TO THE SIMULATION OF LARGE PARA-HYDROGEN CLUSTERS AND DROPLETS

JING YANG and PIERRE-NICHOLAS ROY, Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada.
TJ15 15 min 5:32
SIMULATION STUDIES OF THE VIBRATIONAL DYNAMICS OF para-HYDROGEN CLUSTERS

NABIL F. FARUK, JING YANG, ROBERT J. LE ROY, PIERRE-NICHOLAS ROY, Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada.

TJ16 15 min 5:49
MIXED CLUSTERS OF H₂ AND H₂O: INSIGHTS FROM THEORY AND SIMULATIONS

TAO ZENG, HUI LI, ROBERT J. LE ROY, PIERRE-NICHOLAS ROY, Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada.
WA. PLENARY
WEDNESDAY, JUNE 22, 2011 – 8:30 am
Room: AUDITORIUM, INDEPENDENCE HALL

Chair: MALCOLM CHISHOLM, The Ohio State University, Columbus, Ohio

WA01 40 min 8:30
THE ATMOSPHERIC CHEMISTRY EXPERIMENT, ACE: LATEST RESULTS

P. F. BERNATH, Department of Chemistry, University of York, Heslington, York, YO10 5DD, UK.

WA02 40 min 9:15
CHASING NONEXISTENT COMPOUNDS WITH LASERS: ELECTRONIC SPECTROSCOPY OF MAIN GROUP TRANSIENT MOLECULES, FREE RADICALS, AND IONS

DENNIS J. CLOUTHIER, Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055.

Intermission

WA03 40 min 10:20
WATCHING CONFORMATIONS OF BIOMOLECULES: A MICROWAVE SPECTROSCOPY APPROACH


WA04 40 min 11:05
POLAR MOLECULES IN THE QUANTUM REGIME

DEBORAH S. JIN, JUN YE, JILA, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY AND UNIVERSITY OF COLORADO, BOULDER, CO 80309-0440, USA.
WF01  15 min  1:30
INTERSTELLAR NITRILE CHEMISTRY AS REVEALED BY CHIRPED-PULSE FTMW SPECTROSCOPY

DANIEL P. ZALESKI, JUSTIN L. NEILL, MATT T. MUCKLE, AMANDA L. STEBER, and BROOKS H. PATE, Department of Chemistry, University of Virginia, McCormick Rd., P.O. Box 400319, Charlottesville, VA 22904.; JOANNA F. CORBY, Department of Astronomy, University of Virginia, McCormick Rd., P.O. Box 400325, Charlottesville, VA 22904.; VALERIO LATTANZI and MICHAEL C. MCCARTHY, Harvard-Smithsonian Center for Astrophysics, 60 Garden St., Cambridge, MA 02138, and School of Engineering and Applied Sciences, Harvard University, 29 Oxford St., Cambridge MA 02138.; ANTHONY J. REMIJAN, National Radio Astronomy Observatory, 520 Edgemont Rd., Charlottesville, VA 22904-2475.

WF02  15 min  1:47
3-D SUBMILLIMETER SPECTROSCOPY OF ASTROPHYSICAL 'WEEDS' – CONTINUED ANALYSIS

SARAH M. FORTMAN, IVAN R. MEDVEDEV, CHRISTOPHER F. NEESE, and FRANK C. DE LUCIA, Department of Physics, 191 W. Woodruff Ave., The Ohio State University, Columbus, OH 43210-1106 USA.

WF03  10 min  2:04
PERFORMANCE OF THE NEW 0.4 mm RECEIVER (602-720 GHz) AT THE SUB-MILLIMETER TELESCOPE OF THE ARIZONA RADIO OBSERVATORY


WF04  15 min  2:16
HIGHLY ACCURATE QUARTIC FORCE FIELDS, VIBRATIONAL FREQUENCIES, AND SPECTROSCOPIC CONSTANTS FOR CYCLIC AND LINEAR C3H3H3+ INCLUDING 13C AND DEUTERIUM ISOTOPOLOGUES

TIMOTHY J. LEE, MS 245-1, NASA Ames Research Center, Moffett Field, CA, 94035; XINCHUAN HUANG, SETI Institute, 189 Bernardo Ave, Suite 100, Mountain View, CA, 94043; and PETER R. TAYLOR, Victorian Life Sciences Computation Initiative and Department of Chemistry, University of Melbourne, Vic 3010, Australia.

WF05  15 min  2:33
A SEARCH FOR HYDROXYLAMINE (NH2OH) TOWARDS IRC+10216, ORION-S, ORION(KL), SGRB2(N), SGRB2(OH), W51M AND W3(IRS5)

ROBIN L. PULLIAM, ANTHONY J. REMIJAN, National Radio Astronomy Observatory, Charlottesville, VA 22903; JOANNA CORBY, Dept. of Astronomy, Dept. of Chemistry, University of Virginia and National Radio Astronomy Observatory, Charlottesville, VA 22903.
WF06 10 min 2:50
A SEARCH FOR INTERSTELLAR CARBON-CHAIN ALCOHOL HC₅OH IN THE STAR FORMING REGION L1527

MITSUNORI ARAKI, Department of Chemistry, Faculty of Science Division I, Tokyo University of Science, 1-3 Kagurazaka, Shinjuku-ku, Tokyo, 162-8601, Japan; SHURO TAKANO, Nobeyama Radio Observatory, 462-2 Nobeyama, Minamimaki, Minamisaku, Nagano, 384-1305, Japan; HIROMICHI YAMABE NAHITO KOSHIKAWA, KOICHI TSUKIYAMA, Department of Chemistry, Faculty of Science Division I, Tokyo University of Science, 1-3 Kagurazaka, Shinjuku-ku, Tokyo, 162-8601, Japan; AYA NAKANE, TOSHIKI OKABATYASHI, Department of Chemistry, Faculty of Science, Shizuoka University, 836 Oya, Suruga-ku, Shizuoka 422-8529, Japan; ARISA KUNIMATSU and NOBUHIKO KUZE, Department of Materials and Life Sciences, Faculty of Science and Technology, Sophia University, 7-1 Kioi-cho, Chiyoda-ku, Tokyo, 102-8554, Japan.

WF07 5 min 3:02
LABORATORY SUBMILLIMETER SPECTROSCOPY AS A PROBE OF METHANOL PHOTODISSOCIATION

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

WF08 10 min 3:09
NEW ACETYLENE HC₅H MEASUREMENTS USING SOLEIL SYNCHROTRON

D. JACQUEMART, N. LACOME, Université Pierre et Marie Curie-Paris 6; CNRS; Laboratoire de Dynamique, Interactions et Réactivité (LADIR), UMR 7075, Case Courrier 49, 4 Place Jussieu, 75252 Paris Cedex 05, France; O. PIRALI, Synchrotron SOLEIL, L Orme des Merisiers Saint-Aubin, 91192 Gif-sur-Yvette Cedex, France.

WF09 15 min 3:21
THE MILLIMETERWAVE SPECTRUM OF n-BUTYL CYANIDE

MATTHIAS H. ORDU, HOLGER S. P. MÜLLER, FRANK LEWEN, STEPHAN SCHLEMMER, I. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany; MARC NUNEZ, and ADAM WALTERS, IRAP: Université de Toulouse, UPS-OMP, CNRS; 9 Av. colonel Roche, BP 44346, 31028 Toulouse Cedex 4, France.

WF10 15 min 3:38
ROTATIONALLY RESOLVED SPECTRA OF THE B²Π - X²Π 0₀₀ AND μ²Σ - μ²Σ 11₁¹ TRANSITIONS OF C₆H AND C₆D

D. ZHAO, M.A. HADDAD, Institute for Lasers, Life and Biophotonics Amsterdam, De Boelelaan-1081, NL 1081 HV Amsterdam, Netherlands; H. LINNARTZ, Raymond and Beverly Sackler Laboratory for Astrophysics, Leiden Observatory, Leiden University, P.O. Box 9513, NL-2300 RA Leiden, and Institute for Lasers, Life and Biophotonics Amsterdam, De Boelelaan 1081, NL-1081 HV Amsterdam, Netherlands; W. UBACHS, Institute for Lasers, Life and Biophotonics Amsterdam, De Boelelaan-1081, NL 1081 HV Amsterdam, Netherlands.

Intermission
WF11 10 min 4:15
PROSPECTIVE WORK FOR ALMA: THE MILLIMETERWAVE AND SUBMILLIMETERWAVE SPECTRUM OF DEUTERATED GLYCOLALDEHYDE

A. BOUCHEZ, L. MARGULÈS, R. A. MOTIYENKO, Laboratoire PhLAM, CNRS UMR 8523, Université de Lille 1, 59655 Villeneuve d’Ascq Cedex, France; A. WALTERS, S. BOTTINELLI, IRAP, Université de Toulouse, UPS-OMP, CNRS; 9 Av. colonel Roche, BP 44346, 31028 Toulouse Cedex 4, France; C. CEC-CARELLI, C. KAHANE, IPAG: Université Joseph Fourier, CNRS, BP 53 F-38041, GRENOBLE Cedex 9; and J.-C. GUILLEMIN, Sciences Chimiques de Rennes, UMR 6226 CNRS-ENSCR, Avenue du Général Leclerc, CS 50837, 35708 Rennes Cedex 7, France.

WF12 15 min 4:27
THE MICROWAVE SPECTRUM OF PARTIALLY DEUTERATED SPECIES OF DIMETHYL ETHER

D. LAUVERGNAT, Laboratoire de Chimie Physique, Bât. 349, CNRS, UMR8000, Université Paris-Sud, Orsay, F-91405, France; L. MARGULÈS, R. A. MOTIYENKO, Laboratoire PhLAM, CNRS/Université des Sciences et Technologies de Lille 1, Bât. P5, 59655 Villeneuve d’Ascq, France; J.-C. GUILLEMIN, Sciences Chimiques de Rennes, UMR6226 CNRS-ENSCR, Avenue du Général Leclerc, CS 50837, 35708 Rennes Cedex 7, France; AND L. H. COUDERT, LISA, CNRS/Universités Paris Est et Paris Diderot, 61 Avenue du Général de Gaulle, 94010 Créteil, France.

WF13 15 min 4:44
PROSPECTIVE WORK FOR ALMA: THE MILLIMETERWAVE AND SUBMILLIMETERWAVE SPECTRUM OF $^{13}$C-GLYCOLALDEHYDE

IMANE HAYKAL, LAURENT MARGULÈS, THERESE R. HUET, ROMAN MOTIYENKO, Laboratoire PhLAM, UMR8523 CNRS-Université Lille 1, F-59655 Villeneuve d’Ascq Cedex, France; and J.-C. GUILLEMIN, UMR6226 CNRS-Ecole Nationale Supérieure de Chimie de Rennes,F-35700 Rennes, France.

WF14 15 min 5:01
EXPERIMENTAL ELECTRONIC SPECTROSCOPY OF TWO PAHS: NAPHTHALENE AND 2-METHYL NAPHTHALENE

H. FRIHA, ISMO, CNRS, Université Paris- Sud, Orsay, 91400, France; G. FERAUD, ISMO, CNRS, Université Paris- Sud, Orsay, 91400, France; T. PINO, ISMO, CNRS, Université Paris- Sud, Orsay, 91400, France; PH. BRECHIGNAC, ISMO, CNRS, Université Paris- Sud, Orsay, 91400, France; P. PARNEIX, ISMO, CNRS, Université Paris- Sud, Orsay, 91400, France; Z. DHAOUDI, LSAMA, Faculté des Sciences de Tunis, Campus Universitaire 2092, Manar II, Tunisie; N. JAIMANE, LSAMA, Faculté des Sciences de Tunis, Campus Universitaire 2092, Manar II, Tunisie; H. GALILA, LSAMA, Faculté des Sciences de Tunis, Campus Universitaire 2092, Manar II, Tunisie; T. TROY, School of Chemistry, The University of Sydney, NSW 2006, Australia; T. SCHMIDT, School of Chemistry, The University of Sydney, NSW 2006, Australia.
WF15  15 min  5:18
HIGH RESOLUTION SPECTROSCOPY AND GLOBAL ANALYSIS OF THE TETRADECAD REGION OF METHANE $^{12}$CH$_4$
A. NIKITIN, Institute of Atmospheric Optics, 634055 Tomsk, Russia and Laboratoire GSMA, UMR 6089 CNRS-Université de Reims Champagne Ardenne, Moulin de la Housse BP 1039, Cases 16-17, F-51687 Reims Cedex 2, France; V. BOUDON, C. WENGER, Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR 5209 CNRS-Université de Bourgogne, 9, Av. A. Savary, BP 47870, F-21078 Dijon Cedex, France; L. R. BROWN, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Drive, Pasadena, California 91109, USA; S. BAUERECKER, Physical Chemistry, ETH Zürich, CH-8093 Zürich, Switzerland and Institut für Physikalische und Theoretische Chemie, Technische Universität Braunschweig, D-38106, Germany; S. ALBERT, M. QUACK, Physical Chemistry, ETH Zürich, CH-8093 Zürich, Switzerland.

WF16  5 min  5:35
LONG PATH- HIGH RESOLUTION SPECTRUM OF METHANE. TOWARDS TITAN’S ATMOSPHERE
LUDOVIC DAUMONT, VLADIMIR TYUTEREV, LAURENCE REGALIA, XAVIER THOMAS, PIERRE VON DER HEYDEN, Groupe de Spectrométrie Moléculaire et Atmosphérique, UMR CNRS 6089, Université de Reims Champagne-Ardenne, U.F.R. Sciences, B.P. 1039, 51687 Reims Cedex 2, France; ANDREI NIKITIN, Laboratory of Theoretical Spectroscopy, Institute of Atmospheric Optics, Russian Academy of Sciences, 1, Akademichesky Avenue, 634055 Tomsk, Russian Federation; LINDA BROWN, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Drive, Pasadena, CA 91109, USA.

WF17  15 min  5:42
THE $4\nu_3$ SPECTRAL REGION OF METHANE
D. CHRIS BENNER, V. MALATHY DEVI, JENNIFER HAYS, Department of Physics, College of William and Mary, Williamsburg, VA 23187-8795; J. J. O’BRIEN, S. SHAJI, Department of Chemistry and Biochemistry, University of Missouri - St. Louis, St. Louis, MO 63121-4400; P. T. SPICKLER, C. P. HOUCK, J. A. COAKLEY, KASIE J. HAGA, JUSTIN D. DOLPH, Department of Physics, Bridgewater College, Bridgewater, VA 22812.
WG. ELECTRONIC
WEDNESDAY, JUNE 22, 2011 – 1:30 pm
Room: 170 MATH ANNEX
Chair: ALLAN S-C. CHEUNG, The University of Hong Kong, Hong Kong

WG01 15 min 1:30
APPROXIMATE THEORETICAL MODEL FOR THE FIVE ELECTRONIC STATES (Ω = 5/2, 3/2, 3/2, 1/2, 1/2) ARISING FROM THE GROUND 3d9 CONFIGURATION IN NICKEL HALIDE MOLECULES AND FOR ROTATIONAL LEVELS OF THE TWO Ω = 1/2 STATES IN THAT MANIFOLD

JON T. HOUGEN, Optical Technology Division, NIST, Gaithersburg, MD 20899-8441, USA.

WG02 15 min 1:47
OBSERVATION OF Ω = 1/2 STATES IN NiH THROUGH COLLISIONALLY INDUCED FLUORESCENCE

C. RICHARDa, P. CROZET, A. J. ROSS, Université Lyon 1; CNRS; LASIM UMR 5579, 43 Bd du 11 novembre 1918, F-69622 Villeurbanne, France; D. W. TOKARYK, Department of Physics and Center for Laser, Atomic, and Molecular Sciences, University of New Brunswick, Fredericton, Canada E3B 5A3.

aCurrent address: Harvard-Smithsonian Center for Astrophysics, Atomic and Molecular Physics Division, Cambridge MA 02138, USA

WG03 15 min 2:04
NEW BANDS OF NICKEL FLUORIDE IN THE NEAR INFRARED BY INTRACAVITY LASER ABSORPTION SPECTROscopy

LEAH C. O’BRIEN, KIMBERLY HANDLER, 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.

WG04 10 min 2:21
INTRACAVITY LASER ABSORPTION SPECTROscopy OF PLATINUM FLUORIDE IN THE NEAR INFRARED

LEAH C. O’BRIEN, KAITLIN WOMACK, Department of Chemistry, Southern Illinois University, Edwardsville, IL 62026-1652; JAMES J. O’BRIEN, MEREDITH REDDICK, REBECCA STEINBERG, Department of Chemistry and Biochemistry, University of Missouri, St Louis, MO 63121-4499.

WG05 15 min 2:33
THE ELECTRONIC SPECTRUM AND MOLECULAR STRUCTURE OF HAsO, THE ARSENIC ANALOG OF HNO

ROBERT A. GRIMMINGER, DENNIS J. CLOUTHIER, Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055, USA.

WG06 15 min 2:50
THE PFI-ZEKE SPECTROscopy STUDY OF HIS+ AND THE IONIZATION ENERGY OF HIS

I. O. ANTONOV, B. J. BARKER, M. C. HEAVEN, Department of Chemistry, Emory University, Atlanta, GA 30322.
Intermission

WG07
THEORETICAL STUDIES OF ELECTRONIC SPECTRA AND BONDING OF AlCl/AlF(X^1Σ^+, a^3Π, A^1Π) WITH EXCITED STATES EXHIBITING RECOUPLED PAIR BONDING

JEFF LEIDING, DAVID E. WOON and THOM H. DUNNING, JR., Department of Chemistry, University of Illinois at Urbana-Champaign, Box 86-6, CLSL, 600 South Mathews, Urbana IL, 61801.

WG08
ELECTRONIC SPECTROSCOPY OF THE 6p ← 6s TRANSITION IN Au-Ne

ADRIAN M. GARDNER, RICHARD J. PLOWRIGHT, CAROLYN D. WITHERS, TIMOTHY G. WRIGHT, School of Chemistry, University of Nottingham, University Park, Nottingham, NG7 2RD, United Kingdom; MICHAEL D. MORSE and W. H. BRECKENRIDGE, Department of Chemistry, 315 South 1400 East, Room 2020, University of Utah, Salt Lake City, Utah 84112.

WG09
ELECTRONIC TRANSITIONS AND SPIN-ORBIT SPLITTING OF LANTHANUM DIMER

YANG LIU, LU WU, CHANGHUA ZHANG, and DONG-SHENG YANG, Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055.

WG10
LASER INDUCED FLUORESCENCE SPECTROSCOPY OF COBALT MONOBORIDE

H. F. PANG, Y. W. NG AND A. S-C. CHEUNG, Department of Chemistry, The University of Hong Kong, Pokfulam Road, Hong Kong.

WG11
HIGH RESOLUTION LASER SPECTROSCOPY OF RHODIUM MONOBROMIDE.

A. G. ADAM, T. F. ALLEN, L. E. DOWNIE, and A. D. GRANGER, Chemistry Department, and Centre for Lasers, and Atomic, and Molecular Sciences, University of New Brunswick, Fredericton, NB, E3B 5A3; and C. LINTON, and D. W. TOKARYK, Physics Department, and Centre for Lasers, and Atomic, and Molecular Sciences, University of New Brunswick, Fredericton, NB, E3B 5A3.

WG12
THE VISIBLE SPECTRUM OF IRIDIUM MONOHYDRIDE AND MONODEUTERIDE.

A. G. ADAM, and A. D. GRANGER, Chemistry Department, and Centre for Lasers, and Atomic, and Molecular Sciences, University of New Brunswick, Fredericton, NB, E3B 5A3; and C. LINTON, and D. W. TOKARYK, Physics Department, and Centre for Lasers, and Atomic, and Molecular Sciences, University of New Brunswick, Fredericton, NB, E3B 5A3.

WG13
THE VISIBLE SPECTRUM OF ZIRCONIUM DIOXIDE, ZrO_2

ANH LE AND TIMOTHY C. STEIMLE, Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287; VARUN GUPTA AND JOHN P. MAIER, Department of Chemistry, University of Basel, Basel, Switzerland.
SEQUENTIAL OXIDATION OF TRANSITION METAL SUBOXIDE CLUSTER ANIONS

CAROLINE CHICK JARROLD, JENNIFER E. MANN, SARAH E. WALLER, and DAVID W. ROTHGEB,
Department of Chemistry, Indiana University, 800 E. Kirkwood Avenue, Bloomington, IN 47405.
**WH. MICROWAVE**

**WEDNESDAY, JUNE 22, 2011 – 1:30 pm**

**Room: 1000 McPHERSON LAB**

<table>
<thead>
<tr>
<th>Chair: DeWAYNE T. HALFEN, University of Arizona, Tucson, Arizona</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Time</th>
<th>Title</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>WH01</strong> 15 min 1:30</td>
<td>REASSIGNMENT OF MILLIMETERWAVE SPECTRUM OF THE HCN INTERNAL ROTATION BANDS OF H$_2$-HCN</td>
<td>KENSUKE HARADA, RISA YAMANAKA, and KEIICHI TANAKA, Department of Chemistry, Faculty of Sciences, Kyushu University, Fukuoka, 812-8581 JAPAN.</td>
</tr>
<tr>
<td><strong>WH02</strong> 15 min 1:47</td>
<td>MILLIMETERWAVE SPECTROSCOPY OF THE INTERNAL ROTATION BANDS OF Ne-DCN</td>
<td>NAOKO OYAMADA, KENSUKE HARADA, and KEIICHI TANAKA, Department of Chemistry, Faculty of Science, Kyushu University, Hakozaki, Higashiku, Fukuoka, 812-8581 JAPAN.</td>
</tr>
<tr>
<td><strong>WH03</strong> 15 min 2:04</td>
<td>STUDY OF He$_N$-HCN CLUSTERS USING ROTATIONAL SPECTROSCOPY</td>
<td>STEVE DEMPSTER, OLEKSANDR SUKHORUKOV, QI-YI LEI, and WOLFGANG JÄGER, Department of Chemistry, University of Alberta, Edmonton, Canada T6G 2G2.</td>
</tr>
<tr>
<td><strong>WH04</strong> 15 min 2:21</td>
<td>MICROWAVE SPECTRA AND STRUCTURES OF H$_2$O···AgF</td>
<td>S. L. STEPHENS, N. R. WALKER, D. P. TEW AND A. C. LEGON, School of Chemistry, University of Bristol, Bristol, BS8 1TS, U.K.</td>
</tr>
<tr>
<td><strong>WH05</strong> 15 min 2:38</td>
<td>INTERNAL ROTATION IN CF$_3$I···NH$_3$ AND CF$_3$I···N(CH$_3$)$_3$ PROBED BY CP-FTMW SPECTROSCOPY</td>
<td>N. R. WALKER, S. L. STEPHENS AND A. C. LEGON, School of Chemistry, University of Bristol, Bristol, BS8 1TS, U.K.</td>
</tr>
<tr>
<td><strong>WH06</strong> 15 min 2:55</td>
<td>INTERNAL MOTION EFFECTS IN THE MICROWAVE SPECTRUM OF ARGON-CIS-1,2-DIFLUOROETHYLENE</td>
<td>HELEN O. LEUNG AND MARK D. MARSHALL, Department of Chemistry, Amherst College, P.O. Box 5000, Amherst, MA 01002-5000.</td>
</tr>
<tr>
<td><strong>WH07</strong> 15 min 3:12</td>
<td>THE MICROWAVE SPECTRUM OF ARGON-VINYL CHLORIDE</td>
<td>HELEN O. LEUNG AND MARK D. MARSHALL, Department of Chemistry, Amherst College, P.O. Box 5000, Amherst, MA 01002-5000.</td>
</tr>
</tbody>
</table>
Intermission

WH08 10 min 3:45
HALOGEN BOND AND INTERNAL DYNAMICS IN CClF3-H2O

L. EVANGELISTI, G. FENG and W. CAMINATI, Dipartimento di Chimica “G. Ciamici” dell’Università, Via Selmi 2, I-40126 Bologna, Italy; P. ECJIA, E.J. COCINERO and F. CASTANO, Departamento de Quimica Fisica, Facultad de Ciencia y Tecnologia, Universidad del Pais Vasco (UPV-EHU), Apartado 644, E-48080 Bilbao, Spain.

WH09 15 min 3:57
WEAK C–H· · ·O INTERACTIONS AND H2O INTERNAL ROTATION IN THE HCCIF2–H2O AND HCBrF2–H2O DIMERS

REBECCA A. PEEBLES, SEAN A. PEEBLES, BRANDON J. BILLS, LENA F. ELMUTI, DANIEL A. OBENCHAIN, AMELIA J. SANDERS, AMANDA L. STEBER, Department of Chemistry, Eastern Illinois University, 600 Lincoln Ave., Charleston, IL 61920; PETER GRONER, Department of Chemistry, University of Missouri - Kansas City, Kansas City, MO 64110; BROOKS H. PATE, JUSTIN L. NEILL, MATT T. MUCKLE, Department of Chemistry, University of Virginia, McCormick Rd., PO Box 400319, Charlottesville, VA 22904.

WH10 15 min 4:14
CHIRPED-PULSE, FTMW SPECTROSCOPY OF THE LACTIC ACID-H2O SYSTEM

ZBIGNIEW KISIEL, EWA BIAŁKOWSKA-JAWORSKA, Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warszawa, Poland; DANIEL P. ZALESKI, JUSTIN L. NEILL, AMANDA L. STEBER, BROOKS H. PATE, Department of Chemistry, University of Virginia, McCormick Rd., Charlottesville, VA 22904-4319.

WH11 15 min 4:31
STRUCTURE STUDY OF THE CHIRAL LACTIDE MOLECULES BY CHIRPED-PULSE FTMW SPECTROSCOPY

DANIEL P. ZALESKI, JUSTIN L. NEILL, and BROOKS H. PATE, Department of Chemistry, University of Virginia, McCormick Rd., P.O. Box 400319, Charlottesville, VA 22904; EWA BIAŁKOWSKA-JAWORSKA and ZBIGNIEW KISIEL, Institute of Physics, Polish Academy of Sciences, Al. Lotnikw 32/46, 02-668 Warszawa, Poland.

WH12 15 min 4:48
THE CHIRPED-PULSE AND CAVITY BASED FTMW SPECTROSCOPY OF THE METHYL LACTATE-WATER AND METHYL LACTATE-DEUTERIUM OXIDE DIMERS

JAVIX THOMAS, OLEKSANDR SUKHORUKOV, WOLFGANG JÄGER, YUNJIE XU, Department of Chemistry, University of Alberta, Edmonton, AB, T6G 2G2, Canada.

WH13 15 min 5:05
THE PURE ROTATIONAL SPECTRUM OF PERFLUOROOCTANONITRILE, C7F15CN, STUDIED USING CAVITY-AND CHIRPED-PULSED FOURIER TRANSFORM MICROWAVE SPECTROSCOPIES

C. T. DEWBERRY, G. S. GRUBBS II, S. A. COOKE, Department of Chemistry, The University of North Texas, 1155 Union Circle, # 305070 Denton, TX 76203-5017, USA; W. C. BAILEY, Chemistry-Physics Department, Kean University, 1000 Morris Avenue, Union, NJ 07080, USA.
EVIDENCE FOR A NON-PLANAR C=(CCC) STRUCTURE IN HEXAFLUOROISOBUTENE AND HEXAFLUOROACETONE IMINE: A PURE ROTATIONAL SPECTROSCOPIC STUDY

G. S. GRUBBS II, C. T. DEWBERRY, B. E. LONG, S. A. COOKE, Department of Chemistry, The University of North Texas, 1155 Union Circle, # 305070 Denton, TX 76203-5017, USA; W. C. PRINGLE, Department of Chemistry, Wesleyan University, Hall-Atwater Laboratories, 52 Lawn Ave, Middletown, CT 06459-0180.
WI. MINI-SYMPOSIUM: SPECTROSCOPIC PERTURBATIONS  
WEDNESDAY, JUNE 22, 2011 – 1:30 pm  
Room: 1015 McPherson Lab  

Chair: ROBERT W. FIELD, Massachusetts Institute of Technology, Cambridge, Massachusetts

W101  INVITED TALK  30 min  1:30

INVISIBLE ELECTRONIC STATES AND THEIR DYNAMICS REVEALED BY PERTURBATIONS

ANTHONY J. MERER, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan.

W102  15 min  2:05

INTERNAL AND EXTERNAL PERTURBATIONS IN ELECTRONIC SPECTROSCOPY. THE STARK SPECTRUM OF INDOLE-NH₃⁺

ADAM J. FLEISHER, JUSTIN W. YOUNG, and DAVID W. PRATT, Department of Chemistry, University of Pittsburgh, Pittsburgh, PA 15260.

*Work supported by NSF (CHE-0911117).

W103  15 min  2:22

NOVEL PATTERNS OF TORSION - INVERSION TUNNELING AND TORSION - ROTATION COUPLING IN THE ν₁₁ CH - STRETCH REGION OF CH₃NH₂

MAHESH B DAWADI, SYLVESTRE TWAGIRAYEUZU, C. MICHAEL LINDSAY, and DAVID S. PERRY, Department of Chemistry, The University of Akron, OH 44325-3601; LI-HONG XU, Department of Physics, Centre for Laser, Atomic and Molecular Studies (CLAMS) University of New Brunswick, Saint John, New Brunswick, Canada E2L 4L5.

*Present address: U.S. Air Force Research Laboratory, 2306 Perimeter Rd, Eglin AFB, FL 32542-5910

W104  15 min  2:39

EXTENDED PERMUTATION-INVERSION GROUPS FOR SIMULTANEOUS TREATMENT OF THE ROVIBRONIC STATES OF TRANS-ACETYLENE, CIS-ACETYLENE, AND VINYLIDENE

JON T. HOUGEN, Optical Technology Division, NIST, Gaithersburg, MD 20899-8441, MD, USA; ANTHONY J. MERER, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan 10617 and Department of Chemistry, University of British Columbia, Vancouver, B.C., Canada V6T 1Z1.

W105  15 min  2:56

THE VISIBLE SPECTRUM OF Si₃

XIUJUAN ZHUANG, TIMOTHY C. STEIMLE, Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287; N. REILLY, D. KOKKIN and M. C. McCARTHY, Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts 02138, USA; J. F. STANTON, Chemistry Department and Biochemistry, U. of Texas, Austin, TX 78712, USA; T. D. CRAWFORD and B. FORTEENBERRY, Chemistry Department, Virginia Tech, Blackbury VA 24061, USA; J. P. MAIER, Department of Chemistry, University of Basel, Basel, Switzerland.
EXPERIMENTAL CHARACTERIZATION OF THE WEAKLY ANISOTROPIC CN $^2\Sigma^+ + \text{Ne}$ POTENTIAL FROM IR-UV DOUBLE RESONANCE STUDIES OF THE CN-Ne COMPLEX

JOSEPH M. BEAMES, BRIDGET A. O’DONNELL, MELODIE TING, MARSHA I. LESTER, Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104; THOMAS A. STEPHENSON, Department of Chemistry and Biochemistry, Swarthmore College, Swarthmore, PA 19081.

*Research is supported by the Chemistry Division of the NSF.

INTERMISSION

TERAHERTZ SPECTROSCOPY OF HIGH $K$ METHANOL TRANSITIONS

JOHN C. PEARSON, SHANSHAN YU, HARSHAL GUPTA and BRIAN J DROUIN, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr., Pasadena CA 91109.

* A part of this work was performed at the Jet Propulsion Laboratory, California Institute of Technology under contract with the National Aeronautics and Space Administration. Copyright 2010 © California Institute of Technology. All rights reserved.

SYMMEtRY DEPENDENCE OF THE RO-VIBRONIC DISTRIBUTIONS OF THE ND$_2$ $^2A_2$ $^1A_1$ FRAGMENTS FROM THE PHOTODISSOCIATION OF THE A STATES OF ND$_3$ AND ND$_2$H AT 193.3 NM

G. DUXBURY, Department of Physics, SUPA, John Anderson Building, University of Strathclyde, 107 Rottenrow, Glasgow G4 0NG, Scotland, UK; J.P. REID, School of Chemistry, University of Bristol, Bristol BS8 1TS.

VIBRATIONAL COUPLING PATHWAYS IN THE CH STRETCH REGION OF CH$_3$OH AND CH$_3$OD AS REVEALED BY IR AND FTMW-IR SPECTROSCOPIES

SYLVESTRE TWAGIRAYEU, XIAOLIANG WANG, AND DAVID S. PERRY, Department of Chemistry, The University of Akron, Akron OH 44325; JUSTIN L. NEILL, MATT T. MUCKLE, BROOKS H. PATE, Department of Chemistry, University of Virginia, McCormick Rd., Charlottesville, VA 22904; LI-HONG XU, Department of Physics, Centre for Laser, Atomic and Molecular Studies (CLAMS), University of New Brunswick, Saint John, New Brunswick E2L 4L5, Canada.

CONFORMATION SPECIFIC ELECTRONIC AND INFRARED SPECTROSCOPY OF ISOLATED [2,2,2]-PARATRICYLCLOPHANE AND ITS MONOHYDRATED CLUSTER

EVAN G. BUCHANAN, JACOB C. DEAN, BRETT M. MARSH, and TIMOTHY S. ZWIER, Department of Chemistry, Purdue University, West Lafayette, IN 47907.

CONFORMATION-SPECIFIC EFFECTS ON INTERNAL MIXING: INFRARED AND ULTRAVIOLET SPECTROSCOPY OF 1,1-DIPHENYLPROPANE

NATHANAEL M. KIDWELL, EVAN G. BUCHANAN, JACOB C. DEAN, and TIMOTHY S. ZWIER, Department of Chemistry, Purdue University, West Lafayette, IN 47907.
WI12  15 min  5:10
OPTICAL PUMPING AND ELECTRON SPIN RESONANCE OF SINGLE \textsuperscript{87}Rb ATOMS ON HELIUM NANODROPLETS

MARKUS KOCH, JOHANNES POMS, ALEXANDER VOLK, and WOLFGANG E. ERNST, Institute of Experimental Physics, TU Graz, Petersgasse 16, 8010 Graz, Austria.

WI13  15 min  5:27
HIGHLY EXCITED STATES OF Cs ATOMS ON HELIUM NANODROPLETS

F. LACKNER, M. THEISEN, M. KOCH, and W.E. ERNST, Institute of Experimental Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria.
WJ. RADICALS AND IONS
WEDNESDAY, JUNE 22, 2011 – 1:30 pm
Room: 2015 McPherson Lab
Chair: Gary E. Douverly, University of Georgia, Athens, Georgia

WJ01
15 min 1:30
RECONCILING EXPERIMENT AND THEORY: THE INTERESTING AND UNUSUAL CASE OF THE HOOO RADICAL

Valerio Lattanzi, M.C. McCarthy, Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, and School of Engineering and Applied Science, Harvard University, Cambridge, MA 02138; and John F. Stanton, Institute for Theoretical Chemistry, Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, TX 78712, United States.

WJ02
15 min 1:47
FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF THE HOSO RADICAL

Valerio Lattanzi, M.C. McCarthy, Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, and School of Engineering and Applied Science, Harvard University, Cambridge, MA 02138; and Filippo Tassia, Dipartimento di Chimica Fisica e Inorganica, Università di Bologna, V.le Risorgimento 4, I-40136 Bologna, Italy.

WJ03
15 min 2:04
HIGH RESOLUTION INFRARED SPECTROSCOPY OF THE PO2 RADICAL

Michael A. Lawson, Kristian J. Hoffman and Paul B. Davies, Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge, CB2 1EW, U.K.

WJ04
15 min 2:21
SUBMILLIMETER-WAVE ROTATIONAL SPECTRA OF DNC

T. Amano, Department of Chemistry and Department of Physics and Astronomy, University of Waterloo, Waterloo, ON N2L 3G1, Canada.

WJ05
15 min 2:38
HIGH RESOLUTION FOURIER TRANSFORM SPECTROSCOPY OF TRANSIENT SPECIES ON THE FAR INFRARED "AILES" BEAMLINE OF SOLEIL SYNCHROTRON.

M. A. Martin-Drumel, O. Pirali, D. Balcon, P. Brechignac, Institut des Sciences Moléculaires d’Orsay (ISMO), CNRS, Université Paris XI, Orsay, France; M. Vervloet, P. Roy, SOLEIL Synchrotron, AILES beamline, Saint-Aubin, France.

WJ06
15 min 2:55
CALCULATION OF THE TRANSITION DIPOLE MOMENT OF THE $\tilde{A} \leftarrow \tilde{X}$ ELECTRONIC TRANSITION OF THE C2H5O2 FROM THE PEAK ABSORPTION CROSS-SECTION

Dmitry G. Melnik, Phillip S. Thomas and Terry A. Miller, Laser Spectroscopy Facility, Department of Chemistry, The Ohio State University, 120 W. 18th Avenue, Columbus, Ohio 43210.
ELECTRONIC SPECTROSCOPY OF COBALT-NEON CATION

J. MOSLEY, S. HASBROUCK, and M. A. DUNCAN, Department of Chemistry, University of Georgia, Athens, GA 30602-2556.

Intermission

ROVIBRATIONAL SPECTROSCOPY OF ALUMINUM CARBONYL CLUSTERS IN HELIUM NANODROPLETS


PYROLYSIS OF ACETALDEHYDE: A FLEETING GLIMPSE OF VINYLIDENE

A.J. VASILLOU, K.M. PIECH, G.B. ELLISON, Department of Chemistry, University of Colorado, Boulder, CO, 80303; A. GOLAN, O. KOSTKO, M. AHMED, Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720; D.L. OSBORN, Sandia National Laboratories, Livermore, CA 94551; J.W. DAILY, Department of Mechanical Engineering, University of Colorado, Boulder, CO 80302; M.R. NIMLOS, Center for Renewable Chemical Technologies and Materials, NREL, Golden, CO 80401; and J.F. STANTON, Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, TX 78712.

SPECTROSCOPIC STUDIES OF THE $\tilde{\text{A}} - \tilde{\text{X}}$ ELECTRONIC SPECTRUM REVEAL BOTH THE STRUCTURE AND DYNAMICS OF $\beta$-HYDROXYETHYLPEROXY RADICAL

MING-WEI CHEN, GABRIEL M. P. JUST*, TERRANCE J. CODD, TERRY A. MILLER, Laser Spectroscopy Facility, Department of Chemistry, The Ohio State University, 120 W. 18th Avenue, Columbus, Ohio 43210; W. LEO MEERTS, Radboud University Nijmegen, Institute for Molecules and Materials, Heyendaalseweg 135, NL-6525 AJ Nijmegen, The Netherlands.

*present address: Lawrence Berkeley National Laboratory, Berkeley, CA 94720

OBSERVATION OF THE $\tilde{\text{A}} - \tilde{\text{X}}$ ELECTRONIC TRANSITION OF THE 2-HYDROXYPROPYL PEROXY RADICAL VIA CAVITY RINGDOWN SPECTROSCOPY

NEAL D. KLINE and TERRY A. MILLER, Laser Spectroscopy Facility, Department of Chemistry, The Ohio State University, 120 W. 18th Avenue, Columbus OH 43210.

VIBRATIONAL SPECTRUM OF THE THIOMETHOXY ($\text{CH}_3\text{S}$) RADICAL INVESTIGATED WITH INFRARED-VACUUM ULTRAVIOLET PHOTOIONIZATION

HUI-LING HAN, LUNG FU, 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.
CAVITY RING-DOWN SPECTROSCOPY OF THE $1^2B_1 - \tilde{X}^2A_1$ TRANSITION OF THE PHENYL RADICAL

KEITH FREEL, J. PARK, M. C. LIN, MICHAEL C. HEAVEN, Department of Chemistry, Emory University, Atlanta, GA 30322.
RA01

INVITED TALK

TESTS OF PARITY AND TIME-REVERSAL VIOLATION USING DIATOMIC MOLECULES

D. DeMILLE**, Physics Department, Yale University, New Haven, CT 06520.

*This work supported by NSF

RA02

A NEW MEASUREMENT OF THE ELECTRON’S ELECTRIC DIPOLE MOMENT USING YbF MOLECULES

J. J. HUDSON, D. M. KARA, I. J. SMALLMAN, B. E. SAUER, M. R. TARBUTT and E. A. HINDS, Centre for Cold Matter, Blackett Laboratory, Imperial College London, Prince Consort Road, London SW7 2AZ, UK.

RA03

SPECTROSCOPY OF THORIUM MONOXIDE, ThO; E(O^+),F(O^+),-X^1Σ^+ BANDS

FANG WANG AND TIMOTHY C. STEIMLE, Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287; MICHAEL HEAVEN, Department of Chemistry, Emory University, Atlanta, GA 30322.

RA04

PERMANENT ELECTRON ELECTRIC DIPOLE MOMENT SEARCH IN THE X^3Δ_1 GROUND STATE OF TUNGSTEN CARBIDE MOLECULES

JEONGWON LEE, JINHAI CHEN, and AARON LEANHARDT, Department of Physics, University of Michigan, Ann Arbor, MI 48109.

RA05

THEORETICAL STUDY OF THE PbF AND PbO MOLECULES

ALEXANDER N. PETROV, ANATOLY V. TITOV, MIKHAIL G. KOZLOV, Petersburg Nuclear Physics Institute, Gatchina, Leningrad district 188300, Russia; KIRILL I. BAKLANOV, Institute of Physics, Saint Petersburg State University, Saint Petersburg, Petrodvorets 198904, Russia.

*This work supported by RFBR Grants No. 09-03-01034
THE EFFECTIVE HAMILTONIAN FOR THE GROUND STATE OF $^{207}_{\text{Pb}}^{19}_{\text{F}}$ AND NEW MEASUREMENTS OF THE FINE STRUCTURE SPECTRUM NEAR 1.2 µm.

RICHARD MAWHORTER, BENJAMIN MURPHEY, ALEXANDER BAUM, Department of Physics and Astronomy, Pomona College, Claremont, CA 91711; TREvor J. SEARS, Chemistry Department Brookhaven National Laboratory, Upton, NY 11973 and Stony Brook University, Stony Brook, NY 11794; T. ZH. YANG, P. M. Rupasinghe, C. P. McRAVEN*, N. E. Shafer-Ray, Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma, Norman, OK; Lukas D. Alpheland Jens-Uwe. Grabow, Gottfried-Wilhelm-Liebniz-Universität, Institut für Physikalische Chemie & Elektrochemie, D-30167 Hannover, Germany.

*Current Address: Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973

INTERMISSION

A PbF PROBE FOR THE ELECTRON ELECTRIC DIPOLE MOMENT

JOHN MOORE-FURNEAUX, N.E. SHAFER-RAY, Home L. Dodge Department of Physics and Astronomy, University of Oklahoma, Norman OK, 73019.

HIGH RESOLUTION ROTATIONAL SPECTROSCOPY STUDY OF THE ZEEMAN EFFECT IN THE $^2\Pi_{1/2}$ MOLECULE PbF

ALEXANDER BAUM, RICHARD MAWHORTER, and BENJAMIN MURPHY, Department of Physics and Astronomy, Pomona College, Claremont, CA 91711; TREvor J. SEARS, Chemistry Department Brookhaven National Laboratory, Upton, NY 11973 and Stony Brook University, Stony Brook, NY 11794; T. ZH. YANG, P. M. RUPASINGHE, C. P. MCRAVEN*, and N. E. SHAFER-RAY, Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma, Norman, OK; LUKAS D. ALPHEI and JENS-UWE. GRABOW, Gottfried-Wilhelm-Liebniz-Universität, Institut für Physikalische Chemie & Elektrochemie, D-30167 Hannover, Germany.

*Current Address: Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973

STARK SPECTROSCOPY OF PBF MOLECULE

TAO YANG, NEIL SHAFER-RAY, Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma, 440 W.Brooks, NH 100, Norman, OK 73019.

THE PFI-ZEKE SPECTRUM OF HfF$^+$, IN SUPPORT OF FUNDAMENTAL PHYSICS

BEAU J. BARKER, IVAN O. ANTONOV, VLADIMIR E. BONDYBEY, and MICHAEL C. HEAVEN, Department of Chemistry, Emory University, Atlanta, GA 30322.
RB. ATMOSPHERIC SPECIES
THURSDAY, JUNE 23, 2011 – 8:30 am
Room: 170 MATH ANNEX

Chair: BRIAN DROUIN, California Institute of Technology, Pasadena, California

RB01 15 min 8:30
NITROGEN-BROADENED $^{13}$CH$_4$ AT 80 TO 296 K


RB02 15 min 8:47
MEASUREMENT OF CH$_3$D ABSORPTION CROSS SECTIONS, PRESSURE BROADENING, AND SHFT COEFFICIENTS IN THE 1.65 µm SPECTRAL REGION BY USING CONTINUOUS AVE CAVITY RING-DOWN SPECTROSCOPY

YONGXIN TANG, SHAOYUE L. YANG, KEVIN K. LEHMANN, Department of Chemistry and School of Medicine, University of Virginia, Charlottesville VA, 22904-4319; D. CHRIS BENNER, Department of Physics, College of William and Mary, Box 8795, Williamsburg, VA 23187-8795.

RB03 15 min 9:04
HIGH-RESOLUTION SPECTROSCOPY AND PRELIMINARY GLOBAL ANALYSIS OF C–H STRETCHING VIBRATIONS OF C$_2$H$_4$ IN THE 3000 AND 6000 CM$^{-1}$ REGIONS

M. A. LORONO GONZALEZ, Department of Chemistry, Universidad de Oriente, Cumana 6101, Estado Sucre, Venezuela; V. BOUDON, M. LOÈTE, Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR 5209 CNRS-Université de Bourgogne, 9, Av. A. Savary, BP 47870, F-21078 Dijon Cedex, France; M. ROTGER, M.-T. BOURGEOIS, Groupe de Spectrométrie Moléculaire et Atmosphérique, CNRS UMR 6089, Moulin de la Housse, BP 1039, Cases 16-17, F-51687 Reims Cedex 2, France; K. DIDRICH, M. HERMAN, Laboratoire de Chimie quantique et Photophysique, CP160/09, Faculté des Sciences, Université Libre de Bruxelles, 50 ave. Roosevelt, B-1050, Brussels, Belgium; V. A. KAPITANOV, Yu. N. PONOMAREV, A. A. SOLODOV, A. M. SOLODOV, T. M. PETROVA, V.E. Zuev Institute of Atmospheric Optics SB RAS, 1, Zuev Square, Tomsk, 634921, Russia.

RB04 15 min 9:21
THE THZ ABSORPTION OF METHYL BROMIDE (CH$_3$BR)

MARLON RAMOS, BRIAN J. DROUIN, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109-8099.

RB05 15 min 9:38
IMPACT OF ATMOSPHERIC CLUTTER ON DOPPLER-LIMITED GAS SENSORS IN THE SUBMILLIMETER/TERAHERTZ

IVAN R. MEDVEDEV, Department of Physics, Wright State University, 3640 Colonel Glenn Highway, Dayton, OH 45435, USA; CHRISTOPHER F. NEESE, FRANK C. DE LUCIA, Department of Physics, Ohio State University, 191 West Woodruff Ave., Columbus, OH 43210, USA; GRANT M. PLUMMER, Enthalpy Analytical, Inc., 2202 Ellis Road, Durham, North Carolina 27703, USA.
HIGH RESOLUTION SPECTROSCOPY USING A TUNABLE THZ SYNTHESIZER BASED ON PHOTOMIXING

ARNAUD CUISSET, FRANCIS HINDLE, GAEL MOURET, SOPHIE ELIET, MICKAEL GUINET, ROBIN BOCQUET; Laboratoire de Physico-Chimie de l’Atmosphère, Université du Littoral Côte d’Opale, 189A Ave. Maurice Schumann, 59140 Dunkerque, France.

Intermission

SENSORS ACROSS THE SPECTRUM

CHRISTOPHER F. NEESE, FRANK C. DE LUCIA, Department of Physics, The Ohio State University, 191 W. Woodruff Ave., Columbus, OH 43210 USA; IVAN R. MEDVEDEV, Department of Physics, Wright State University, 3640 Colonel Glenn Hwy, Dayton, OH 45435.

NEW CHIRPED-PULSE THZ FOURIER TRANSFORM TECHNIQUES FOR DETERMINATION OF LINESHAPE PARAMETERS FOR ATMOSPHERIC SPECIES

EYAL GERECHT, KEVIN O. DOUGLASS, DAVID F. PLUSQUELLIC, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY, OPTICAL TECHNOLOGY DIVISION, GAITHERSBURG, MD 20899.

INFRARED ABSORPTION OF CH$_3$SONO DETECTED WITH TIME-RESOLVED FOURIER-TRANSFORM SPECTROSCOPY

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; JIN-DAH CHEN, Department of Applied Chemistry, National Chiao Tung University, Hsinchu 30010, Taiwan.

TORSIONAL EXCITATION IN O-H STRETCH OVERTONE SPECTRA OF ETHYL HYDROPEROXIDE CONFORMERS

SHIZUKA HSIEH, MA THIDA, MARGARET NYAMUMBO, and R. G. LINCK, Chemistry Department, Smith College, Northampton, MA 01063.

RULES APPLICABLE FOR SPECTROSCOPIC PARAMETERS OF H$_2$O TRANSITIONS INVOLVING HIGH J STATES

Q. MA, NASA/Goddard Institute for Space Studies and Department of Applied Physics and Applied Mathematics, Columbia University, 2880 Broadway, New York, NY 10025; R. H. TIPPING, Department of Physics and Astronomy, University of Alabama, Tuscaloosa, AL 35487.
RC01 15 min 8:30
FOURIER TRANSFORM MICROWAVE SPECTRUM OF THE Y$_{2}$(X$^{2}$A$_{1}$) RADICAL

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

RC02 15 min 8:47
OBSERVATION OF LOW J TRANSITIONS OF LASER ABLATED ALKALI HALIDES

BROOKE A. TIMP, JAMIE L. DORAN, KENNETH R. LEOPOLD, Department of Chemistry, University of Minnesota, 207 Pleasant St. SE, Minneapolis, MN 55455; JENS-UWE GRABOW, Institut für Physikalische Chemie und Elektrochemie, Gottfried-Wilhelm-Leibniz-Universität Hannover, Callinstraße 3A, 30167 Hannover, Germany.

RC03 15 min 9:04
ROTATIONAL SPECTROSCOPY OF ZnCCH (X$^{2}$Σ$^{+}$) AT MICROWAVE AND MILLIMETER WAVELENGTHS


RC04 15 min 9:21
FOURIER TRANSFORM MICROWAVE SPECTRUM OF MgCCH (X$^{2}$Σ$^{+}$)


RC05 15 min 9:38
A CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE SPECTROMETER COMBINED WITH A LASER ABLATION SOURCE

S. MATA, I. PENA, C. CABEZAS, J. C. LÓPEZ, J. L. ALONSO, Grupo de Espectroscopía Molecular (GEM). Edificio Quijima. Laboratorios de Espectroscopía y Bioespectroscopía. Parque Científico. Universidad de Valladolid, 47011 Valladolid. (Spain); B. H. PATE, Department of Chemistry, University of Virginia, Charlottesville. Virginia 22904 (USA).

RC06 15 min 9:55
TECHNIQUES FOR HIGH-BANDWIDTH (≥30 GHz) CHIRPED-PULSE MILLIMETER/SUBMILLIMETER-WAVE SPECTROSCOPY

JUSTIN L. NEILL, AMANDA L. STEBER, BRENT J. HARRIS, and BROOKS H. PATE, Department of Chemistry, University of Virginia, McCormick Rd., P.O. Box 400319, Charlottesville, VA 22904; KEVIN O. DOUGLASS and DAVID F. PLUSQUELLIC, National Institute of Standards and Technology, Optical Technology Division, Gaithersburg, MD 20899; EYAL GERECHT, National Institute of Standards and Technology, Electromagnetics Division, Boulder, CO 80305.
Intermission

RC07 15 min 10:30
PROBING VITAMINE C, ASPIRIN AND PARACETAMOL IN THE GAS PHASE: HIGH RESOLUTION ROTATIONAL STUDIES


RC08 15 min 10:47
JET COOLED ROTATIONAL STUDIES OF DIPEPTIDES


RC09 15 min 11:04
CHIRPED-PULSED FTMW SPECTRUM OF VALERIC ACID AND 5-AMINOVALERIC ACID. A STUDY OF AMINO ACID MIMICS IN THE GAS PHASE

RYAN G. BIRD, VANESA VAQUERO, and DAVID W. PRATT, Department of Chemistry, University of Pittsburgh, Pittsburgh, Pa 15213; JUSTIN L. NEILL and BROOKS H. PATE, Department of Chemistry, University of Virginia, Charlottesville, Va 22904.

RC10 15 min 11:21
STRUCTURE STUDY OF FORMIC ACID CLUSTERS BY CHIRPED-PULSE FTMW SPECTROSCOPY

DANIEL P. ZALESKI, JUSTIN L. NEILL, MATT T. MUCKLE, AMANDA L. STEBER, and BROOKS H. PATE, Department of Chemistry, University of Virginia, McCormick Rd., P.O. Box 400319, Charlottesville, VA 22904; KEVIN O. DOUGLASS, National Institute of Standards and Technology, Optical Technology Division, Gaithersburg, MD 20899.

RC11 15 min 11:38
A CHIRPED PULSE FTMW STUDY OF THE STRUCTURE OF PHENOL DIMER

AMANDA L. STEBER, JUSTIN L. NEILL, DANIEL P. ZALESKI, and BROOKS H. PATE, Department of Chemistry, University of Virginia, Charlottesville, VA 22904; ALBERTO LESARRI, Departamento Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, 47011 Valladolid, Spain.

RC12 15 min 11:55
OBSERVATION OF C−H···π INTERACTIONS: MICROWAVE SPECTRA AND STRUCTURES OF THE CH₂FX ··HCCH (X=F,Cl) WEAKLY BOUND COMPLEXES

LENA F. ELMUTI, DANIEL A. OBENCHAIN, DON L. JURKOWSKI, AMELIA J. SANDERS, REBECCA A. PEEBLES, SEAN A. PEEBLES, Department of Chemistry, Eastern Illinois University, 600 Lincoln Avenue, Charleston, IL 61920; AMANDA L. STEBER, JUSTIN L. NEILL, BROOKS H. PATE, Department of Chemistry, University of Virginia, McCormick Rd., PO Box 400319, Charlottesville, VA 22904.
RD. MINI-SYMPOSIUM: SPECTROSCOPIC PERTURBATIONS
THURSDAY, JUNE 23, 2011 – 8:30 am
Room: 1015 McPHERSON LAB

Chair: THOMAS BERGEMAN, SUNY Stony Brook, Stony Brook, New York

RD01
INVITED TALK
30 min 8:30
SPECTROSCOPIC SIGNATURES OF BOND BREAKING INTERNAL ROTATION IN HCP

MARK S CHILD, Physical and Theoretical Chemistry Laboratory, South Parks Rd, Oxford, OX1 3QZ, UK.

RD02
15 min 9:05
PERTURBATION FACILITATED DISPERSED FLUORESCENCE AND STIMULATED EMISSION PUMPING SPECTROSCOPIES OF HCP

HARUKI ISHIKAWA, Department of Chemistry, Graduate School of Science, Kobe University, Nada-ku, Kobe 657-8501, Japan; YASUHIKO MURAMOTO, MASAHITO NAMAI, NAOHIKO MIKAMI, Department of Chemistry, Graduate School of Science, Tohoku University, Aoba-ku, Sendai 980-8578, Japan.

RD03
15 min 9:22
COLLISIONAL ORIENTATION TRANSFER FACILITATED POLARIZATION SPECTROSCOPY

JIANMEI BAI, E.H.AHMED, B. BESER, Y. GUAN, A. M. LYYRA, Temple University; S. ASHMAN, C. M. WOLFE, J. HUENNEKENS, Lehigh University.

RD04
10 min 9:39
THE $X^1\Sigma^+$ AND $B^1\Pi$ STATES OF LiRb AND PROSPECTS FOR CREATING ULTRACOLD GROUND STATE LiRb MOLECULES

SOURAV DUTTA, ADEEL ALTAF, JOHN LORENZ, D. S. ELLIOTT AND YONG P. CHEN, Purdue University, West Lafayette, IN 47907.

RD05
15 min 9:51
OPTICAL STARK SPECTROSCOPY OF CHLORO-METHYLENE, HCCl

XIUJUAN ZHUANG AND TIMOTHY C. STEIMLE, Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287; ZHONG WANG, Math and Sciences Department, Suffolk County Community College, East Campus, Riverhead, NY, 11901.

RD06
15 min 10:20
PHASE SPACE EXPLORATION OF ACETYLENE AT ENERGIES UP TO 13,000 cm$^{-1}$

DAVID S. PERRY, JONATHAN MARTENS, Department of Chemistry, The University of Akron, OH 44325-3601; MICHEL HERMAN, BADR AMYAY, Laboratoire de Chimie quantique et Photophysique, Université libre de Bruxelles, B-1050, Belgium.
RD07 15 min 10:37

ACETYLENE DYNAMICS AT ENERGIES UP TO 13,000 cm$^{-1}$

JONATHAN MARTENS, DAVID S. PERRY, Department of Chemistry, The University of Akron, OH 44325-3601; MICHEL HERMAN, BADR AMAY, Laboratoire de Chimie quantique et Photophysique, Universite libre de Bruxelles, B-1050, Belgium.

RD08 15 min 10:54

THE HIGH RESOLUTION SPECTRUM OF THE Ar–C$_2$H$_2$ COMPLEX


RD09 15 min 11:11

IR EMISSION SPECTROSCOPY OF AMMONIA: LINELISTS AND ASSIGNMENTS

R. HARGREAVES and P. F. BERNATH, Department of Chemistry, University of York, Heslington, York YO10 5DD, UK; N. F. ZOBOV, S. V. SHIRIN, R. I. OVSYANNIKOV and O. L. POLYANSKY, Russian Academy of Sciences, Nizhny Novgorod, Russia; S. N. YURCHENKO, R. J. BARBER and J. TENNYSON, Department of Physics and Astronomy, University College London, London WC1E 6BT, UK.

RD10 15 min 11:28

DIRECT EXCITATION OF THE REACTION COORDINATE: OVERTONE-INDUCED PREDISSOCIATION OF THE HYDROXYMETHYL RADICAL

HANNA REISLER, MIKHAIL RYAZANOV and CHIRANTHA P. RODRIGO, Department of Chemistry, University of Southern California, Los Angeles, CA, 90089-0482.

RD11 15 min 11:45

AUTOIONIZATION BRANCHING RATIOS FOR METAL HALIDE MOLECULES

JEFFREY J. KAY, Lawrence Livermore National Laboratory, Livermore, CA 94550; ROBERT W. FIELD, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139.
<table>
<thead>
<tr>
<th>Session</th>
<th>Duration</th>
<th>Time</th>
<th>Title</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>RE01</td>
<td>15 min</td>
<td>8:30</td>
<td>INTER-RING AND HEXYL CHAIN TORSIONAL POTENTIALS IN POLY (3-HEXYLTHIOPHENE) OLIGOMERS: SCALING WITH THE LENGTH OF THE CONJUGATED POLYMER BACKBONE</td>
<td>RAM S. BHATTA, DAVID S. PERRY, Department of Chemistry, The University of Akron, OH 44325-3601; YENENEH YIMER AND MESFIN TSIGE, Department of Polymer Science, The University of Akron, OH 44325-3909.</td>
</tr>
<tr>
<td>RE02</td>
<td>15 min</td>
<td>8:47</td>
<td>VIBRATIONAL STATE DEPENDENT LARGE AMPLITUDE TUNNELING DYNAMICS IN MALONALDEHYDE</td>
<td>GRANT BUCKINGHAM AND DAVID J. NESBITT, JILA, National Institute of Standards and Technology and University of Colorado, and Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO 80309.</td>
</tr>
<tr>
<td>RE03</td>
<td>15 min</td>
<td>9:04</td>
<td>VIBRATIONAL RELAXATION AND CONTROL OF SALICYLIDENE ANILINE</td>
<td>ADAM D. DUNKELBERGER, RYAN D. KIEDA, JAEOYON SHIN, and F. FLEMING CRIM, Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706.</td>
</tr>
<tr>
<td>RE04</td>
<td>15 min</td>
<td>9:21</td>
<td>DEVELOPMENT OF FEMTOSECOND STIMULATED RAMAN SPECTROSCOPY AS A PROBE OF VIBRATIONAL DYNAMICS</td>
<td>RYAN D. KIEDA, KRISTIN A. BRINEY, ADAM D. DUNKELBERGER, and F. FLEMING CRIM, Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706.</td>
</tr>
<tr>
<td>RE05</td>
<td>15 min</td>
<td>9:38</td>
<td>VIBRATIONAL DYNAMICS OF TRICYANOMETHANIDE</td>
<td>DANIEL WEIDINGER, CASSIDY HOCHINS, and JEFFREY C. OWRUTSKY, Code 6111, Naval Research Laboratory, 4555 Overlook Ave SW, Washington, D.C. 20375.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>Intermission</strong></td>
<td></td>
</tr>
<tr>
<td>RE06</td>
<td>15 min</td>
<td>10:10</td>
<td>PHOTOCHEMISTRY OF HALOGENATED TRANSITION METAL DIANIONS</td>
<td>ALEXANDER N. TARNOVSKY, IGOR L. ZHLEDKOV, EVGENIYA V. BUTAEVA, and ANDREY S. MERESHCINENKO, Department of Chemistry, Bowling Green State University, Bowling Green, OH, 43402.</td>
</tr>
</tbody>
</table>
PHOTOCHEMISTRY OF BROMOFORM AND TRIBROMIDES OF OTHER ELEMENTS IN SOLUTION

ANDREY S. MERESHCHEKO, KANYKEY E. KARABAEVA, ALEXANDER N. TARNOVSKY, Department of Chemistry and Center for Photochemical Sciences, Bowling Green State University, Bowling Green, Ohio 43403; PATRICK Z. EL-KHOURY, Institute for Surface and Interface Science, University of California Irvine, Irvine, CA 92697; AND SUMAN K. PAL, School of Basic Sciences IIT Mandi, Vallabh Degree College Campus, Mandi 175001, India.

ISOMERIZATION BETWEEN CH$_2$ClI AND CH$_2$Cl-I IN CRYOGENIC MATRICES STUDIED ON ULTRAFAST TIMESCALE

THOMAS J. PRESTON, MAITREYA DUTTA, BRIAN J. ESSELMAN, MICHAEL A. SHALOSKI, ROBERT J. MCMAHON, and F. FLEMINING CRIM, The University of Wisconsin-Madison Department of Chemistry, 1101 University Avenue, Madison, WI, 53705; AMIABLE KALUME, LISA GEORGE, and SCOTT A. REID, Department of Chemistry, Marquette University, Milwaukee, WI, 53233.

ISOMERIZATION OF CH$_2$Cl-I TO CH$_2$Cl-II IN CRYOGENIC MATRICES: A STUDY ON ULTRAFAST TIMESCALE

THOMAS J. PRESTON, MAITREYA DUTTA, BRIAN J. ESSELMAN, MICHAEL A. SHALOSKI, ROBERT J. MCMAHON and F. FLEMINING CRIM, The University of Wisconsin-Madison Department of Chemistry, 1101 University Avenue, Madison, WI, 53706; AMIABLE KALUME, LISA GEORGE and SCOTT A. REID, Department of Chemistry, Marquette University, Milwaukee, WI, 53233.

PHOTODISSOCIATION DYNAMICS OF A TRIATOMIC PSEUDO-DIHALIDE: ABSORPTION CROSS SECTION AND DYNAMICS OF SOLVATED ICN$^-$

JOSHUA P. MARTIN, QUANLI GU$^a$, JOSHUA P. DARR$^b$, JILA, Department of Chemistry and Biochemistry University of Colorado at Boulder, Boulder, CO 80309; ANNE B. McCOY, Department of Chemistry, The Ohio State University, Columbus, OH 43210; and W. CARL LINEBERGER, JILA, Department of Chemistry and Biochemistry, University of Colorado at Boulder, Boulder, CO 80309.

$^a$Present address: Department of Chemistry, University of Virginia, Charlottesville, VA 22904
$^b$Present address: Department of Chemistry, University of Nebraska, Omaha, NE 68182

EXCITED-STATE DYNAMICS IN 6-THIOGUANOSINE FROM FEMTOSECOND TO MICROSECOND TIME SCALE

CAO GUO, CHRISTIAN REICHARDT AND CARLOS E. CRESPO-HERNÁNDEZ, Department of Chemistry and the Center for Chemical Dynamics, Case Western Reserve University, 10900 Euclid Avenue, Cleveland, Ohio 44106.
RF. MINI-SYMPOSIUM: THE THz COSMOS
THURSDAY, JUNE 23, 2011 – 1:30 pm
Room: 160 MATH ANNEX

Chair: LUCY ZIURYS, University of Arizona, Tucson, Arizona

RF01

INTERSTELLAR HYDRIDE SPECTROSCOPY WITH HERSCHEL

MARYVONNE GERIN, LERMA, CNRS UMR8112, OBSERVATOIRE DE PARIS & ECOLE NORMALE SUPERIEURE, 24 RUE L'HOMOND, 75231 PARIS CEDEX 05, FRANCE; and THE PRISMAS CONSOR-

TIUM.

RF02

CHEMICAL HERSCHEL SURVEYS OF STAR FORMING REGIONS (CHESS)

MARTIN EMPRECHTINGER, California Institute of Technology, Pasadena CA 91125 (email: em-

precht@caltech.edu).

RF03

OBSERVATIONS OF INTERSTELLAR HYDROGEN FLUORINE AND HYDROGEN CHLORIDE IN THE GALAXY

RAQUEL R. MONJE, DAREK C. LIS, THOMAS G. PHILLIPS, PAUL F. GOLDSMITH, MARTIN EM-

PRECHTINGER, California Institute of Technology, 1200 E. California Blvd., Pasadena, CA 91125-4700, USA ; DAVID A. NEUFELD, Johns Hopkins University, USA.

RF04

THE STRATOSPHERIC OBSERVATORY FOR INFRARED ASTRONOMY (SOFIA)

R. D. GEHRZ, Department of Astronomy, University of Minnesota, 116 Church Street, S. E., Minneapolis, MN 55455; E. E. BECKLIN, Universities Space Research Association, NASA Ames Research Center, MS 211-3, Moffett Field, CA 94035.

RF05

INFRARED SPECTROSCOPIC STUDIES WITH THE STRATOSPHERIC OBSERVATORY FOR INFRARED ASTRONOMY (SOFIA)

R. D. GEHRZ, Department of Astronomy, University of Minnesota, 116 Church Street, S. E., Minneapolis, MN 55455; E. E. BECKLIN, Universities Space Research Association, NASA Ames Research Center, MS 211-3, Moffett Field, CA 94035.

RF06

ROTATIONAL SPECTROSCOPY FOR ASTROPHYSICAL APPLICATIONS: THE THz FREQUENCY REGION

CRISTINA PUZZARINI, GABRIELE CAZZOLI, Dipartimento di Chimica "G. Ciamician", Università di Bologna, I-40126 Bologna, Italy.

Intermission
RF07 15 min 3:45
UNRAVELING THE MYSTERIES OF COMPLEX INTERSTELLAR ORGANIC CHEMISTRY USING HIFI LINE SURVEYS

SUSANNA L. WIDICUS WEAVER, MARY L. RADHUBER, JAY A. KROLL, BRETT A. McGUIRE, and JACOB C. LAAS, Department of Chemistry, Emory University, Atlanta, GA 30322; DAREK C. LIS, Department of Physics, California Institute of Technology, Pasadena, CA 91125; and ERIC HERBST, Departments of Physics, Chemistry, and Astronomy, The Ohio State University, Columbus, OH 43210.

RF08 15 min 4:02
PROGRESS TOWARDS THE ROTATIONAL SPECTRUM OF H$_3^+$ AND ITS ISOTOPOLOGUES

BRETT A. McGUIRE, YIMIN WANG, JOEL M. BOWMAN, AND SUSANNA L. WIDICUS WEAVER, Department of Chemistry, Emory University, Atlanta, GA 30033.

RF09 15 min 4:19
ANALYSIS OF NEW DATA SETS PERTAINING TO THE WATER MOLECULE


RF10 15 min 4:36
VIBRATIONALLY HOT HCN IN THE LABORATORY AND IRC+10216

JOHN C. PEARSON*, SHANSHAN YU, HARSHAL GUPTA and BRIAN J. DROUIN, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr., Pasadena, CA 91109.

A part of this work was performed at the Jet Propulsion Laboratory, California Institute of Technology under contract with the National Aeronautics and Space Administration. Copyright 2010 © California Institute of Technology. All rights reserved.

RF11 15 min 4:53
SHOCK-INDUCED MOLECULAR ASTROCHEMISTRY IN DENSE CLOUDS


RF12 15 min 5:10
THE LABORATORY AND OBSERVATIONAL STUDY OF 2-BUTANONE AS A TEST FOR ORGANIC CHEMICAL COMPLEXITY IN VARIOUS INTERSTELLAR PHYSICAL ENVIRONMENTS

JAY A. KROLL, and SUSANNA L. WIDICUS WEAVER, Department of Chemistry, Emory University, Atlanta, GA 30322; STEVEN T. SHIPMAN, Division of Natural Sciences, New College of Florida, Sarasota, FL 34243.
RF13  15min  5:27
HIGH RESOLUTION FAR INFRARED FOURIER TRANSFORM SPECTROSCOPY OF THE NH2 RADICAL.

M. A. MARTIN-DRUMEL, O. PIRALI, D. BALCON, SOLEIL Synchrotron, AILES beamline, Saint-Aubin, France and Institut des Sciences Moléculaires d’Orsay, ISMO, CNRS, Université Paris XI, Orsay, France; M. VERVOLOET, SOLEIL Synchrotron, AILES beamline, Saint-Aubin, France.

RF14  15min  5:44
THE PURE ROTATIONAL SPECTRA OF ACETALDEHYDE AND GLYCOLALDEHYDE ISOTOPOLOGUES MEASURED IN NATURAL ABUNDANCE BY CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE SPECTROSCOPY

P. BRANDON CARROLL, BRETT A. McGuire, and SUSANNA L. WIDICUS WEAVER, Department of Chemistry, Emory University, Atlanta, GA 30322; DANIEL P. ZALESKI, JUSTIN L. NEILL, and BROOKS H. PATE, Department of Chemistry, University of Virginia, McCormick Rd., P.O. Box 400319, Charlottesville, VA 22904.

RF15  15min  6:01
THE THZ SPECTRUM OF GLYCOLALDEHYDE

MANUEL GOUBET, THERESE R. HUET, IMANE HAYKAL, LAURENT MARGULES, Laboratoire PhLAM, UMR8523 CNRS-Université Lille 1, F-59655 Villeneuve d’Ascq Cedex, France; OLIVIER PIRALI, PASCALE ROY, Ligne AILES - Synchrotron SOLEIL, L’Orme des Merisiers Saint Aubin, F-91192 Gif-sur-Yvette, France.
RG. INFRARED/RAMAN
THURSDAY, JUNE 23, 2011 – 1:30 pm
Room: 170 MATH ANNEX

Chair: ROBERT McKELLAR, National Research Council of Canada, Ottawa, Canada

RG01 15 min 1:30
VIBRATIONAL SPECTRA OF CRYOGENIC PEPTIDE IONS USING H₂ PREDISSOCIATION SPECTROSCOPY

CHRISTOPHER M. LEAVITT, ARRON B. WOLK, MICHAEL Z. KAMRATH, ETIENNE GARAND, MARK A. JOHNSON, Sterling Chemistry Laboratory, Yale University, PO Box 208107, New Haven, CT 06520; and MICHAEL J. VAN STIPDONK, Department of Chemistry, Wichita State University, 1845 Fairmont Ave, Wichita, KS 67208.

RG02 15 min 1:47
VIBRATIONAL CHARACTERIZATION OF SIMPLE PEPTIDES USING CRYOGENIC INFRARED PHOTODISSOCIATION OF H₂-TAGGED, MASS-SELECTED IONS

MICHAEL Z. KAMRATH, ETIENNE GARAND, PETER A. JORDAN, CHRISTOPHER M. LEAVITT, ARRON B. WOLK, SCOTT J. MILLER, AND MARK A. JOHNSON, Sterling Chemistry Laboratory, Yale University, P.O. Box 208107, New Haven, CT 06520 USA; MICHAEL J. VAN STIPDONK, Wichita State University, Department of Chemistry, 1845 Fairmont Ave, Wichita, KS, USA.

RG03 15 min 2:04
USING AN ORGANIC SCAFFOLD TO MODULATE THE QUANTUM STRUCTURE OF AN INTRAMOLECULAR PROTON BOND: CRYOGENIC VIBRATIONAL PREDISSOCIATION SPECTROSCOPY OF H₂ ON PROTONATED 8-NAPHTHALENE-1-AMINE

ANDREW F. DEBLASE, TIMOTHY L. GUASCO, CHRISTOPHER M. LEAVITT, AND MARK A. JOHNSON, STERLING CHEMISTRY, YALE UNIVERSITY, NEW HAVEN, CT, 06520; THOMAS LECTKA, DEPARTMENT OF CHEMISTRY, JOHNS HOPKINS UNIVERSITY, 3400 NORTH CHARLES STREET, BALTIMORE, MD, 21218.

RG04 15 min 2:21
APPLICATION OF INFRARED MULTIPHOTON DISSOCIATION SPECTROSCOPY FOR THE STUDY OF CHIRAL RECOGNITION IN THE PROTONATED SERINE CLUSTERS: PART II

FUMIE X. SUNAHORI, ELENA N. KITOVA, JOHN S. KLASSEN, AND YUNJIE XIU, Department of Chemistry, University of Alberta, Edmonton, Canada T6G 2G2; GUOCHUN YANG, Department of Chemistry, Northeast Normal University, Changchun 130024, Jilin, P.R. China.

RG05 15 min 2:38
ROTATION-VIBRATION SPECTRA OF MALONALDEHYDE OBTAINED WITH FAR-INFRARED SYNCHROTRON RADIATION

D. W. TOKARYK, S. C. ROSS, D. FORTHOMME, J. E. PRESCOTT, Department of Physics and Centre for Laser Atomic and Molecular Sciences, University of New Brunswick, Fredericton, NB, Canada E3B 5A3; K. M. T. YAMADA, F. ITO, EMTech, AIST, Tsukuba-West, Tsukuba, Ibaraki, Japan.
IR SPECTROSCOPIC AND THEORETICAL STUDY OF NEW PHOTOCHROMIC SYSTEMS BASED ON CY- 
MANTRENNE DERIVATIVES.

B. V. LOKSHIN, M. G. EZERNITSKAYA, Yu. B. BORISOV, E. S. KELBYSHEVA, and N. M. LOIM,
A. N. Nesmeyanov Institute of organoelement compounds of Russian Academy of Sciences, Vavilov street, 28,
119991 GSP-1, Moscow, Russia.

Intermission

VIBRATIONAL ANALYSIS AND VALENCE FORCE FIELD FOR NITROTOLUENES, DIMETHYLANILINES AND 
SOME SUBSTITUTED METHYLBENZENES

B. VENKATRAM REDDY, Department of Physics, Kakatiya University, Warangal-506 009, A.P., India 
Email: bvreddy67@yahoo.com; JAI KISHAN OJHA, Department of Physics, Government Degree College, 
Mancherial-504 208, A.P., India; G. RAMANA RAO, Department of Physics, Varada Reddy College of 
Engineering, Ananthasagar, Warangal-506 371, A.P., India.

THE HIGH RESOLUTION SPECTRUM OF JET-COOLED METHYL ACETATE IN THE C=O STRETCH REGION

FUMIE X. SUNAHORI, NICOLE BORHO, XUNCHEN LIU, AND YUNJIE XU, Department of Chemistry, 
University of Alberta, Edmonton, Canada T6G 2G2.

INFRARED FLUORESCENCE MEASUREMENTS OF GASEOUS BENZENE WITH A NEW HOME-MADE SPECTROMETER

G. FÉRAUD, Y. CARPENTIER*, T. PINO, P. PARNEIX, T. CHAMAILLÉ, Institut des Sciences Moléculaires 
d’Orsay, Université Paris-Sud 11, Orsay, France; E. DARTOIS, Y. LONGVAL, Institut d’Astrophysique Spatiale, 
Université Paris-Sud 11, Orsay, France; R. VASQUEZ and Ph. BRÉCHIGNAC, Institut des Sciences 
Moléculaires d’Orsay, Université Paris-Sud 11, Orsay, France.

*Present address: Laboratory Astrophysics Group of the Max Planck Institute for Astronomy at the Friedrich Schiller University Jena, Institute of 
Solid State Physics, Helmholtzweg 3, D-07743 Jena, Germany

INFRARED ION-GAIN SPECTROSCOPY AND FRACTIONAL ABUNDANCE MEASUREMENTS OF CON-
FORMER POPULATIONS

EVAN G. BUCHANAN, JACOB C. DEAN, BRETT M. MARSH, and TIMOTHY S. ZWIER, Department of 
Chemistry, Purdue University, West Lafayette, IN 47907-2804.

SINGLE-CONFORMATION SPECTROSCOPY OF A DIASTEREOEMERIC LIGNIN MONOMER: EXPLORING THE HYDROGEN BONDING ARCHITECTURES OF A TRIOL CHAIN

JACOB C. DEAN, EVAN G. BUCHANAN, ANNA GUTBERLET, WILLIAM H. JAMES III, BIDYUT 
BISWAS, P. V. RAMACHANDRAN, and TIMOTHY S. ZWIER, Department of Chemistry, Purdue Uni-
versity, West Lafayette, IN 47907.
THE TORSIONAL FUNDAMENTAL BAND OF METHYLFORMATE

M. TUDORIE, Service de Chimie Quantique et Photophysique, Université Libre de Bruxelles, CP 160/09, 50 avenue F.D. Roosevelt, B-1050 Brussels, Belgium; V. ILYUSHIN, Department of Microwave Radiospectrometry, Institute of Radio Astronomy of NASU, Chervonopraporna 4, 61002 Kharkov, Ukraine; J. VANDER AUWERA, Service de Chimie Quantique et Photophysique, Université Libre de Bruxelles, CP 160/09, 50 avenue F.D. Roosevelt, B-1050 Brussels, Belgium; O. PIRALI, P. ROY, Ligne AILES – Synchrotron SOLEIL, L’Orme des Merisiers, F-91192 Gif-sur-Yvette, France; T. R. HUET, Laboratoire de Physique des Lasers, Atomes et Molécules, UMR CNRS 8523, Université Lille 1, 59655 Villeneuve d’Ascq Cedex, France.

A FAR INFRARED SYNCHROTRON-BASED INVESTIGATION OF 3-OXETANONE

ZIQIU CHEN, JENNIFER VAN WIJNGAARDEN, Department of Chemistry, University of Manitoba, Winnipeg MB R3T 2N2 Canada.

FAR-INFRARED SYNCHROTRON-BASED SPECTROSCOPY OF FURAN: ANALYSIS OF THE \( \nu_{14} - \nu_{11} \) PERTURBATION AND THE \( \nu_{18} \) AND \( \nu_{19} \) LEVELS

D. W. TOKARYK, S. D. CULLIGAN\(^a\), Department of Physics and Centre for Laser, Atomic and Molecular Sciences, University of New Brunswick, Fredericton, NB, Canada E3B 5A3; B. E. BILLINGHURST, Canadian Light Source, Inc., 101 Perimeter Road, University of Saskatchewan, Saskatoon, SK, Canada S7N 0X4; and J. A. van WIJNGAARDEN, Department of Chemistry, University of Manitoba, Winnipeg, MB, Canada R3T 2N2.

\(^a\)Current address: Inorganic Chemistry Laboratory, South Parks Road, University of Oxford, UK OX1 3QR
<table>
<thead>
<tr>
<th>RH01</th>
<th>15 min 1:30</th>
</tr>
</thead>
<tbody>
<tr>
<td>WAVEGUIDE CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE (CP-FTMW) SPECTRUM OF ALLYL CHLORIDE</td>
<td></td>
</tr>
<tr>
<td>ERIN B. KENT, MORGAN N. McCABE, MARIA A. PHILLIPS, BRITTANY P. GORDON and STEVEN T. SHIPMAN, Division of Natural Sciences, New College of Florida, Sarasota, FL 34243.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>RH02</th>
<th>15 min 1:47</th>
</tr>
</thead>
<tbody>
<tr>
<td>WAVEGUIDE CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE (CP-FTMW) SPECTRUM OF ORTHO-FLUOROTOLUENE</td>
<td></td>
</tr>
<tr>
<td>IAN A. FINNERAN and STEVEN T. SHIPMAN, Division of Natural Sciences, New College of Florida, Sarasota, FL 34243.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>RH03</th>
<th>15 min 2:04</th>
</tr>
</thead>
<tbody>
<tr>
<td>A LOOK AT A SERIES OF ALKYL AND PERFLUOROALKYL BROMIDES AND CHLORIDES</td>
<td></td>
</tr>
<tr>
<td>BRITTANY E. LONG, STEPHEN A. COOKE, Department of Chemistry, The University of North Texas, 1155 Union Circle, #305070, Denton, TX 76203-5017, U.S.A.; GARRY S. GRUBBS II, Department of Chemistry, Wesleyan University, Hall-Atwater Laboratories, 52 Lawn Ave., Middletown, CT 06459-0180, U.S.A.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>RH04</th>
<th>15 min 2:21</th>
</tr>
</thead>
<tbody>
<tr>
<td>METHYL GROUP INTERNAL ROTATION IN THE PURE ROTATIONAL SPECTRUM OF 1,1-DIFLUOROACETONE</td>
<td></td>
</tr>
<tr>
<td>G. S. GRUBBS II, S. A. COOKE, Department of Chemistry, The University of North Texas, 1155 Union Circle, #305070 Denton, TX 76203-5017, USA; P. GRONER, Department of Chemistry, University of Missouri-Kansas City, 5100 Rockhill Road, Kansas City, MO 64110.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>RH05</th>
<th>15 min 2:38</th>
</tr>
</thead>
<tbody>
<tr>
<td>FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF ALKALI METAL ACETYLIDES</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>RH06</th>
<th>15 min 2:55</th>
</tr>
</thead>
<tbody>
<tr>
<td>ANALYSIS OF ROTATIONAL STRUCTURE IN THE HIGH-RESOLUTION INFRARED SPECTRA OF THE TRANS-HEXATRIENE-1,1-D₂ AND -CIS-1-D₂ SPECIES</td>
<td></td>
</tr>
<tr>
<td>NORMAN C. CRAIG, HANNAH A. FUSON, and HENGFENG TIAN, Department of Chemistry and Biochemistry, Oberlin College, Oberlin, OH 44074; THOMAS A. BLAKE, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA 99352.</td>
<td></td>
</tr>
</tbody>
</table>
ANALYSIS OF THE ROTATIONAL STRUCTURE IN THE HIGH-RESOLUTION INFRARED SPECTRUM OF TRANS-HEXATRIENE-1,13C1

NORMAN C. CRAIG and HENGFENG TIAN, Department of Chemistry and Biochemistry, Oberlin College, Oberlin, OH 44074; THOMAS A. BLAKE, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA 99352.

Intermission

ROTATIONAL SPECTRUM SPECTRUM AND COUPLED-CLUSTER CALCULATIONS OF SILICON OXYSULFIDE, O=Si=S

S. THORWIRTH, J. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany; L. A. MÜCK, J. GAUSS, Institut für Physikalische Chemie, Universität Mainz, 55099 Mainz, Germany; F. TAMASSIA, Dipartimento di Chimica Fisica e Inorganica, Università di Bologna, I-40136 Bologna, Italy; V. LATTANZI, M. C. McCARTHY, Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, and School of Engineering and Applied Science, Harvard University, Cambridge, MA 02138.

STRUCTURAL DETERMINATION OF SILACYCLOBUTANE AND SILACYCLOPENTANE USING FOURIER TRANSFORM MICROWAVE (FTMW) AND CHIRPED PULSE FOURIER TRANSFORM MICROWAVE (cp-FTMW) SPECTROSCOPY

ZIQIU CHEN, CODY VAN DIJK AND JENNIFER VAN WIJNGAARDEN, Department of Chemistry, University of Manitoba, Winnipeg MB R3T 2N2 Canada.

ROOM-TEMPERATURE CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE (CP-FTMW) SPECTRUM OF 2-METHYLFURAN

IAN A. FINNERAN and STEVEN T. SHIPMAN, Division of Natural Sciences, New College of Florida, Sarasota, FL 34243.

THE MICROWAVE SPECTRUM OF METHYL VINYL KETONE REVISITED

DAVID S. WILCOX, AMANDA J. SHIRAR, OWEN L. WILLIAMS, BRIAN C. DIAN, Department of Chemistry, Purdue University, West Lafayette, IN, 47907.

HIGH RESOLUTION ROTATIONAL SPECTROSCOPY OF A FLEXIBLE CYCLIC ETHER

THE PURE ROTATIONAL SPECTRA OF THE TWO LOWEST ENERGY CONFORMERS OF \( n \)-BUTYL ETHYL ETHER

B. E. LONG, G. S. GRUBBS II, S. A. COOKE, Department of Chemistry, The University of North Texas, 1155 Union Circle, # 305070 Denton, TX 76203-5017, USA.
RI. THEORY
THURSDAY, JUNE 23, 2011 – 1:30 pm
Room: 1015 McPHERSON LAB

Chair: RUSSELL PITZER, The Ohio State University, Columbus, Ohio

RI01  
INVITED TALK  30 min  1:30
COMPOSITE APPROACHES FOR AB INITIO SPECTROSCOPY: THE CCN, CCSb, AND HNNO RADICALS

KIRK A. PETERSON, J. GRANT HILL, JAMES SHEAROUSE, Department of Chemistry, Washington State University, Pullman, WA 99164; ALEXANDER MITRUSHCHENKOV, Laboratoire de Modélisation et Simulation Multi Echelle, Université Paris-Est Marne-la-Vallée, 77454 Marne la Vallée, Cedex 2, France; and JOSEPH S. FRANCISCO, Department of Chemistry, Purdue University, West Lafayette, IN 47907.

RI02  15 min  2:05
EMPLOYING DIFFUSION MONTE CARLO IN THE CALCULATION OF MINIMIZED ENERGY PATHS OF THE
\[ \text{CH}_3^+ + \text{H}_2 \leftrightarrow \text{CH}_3^+ \leftrightarrow \text{CH}_4^+ + \text{H}_2 \]
REACTION AND ITS ISOTOPIC VARIANTS

CHARLOTTE E. HINKLE, ANNE B. MCCOY, Department of Chemistry, The Ohio State University, Columbus, OH 43210.

RI03  15 min  2:22
POTENTIAL ENERGY SURFACES OF M+NG, M = K, RB, CS AND NG = HE, NE, AR

L BLANK, DAVID E. WEEKS, Engineering Physics Department, Air Force Institute of Technology, 2950 Hobson Way, WPAFB, OH 45433-7765; GARY S. KEDZORIA, High Performance Technologies, Inc. 2435 5th St., WPAFB, OH USA 45433-7765.

RI04  15 min  2:39
A QUANTUM CHEMICAL STUDY OF XH AND XH$_2$ (X=Be,C,N,O): 2s$^2$ RECOUPLED PAIR BONDING

LU XU, D. E. WOON, and T. H. DUNNING, JR., Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801.

RI05  15 min  2:56
COMPUTATIONAL AND SPECTROSCOPIC STUDY OF THE B-N DATIVE BOND IN AMMONIA BORANE

ASHLEY M. WRIGHT, GREGORY S. TSCHUMPER, and NATHAN I. HAMMER, University of Mississippi, Department of Chemistry & Biochemistry, Oxford, MS 38677.

RI06  15 min  3:13
EXCITED STATES IN SOLUTION AT EOM-CCSD LEVEL WITH THE POLARIZABLE CONTINUUM MODEL OF SOLVATION

M. CARICATO, Gaussian, Inc., 340 Quinnipiac St., Bldg 40, Wallingford, CT 06492.

Intermission
RI07 15 min 3:45
EXPLORING TRANSITION METAL CATALYZED REACTIONS VIA AB INITIO REACTION PATHWAYS

HRANT P. HRATCHIAN, Gaussian, Inc., 340 Quinnipiac St., Bldg. 40, Wallingford, CT 06492.

RI08 15 min 4:02
NON-PRODUCT SMOLYAK GRIDS FOR COMPUTING SPECTRA: HOW AND WHY?

GUSTAVO AVILA and TUCKER CARRINGTON JR., Chemistry Department, Queen’s University, Kingston, Ontario K7L 3N6, Canada.

RI09 15 min 4:19
USING A NON-PRODUCT QUADRATURE GRID TO COMPUTE THE VIBRATIONAL SPECTRUM OF C₂H₄

GUSTAVO AVILA and TUCKER CARRINGTON JR., Chemistry Department, Queen’s University, Kingston, Ontario K7L 3N6, Canada.

RI10 15 min 4:36
PROGRESS TOWARDS THE ACCURATE CALCULATION OF ANHARMONIC VIBRATIONAL STATES OF FLUXIONAL MOLECULES AND CLUSTERS WITHOUT A POTENTIAL ENERGY SURFACE

ANDREW S. PETIT and ANNE B. McCoy, Department of Chemistry, The Ohio State University, Columbus, OH 43210.

RI11 15 min 4:53
HOW LIGAND PROPERTIES AFFECT THE FORMATION AND CHARACTERISTICS OF RECOUPLED PAIR BONDS

BETH A. LINDQUIST, D. E. WOON and T. H. DUNNING, JR., Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana IL, 61801.

RI12 15 min 5:10
A QUANTUM CHEMICAL STUDY OF THE STRUCTURE AND CHEMISTRY OF HZnCH₃, A TRANSITION METAL COMPOUND WITH 4s² RECOUPLED PAIR BONDING

D. E. WOON and T. H. DUNNING, JR., Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801.

RI13 15 min 5:27
THE SEARCH FOR AN OBSERVABLE HELIUM COMPLEX

ADRIAN M. GARDNER, TIMOTHY G. WRIGHT, School of Chemistry, University of Nottingham, University Park, Nottingham, NG7 2RD, United Kingdom; and COREY J. EVANS, Department of Chemistry, University of Leicester, University Road, Leicester, LE1 7RH, United Kingdom.
RJ. RADICALS AND IONS
THURSDAY, JUNE 23, 2011 – 1:30 pm
Room: 2015 McPHERSON LAB

Chair: LAURA McCUNN, Marshall University, Huntington, West Virginia

RJ01 15 min 1:30
DEHYROGENATION OF ETHYLENE: SPECTROSCOPY AND STRUCTURES OF La(C\textsubscript{2}H\textsubscript{2}) AND La(C\textsubscript{4}H\textsubscript{6}) COMPLEXES

SUDESH KUMARI, MOURAD ROUDJANE, and DONG-SHENG YANG, Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055.

RJ02 15 min 1:47
DEHYDROGENATION AND C-H BOND INSERTION OF PROPENE: La(\eta\textsuperscript{2}-C\textsubscript{3}H\textsubscript{4}) AND HLa(\eta\textsuperscript{3}-C\textsubscript{3}H\textsubscript{5})

SUDESH KUMARI and DONG-SHENG YANG, Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055.

RJ03 15 min 2:04
OBSERVATION OF TWO La(C\textsubscript{3}H\textsubscript{2}) ISOMERS FORMED BY DEHYDROGENATION OF PROPYNE

DILRUKSHI HEWAGE, MOURAD ROUDJANE, AND DONG-SHENG YANG, Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055.

RJ04 15 min 2:21
VIBRONIC SPECTROSCOPY OF THE PHENYLCYANOMETHYL RADICAL

DEEPALI N. MEHTA, NATHANIEL M. KIDWELL, and TIMOTHY S. ZWIER, Department of Chemistry, Purdue University, West Lafayette, IN 47907.

RJ05 15 min 2:38
SPECTROSCOPIC IDENTIFICATION OF ISOMERIC TRIMETHYLBENZYL RADICALS GENERATED IN CORONA DISCHARGE OF TETRAMETHYLBENZENE

YOUNG WOOK YOON, SANG KUK LEE, Department of Chemistry, Pusan National University, Pusan 609-735, Korea; and GI WOO LEE, Korea Basic Science Institute, Pusan 609-735, Korea.

RJ06 15 min 2:55
INFRARED SPECTRA OF PRODUCTS OF THE ULTRAVIOLET AND VACUUM ULTRAVIOLET IRRADIATION OF BENZENE TRAPPED IN SOLID NEON

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

Intermission
INFRARED SPECTROSCOPY OF PROTONATED MIXED BENZENE-WATER CLUSTERS

T. CHENG, B. BANDYOPADHYAY and M. A. DUNCAN, Department of Chemistry, University of Georgia, Athens, GA 30602.

MASS-ANALYZED THRESHOLD IONIZATION AND STRUCTURES OF M$_3$C$_2$(M=Sc, La)

LU WU, ROUDJANE MOURAD and D. S. YANG, Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055.

VIBRATIONAL AND GEOMETRIC STRUCTURES OF La$_3$C$_2$O AND La$_3$C$_2$O$^+$ FROM MASS-ANALYZED THRESHOLD IONIZATION

ROUDJANE MOURAD, LU WU and D. S. YANG, Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055.

AN UNEXPECTED GAS-PHASE BINDING MOTIF FOR METAL DICATION COMPLEXATION WITH PEPTIDES: IRMPD SPECTROSCOPIC STRUCTURE DETERMINATION

ROBERT C. DUNBAR, Chemistry Department, Case Western Reserve Univ., Cleveland, OH 44106; JEFFREY STEILL, Sandia National Laboratory, Livermore, CA; NICOLAS POLFER, Chemistry Department, University of Florida, Gainesville, FL; GIJ EL BERDEN, FOM Institute for Plasma Physics, Nieuwegein, Netherlands; JOS OOMENS, FOM Institute for Plasma Physics, Nieuwegein, and University of Amsterdam, Netherlands.

SPECTROSCOPIC INVESTIGATION OF ELECTRON-INDUCED PROTON TRANSFER IN THE FORMIC ACID DIMER, (HCOOH)$_2$

HELEN K. GERARDI, CHRIS M. LEAVITT, ANDREW F. DEBLASE, AND MARK A. JOHNSON, Yale University, Department of Chemistry, New Haven, CT.

VIBRATIONALLY MEDIATED ELECTRON CAPTURE IN THE CO$_2$(H$_2$O)$_6$ ANION

KRISTIN J. BRENN, Sterling Chemistry Laboratory, Yale University, P.O. Box 208107, New Haven, CT 06520; ANDREW F. DEBLASE, Sterling Chemistry Laboratory, Yale University, P.O. Box 208107, New Haven, CT 06520; and MARK A. JOHNSON, Sterling Chemistry Laboratory, Yale University, P.O. Box 208107, New Haven, CT 06520.

INFRARED PREDISSOCIATION SPECTROSCOPY OF H$_2$-TAGGED DICARBOXYLIC ACID ANIONS

ARRON B. WOLK, Chemistry Laboratory, Yale University, P.O. Box 208107, New Haven, CT 06520; MICHAEL Z. KAMRATH, Chemistry Laboratory, Yale University, P.O. Box 208107, New Haven, CT 06520; CHRISTOPHER M. LEAVITT, Chemistry Laboratory, Yale University, P.O. Box 208107, New Haven, CT 06520; and MARK A. JOHNSON, Chemistry Laboratory, Yale University, P.O. Box 208107, New Haven, CT 06520.
FA01  INVITED TALK  30 min  8:30
EXPLORING NEW SPECTRAL WINDOWS WITH THE HERSCHEL SPACE OBSERVATORY

EDWIN A. BERGIN AND THE HEXOS TEAM, Department of Astronomy, University of Michigan (email to: ebergin@umich.edu).

FA02  15 min  9:05
HERSCHEL OBSERVATIONS OF EXTRA-ORDINARY SOURCES (HEXOS): ANALYSIS OF THE HIFI 1.2 THz WIDE SPECTRAL SURVEY TOWARD ORION KL

N. R. CROCKETT, E. A. BERGIN, S. WANG, Department of Astronomy, University of Michigan, 500 Church Street, Ann Arbor, MI 48109, USA; G. BLAKE, M. EMPRECHTINGER, D. LIS, California Institute of Technology, Cahill Center for Astronomy and Astrophysics 301-17, Pasadena, CA 91125 USA; H. GUPTA, J. PEARSON, S. YU, Jet Propulsion Laboratory, Caltech, Pasadena, CA 91109, USA; T. BELL, J. CERNICHARO, Centro de Astrobiología (CSIC/INTA), Laboratorio de Astrofísica Molecular, Ctra. de Torrejón a Ajalvir, km 428850, Torrejón de Ardoz, Madrid, Spain; S. LORD, Infrared Processing and Analysis Center, California Institute of Technology, MS 100-22, Pasadena, CA 91125; R. PLUME, Department of Physics and Astronomy, University of Calgary, 2500 University Drive NW, Calgary, AB T2N 1N4, Canada; P. SCHILKE, Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany; and F. VAN DER TAK, SRON Netherlands Institute for Space Research, PO Box 800, 9700 AV, Groningen, The Netherlands.

FA03  15 min  9:22
DETECTION OF OH$^+$ AND H$_2$O$^+$ TOWARD ORION KL

HARSHAL GUPTA$, JOHN C. PEARSON, SHANSHAN YU, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109; PAUL RIMMER, ERIC HERBST, Departments of Physics, Chemistry, and Astronomy, The Ohio State University, Columbus, OH 43210; EDWIN A. BERGIN, Department of Astronomy, University of Michigan, Ann Arbor, MI 48109; and the HEXOS TEAM, HTTP://WWW.HEXOS.ORG/TEAM.PHP.

$A$ part of this work was performed at the Jet Propulsion Laboratory, California Institute of Technology under contract with the National Aeronautics and Space Administration. Copyright 2010© California Institute of Technology. All rights reserved.

FA04  15 min  9:39
IS WATER ICE THE PRECURSOR TO OH$^+$ AND H$_2$O$^+$ IN ORION KL?

PAUL B. RIMMER, Department of Physics, The Ohio State University, Columbus, OH 43210; ERIC HERBST, Departments of Astronomy, Chemistry and Physics, The Ohio State University, Columbus, OH 43210.

Intermission
FA05 15 min 10:10
REACHING THE LINE CONFUSION LIMIT: ANALYSIS OF THE $\lambda = 1.3$ mm SPECTRUM OF ORION-KL

MARY L. RADHUBER, JAY A. KROLL, SUSANNA L. WIDICUS WEAVER, 1515 DICKEY DR. ATLANTA, GA 30322.

FA06 15 min 10:27
$^{15}$N/$^{14}$N RATIO DETERMINATION IN THE ISM WITH HERSCHEL WITH HIGH RESOLUTION SPECTROSCOPY OF NITROGEN RADICALS

L. MARGULÈS, S. BAILLEUX, G. WLODARCZAK, Laboratoire PhLAM, CNRS UMR 8523, Université Lille 1, 59655 Villeneuve d’Ascq Cedex, France; O. PIRALI, M.-A. MARTIN-DRUMEL, P. ROY, Ligne AILES - Synchrotron SOLEIL, L’Orme des Merisiers Saint Aubin, 91192 Gif-sur-Yvette, France; E. ROUEFF, Laboratoire de l’Univers et de ses Théories, Observatoire de Paris-Meudon, 92195, Meudon, France; and M. GERIN, LERMA, CNRS UMR 8112, 24 rue Lhomond, 75231 Paris Cedex 05, France.

FA07 15 min 10:44
THZ SPECTROSCOPY OF $^{13}$C ISOTOPIC SPECIES OF A "WEED": ACETALDEHYDE

Sciences Chimiques de Rennes, UMR 6226 CNRS-ENSCR, Avenue du Général Leclerc, CS 50837, 35708 Rennes Cedex 7, France; L. MARGULÈS, and 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.

FA08 15 min 11:01
THE ROTATIONAL SPECTRUM OF $^{13}$CH$_3$NH$_2$ UP TO 1 THz

ROMAN A. MOTIYENKO, LAURENT MARGULÈS, Laboratoire PhLAM, CNRS UMR 8523, Université de Lille 1, 59655 Villeneuve d’Ascq Cedex, France; VADIM V. ILYUSHIN, Institute of Radio Astronomy of NASU, Chervonopraporna 4, 61002 Kharkov, Ukraine.

FA09 10 min 11:18
THE EXTENDED SPECTROSCOPIC DATABASE ON FORMAMIDE: PARENT, $^{13}$C AND DEUTERATED SPECIES UP TO 1 THz

A. S. KUTSENKO, Institute of Radio Astronomy of NASU, Chervonopraporna 4, 61002 Kharkov, Ukraine; R. A. MOTIYENKO, L. MARGULÈS, Laboratoire PhLAM, CNRS/Université des Sciences et Technologies de Lille 1, Bât. P5, 59655 Villeneuve d’Ascq Cedex, France; J.-C. GUILLEMIN, Sciences Chimiques de Rennes-Ecole Nationale Supérieure de Chimie de Rennes-CNRS, 35700 Rennes, France.

FA10 Post-deadline Abstract 10 min 11:30
MONTE CARLO MODELING OF GAS-GRAIN CHEMISTRY IN STAR-FORMING REGIONS

A.I. VASYUNIN, E. HERBST, The Ohio State University.
FB01 15 min 8:30
AUGER ELECTRONS VIA Kα X-RAY LINES OF PLATINUM COMPOUNDS FOR NANOTECHNOLOGICAL APPLICATIONS

SULTANA N. NAHAR, Dept of Astronomy, The Ohio State University, Columbus, OH 43210; SARA LIM, Biophysics Program, The Ohio State University, Columbus, OH 43210; A.K. PRADHAN, Dept of Astronomy, and Chemical Physics Program, The Ohio State University, Columbus, OH 43210; R.M. PITZER, Dept of Chemistry, The Ohio State University, Columbus, OH 43210.

FB02 15 min 8:47
A QUANTUM CHEMICAL EXPLORATION OF THE SFₙO SERIES (n = 1 – 5): AN ATOM-BY-ATOM APPROACH

TYLER Y. TAKESHITA, D. E. WOON, and T. H. DUNNING, JR., Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801.

FB03 10 min 9:04
A COMPUTATIONAL INVESTIGATION OF c-C₃H₂·HX(X = F, Cl, Br) H-BONDED COMPLEXES

PRADEEP R. VARADWAJ, ARPITA VARADWAJ, GILLES H. PESLHERBE, Centre for Research in Molecular Modeling & Department of Chemistry and Biochemistry, Concordia University, Montreal, QC, Canada.

FB04 15 min 9:16
ELECTRONIC STRUCTURE OF ETHYNYL SUBSTITUTED CYCLOBUTADIENES

FRANK LEE EMMENT III, STEPHANIE J. THOMPSON, and LYUDMILA V. SLIPCHENKO, Department of Chemistry, Purdue University, West Lafayette, IN 47907.

FB05 15 min 9:33
AB INITIO INVESTIGATION OF THE EXCITED STATES OF NUCLEOBASES AND NUCLEOSIDES

PÉTER G. SZALAY, GÉZA FOGARASI, Eötvös Loránd University, Budapest, Hungary; THOMAS WATSON, AJITH PERERA, VICTOR LOTRICH, ROD J. BARTLETT, Quantum Theory Project, University of Florida, Gainesville, FL.

FB06 15 min 9:50
APPLICATIONS OF PATH INTEGRAL LANGEVIN DYNAMICS TO WEAKLY BOUND CLUSTERS AND BIOLOGICAL MOLECULES

CHRISTOPHER ING, Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada; CONRAD HINSEN, Centre de Biophysique Moléculaire, CNRS, Rue Charles Sadron, 45071 Orleans, France; JING YANG, PIERRE-NICHOLAS ROY, Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada.
Intermission

FB07  15 min  10:30
INTERPRETATION OF THE IR/UV SPECTRA OF Ac-Trp-Tyr-NH₂ and Ac-Trp-Tyr-Ser-NH₂ USING MOLECULAR DYNAMICS AND AB INITIO METHODS.¹

JESSICA A. THOMAS and DAVID W. PRATT, Department of Chemistry, University of Pittsburgh, Pittsburgh, PA 15260; ERIC GLOAGUEN, BENJAMIN TARDIVEL, FRANÇOIS PIUZZI, and MICHEL MONS, Laboratoire Francis Perrin, URA 2453 CRNS, Service des Photons, Atomes et Molécules CEA Saclay, Bât 522, 91191 Gif-sur-Yvette Cedex, France.

¹Work supported in part by NSF CHE-0911117

FB08  15 min  10:47
APPLICATION OF EFFECTIVE FRAGMENT POTENTIAL METHODS TO THE REDOX POTENTIAL OF GREEN FLUORESCENT PROTEIN

DEBASHREE GHOSH, ANNA I. KRYLOV, Department of Chemistry, University of Southern California, Los Angeles, CA 90089 (email to D. G.: debashree.ghosh@gmail.com).

FB09  15 min  11:04
VIBRONIC COUPLING IN ASYMMETRIC DIMERS: GENERALIZATION OF THE FULTON-GOUTERMAN APPROACH

B. NEBGEN and L. V. SLIPCHENKO, Department of Chemistry, Purdue University, West Lafayette, IN 47907.

FB10  15 min  11:21
Post-deadline Abstract
PREDICTION OF FUNDAMENTAL VIBRATIONAL FREQUENCIES AND INFRARED INTENSITIES: A BENCHMARK STUDY

JUANA VÁZQUEZ, MICHAEL E. HARDING, JOHN F. STANTON, Institute for Theoretical Chemistry, Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, TX 78712.

FB11  10 min  11:38
Post-deadline Abstract
VIBRATIONAL CORRECTIONS TO MOLECULAR PROPERTIES: SECOND-ORDER VIBRATIONAL PERTURBATION THEORY VS VARIATIONAL COMPUTATIONS

MICHAEL E. HARDING, JUANA VÁZQUEZ, JOHN F. STANTON, Institute for Theoretical Chemistry, Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, TX 78712, USA; GREGOR DIEZEMANN, and JÜRGEN GAUSS, Institut für Physikalische Chemie, Universität Mainz, Jakob-Welder-Weg 11, D-55128 Mainz, Germany.
FC01 15 min 8:30
NEW METHOD OF FITTING EXPERIMENTAL RO-VIBRATIONAL INTENSITIES TO THE DIPOLE MOMENT FUNCTION: APPLICATION TO HCl

G. LI, P. F. BERNATH, Department of Chemistry, University of York, Heslington, York YO10 5DD; I. E. GORDON, L. S. ROTHMAN, Harvard-Smithsonian Center for Astrophysics, Atomic and Molecular Physics Division, Cambridge MA 02138, USA.

FC02 15 min 8:47
EXTENSIVE AND HIGHLY ACCURATE LINE LISTS FOR HYDROGEN HALIDES

G. LI and P. F. BERNATH, Department of Chemistry, University of York, Heslington, York YO10 5DD, UK; I. E. GORDON, L. S. ROTHMAN, C. RICHARD, Harvard-Smithsonian Center for Astrophysics, Atomic and Molecular Physics Division, Cambridge MA 02138, USA; R. J. LE ROY, Department of Chemistry, University of Waterloo, Waterloo, Ontario, N2L 3G1, Canada; I. A. COXON, Department of Chemistry, Dalhousie University, Halifax, Nova Scotia B3H 4J3, Canada; P. HAJIGEORGIOU, Department of Life and Health Sciences, University of Nicosia, 46 Makedonitissas Ave., P.O. Box 24005, Nicosia 1700, Cyprus.

FC03 15 min 9:04
NEAR-INFRARED OVERTONE SPECTROSCOPY OF TRITIATED WATER

KAORI KOBAYASHI, TOMOYA ENOKIDA, DAISUKE IIO, YUTA YAMADA, Department of Physics, University of Toyama, 3190 Gofuku, Toyama, 930-8555 Japan; MASANORI HARA, YUJI HATANO, Hydrogen Isotope Research Center, University of Toyama, 3190 Gofuku, Toyama, 930-8555 Japan.

FC04 15 min 9:21
ANALYSIS OF THE VIBRATIONAL SPECTRA OF P$_3$N$_3$(OCH$_2$CF$_3$)$_6$ AND P$_4$N$_4$(OCH$_2$CF$_3$)$_8$

ADRIAN K. KING, DAVID F. PLANT, PETER GOLDING, Atomic Weapons Establishment, Aldermaston, Berkshire, RG7 4PR, United Kingdom; MICHAEL A. LAWSON and PAUL B. DAVIES, University of Cambridge, Department of Chemistry, Lensfield Road, Cambridge, CB2 1EW, United Kingdom.

FC05 15 min 9:38
GAS PHASE THZ SPECTROSCOPY OF ORGANOSULFIDE AND ORGANOPHOSPHOROUS COMPOUNDS USING A SYNCHROTRON SOURCE

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

Intermission
HIGH RESOLUTION INFRARED SPECTRA OF SPIROPENTANE, \((\text{C}_5\text{H}_8)\)


C-H STRETCH OVERTONE SPECTRA OF FLUORINATED ETHERS

SHIZUKA HSIEH, Chemistry Department, Smith College, Northampton, MA 01063.

COLLISION-INDUCED INFRARED ABSORPTION BY COLLISIONAL COMPLEXES IN DENSE HYDROGEN-HELIUM GAS MIXTURES AT THOUSANDS OF KELVIN

MARTIN ABEL, LOTHAR FROMMHOLD, Department of Physics, The University of Texas at Austin, Austin, TX 78712; XIAOPING LI, KATHARINE L. C. HUNT, Department of Chemistry, Michigan State University, East Lansing, MI 48824.

ROTATIONALLY-RESOLVED INFRARED SPECTROSCOPY OF THE POLYCYCLIC AROMATIC HYDROCARBON PYRENE \((\text{C}_{16}\text{H}_{10})\) IN THE MID-INFRARED USING A QUANTUM CASCADE LASER-BASED CAVITY RINGDOWN SPECTROMETER

JACOB T. STEWART, BRIAN E. BRUMFIELD, 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.

VIBRATIONAL SPECTROSCOPIC STUDY ON SOME HOFMANN TYPE CLATHRATES: \(\text{M}(2-(1\text{-CYCLOHEXENYL})\text{ETHYLAMINE})_2\text{Ni(CN)}_4\cdot\text{2BENZENE (M=Ni AND Cd)}\)

TEKİN İZG, DEPARTMENT OF PHYSICS, ARTS AND SCIENCE FACULTY, İNiNÜ UNIVERSITY, MALATYA, 44069, TURKEY; CEMAL PARLAK, DEPARTMENT OF PHYSICS, ARTS AND SCIENCE FACULTY, Dumlupınar University, Kütahya, 43100, Turkey; MUSTAFA SENYEL, DEPARTMENT OF PHYSICS, SCIENCE FACULTY, ANADOLU UNIVERSITY, ESKİŞEHİR, 26470, TURKEY.
FD. MINI-SYMPOSIUM: FUNDAMENTAL PHYSICS
FRIDAY, JUNE 24, 2011 – 8:30 am
Room: 1015 McPherson Lab
Chair: Trevor Sears, Brookhaven National Laboratory, Upton, New York

FD01
INVITED TALK
TIME-DOMAIN MW SPECTROSCOPY: FUNDAMENTAL PHYSICS FROM MOLECULAR ROTATION

JENS-UWE GRABOW, Gottfried-Wilhelm-Leibniz-Universität, Institut für Physikalische Chemie & Elektrochemie, Callinstraße 3A, 30167 Hannover, Germany.

FD02
15 min 9:05
HIGH PRECISION UV MEASUREMENTS IN CO, TOWARDS A LABORATORY TEST OF THE TIME-INVARIANCE OF μ.

ADRIAN J. DE NIJS, KJELD S.E. EIKEMA, WIM UBACHS and HENDRICK L. BETHLEM, LaserLab, VU University Amsterdam, the Netherlands.

FD03
15 min 9:22
PROSPECTS FOR RAPID DECELERATION OF DIATOMIC MOLECULES WITH OPTICAL BICHROMATIC FORCES

E. E. EYLER and M. A. CHIEDA, Department of Physics, University of Connecticut, Storrs, CT 06269, USA.

FD04
15 min 9:39
DECELERATION AND TRAPPING OF HEAVY DIATOMIC MOLECULES FOR PRECISION MEASUREMENTS


FD05
15 min 9:56
INVESTIGATION OF THE USE OF HE – DIATOMIC VAN DER WAALS COMPLEXES AS A PROBE OF TIME-REVERSAL VIOLATION

JACOB STINNETT, ERIC ABRAHAM, NEIL SHAFER-RAY, Homer L. Dodge Department of Physics, University of Oklahoma, 440 W. Brooks, NH 100, Norman, OK 73019.

Intermission

FD06
15 min 10:30
FREQUENCY COMB VELOCITY MODULATION SPECTROSCOPY

KEVIN C. COSSEL, LAURA C. SINCLAIR, TYLER COFFEY, ERIC 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.
OPTICAL PULSE-SHAPING FOR INTERNAL COOLING OF MOLECULAR IONS

CHIEN-YU LIEN, SCOTT R. WILLIAMS, and BRIAN ODOM, Department of Physics and Astronomy, Northwestern University, 2145 Sheridan Road, Evanston IL 60208.

RELATIVISTIC COMBINED PSEUDOPOTENTIAL—RESTORATION METHOD FOR STUDYING MULTITUDE OF PROPERTIES IN HEAVY-ATOM SYSTEMS

ANATOLY V. TITOV, ALEXANDER N. PETROV, LEONID V. SKRIPNIKOV, NIKOLAI S. MOSYAGIN, B.P. Konstantinov Petersburg Nuclear Physics Institute, Gatchina, Leningrad district 188300, Russia.

*This work is supported by the RFBR Grant No. 09–03–01034

SPECTROSCOPIC CHARACTERIZATION OF ThF AND THE LOW- LYING STATES OF ThF+

BEAU J. BARKER, IVAN O. ANTONOV, and MICHAEL C. HEAVEN, Department of Chemistry, Emory University, Atlanta, GA 30322.
TOWARD A CONTINUOUS-WAVE SOLID HYDROGEN RAMAN LASER FOR MOLECULAR SPECTROSCOPY APPLICATIONS

W. R. Evans, Department of Physics, University of Illinois at Urbana-Champaign, Urbana, IL 61801; T. Momose, Department of Chemistry, The University of British Columbia, Vancouver, BC Canada V6T 1Z1; B. J. McCall, Departments of Chemistry, Physics, and Astronomy, University of Illinois at Urbana-Champaign, Urbana, IL 61801.

PHOTODISSOCIATION OF FORMIC ACID ISOLATED IN SOLID PARAHYDROGEN

David T. Anderson, Leif O. Paulson, Department of Chemistry, University of Wyoming, Laramie, WY 82071-3838.

RESONANT TWO-STEP IONIZATION OF Rb AND Cs ATOMS ON HELIUM NANODROPLETS

F. Lackner, M. Theisen, and W.E. Ernst, Institute of Experimental Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria.

INFRARED AND MICROWAVE-INFRARED DOUBLE RESONANCE SPECTROSCOPY OF METHANOL EMBEDDED IN SUPERFLUID HELIUM NANODROPLETS

Paul L. Raston and Wolfgang Jäger, Department of Chemistry, University of Alberta, Edmonton, Alberta T6G-2G2, Canada.

LASER SPECTROSCOPY OF HYDROGEN PEROXIDE EMBEDDED IN HELIUM NANODROPLETS

Chriissy J. Knapp, Paul L. Raston, and Wolfgang Jäger, Department of Chemistry, University of Alberta, Edmonton, AB, Canada T6G 2G2.

Intermission

PYRIDINE AGGREGATION IN HELIUM NANODROPLETS

Pablo Nieto, Melanie Letzner, Daniel Habig, Toersten Poerschke, Sarah Angelique Grün, Kenny Hanke, Gerhard Schwaab and Martina Havenith, Department of Physical Chemistry II, Ruhr-Universität Bochum, Germany.
FE07  
Post-deadline Abstract  
15 min  10:27  

IR SPECTROSCOPY STUDY ON THE \((\text{HCl})_n(\text{H}_2\text{O})_m\) AGGREGATION IN HELIUM NANODROPLETS  

**PABLO NIETO, MELANIE LETZNER, DANIEL HABIG, TOERSTEN POERSCHKE, SARAH ANGELIQUE GRÜN, KENNY HANKE, GERHARD SCHWAAB and MARTINA HAVENITH, Department of Physical Chemistry II, Ruhr-Universität Bochum, Germany.**

FE08  
Post-deadline Abstract  
10 min  10:44  

IR-SPECTROSCOPY OF GLYCINE AND ITS COMPLEXES WITH WATER IN HELIUM NANODROPLETS  

**M. LETZNER, S. A. GRÜN, G. SCHWAAB and M. HAVENITH, Department of Physical Chemistry II, Ruhr-University Bochum, D-44780 Bochum, Germany.**

FE09  
Post-deadline Abstract  
15 min  10:56  

INELASTIC SCATTERING OF RADICALS FROM A LIQUID SURFACE  

**MICHAEL ZIEMKIEWICZ and DAVID NESBITT, JILA - UNIVERSITY OF COLORADO, 440 UCB, BOULDER, CO 80309.**
AUTHOR INDEX

A
ABEL, M. – FC08
ABRAHAM, E. – FD05
ADAM, A. G. – WG11, WG12
ADAM, A. G. – TD05
ADAMS, C. L. – MI06, MI07
ADANDE, G. R. – TC10
AHMED, E. H. – RD03
AHMED, M. – WJ09
ALBERT, S. – WF15
ALLEN, J. – TA02
ALLEN, T. F. – WG11
ALonso, J. – TC03
ALonso, J. L. – MH13, MH14, MI06, MI07, RC05, RC07, RC08, RH12
ALPHEI, L. D. – RA06, RA08
ALBERT, A. – RD04
AMANO, T. – TF05, WJ04
AMICANGELO, J. C. – MJ06
AMYAY, B. – RD06, RD07
ANDERSEN, M. – RF11
ANDERSON, D. T. – FE02
ANNESLEY, C. J. – TB09
ANTONOV, I. O. – TD01, TH02, WG06, RA10, FD09
ARAKI, M. – WF06
ASHMAN, S. – RD03
ASVANY, O. – MI13
AUWERA, J. V. – MG05, RG12
AVILA, G. – RI08, RI09
AYLES, V. – TH12
AZZAM, A. – TJ09

B
BAHOU, M. – MJ06, MJ09
BAI, J. – RD03
BAILEY, W. C. – WH13
BAILLEUX, S. – FA06
BAKLANOY, K. I. – RA05
BALCON, D. – RF09, RF13
BALDACCI, A. – TC03
BALDAN, A. – TC03
BANDYOPADHYAY, B. – MG12, MI05, TG08, RJ07
BANERJEE, J. – MF02
BANISKAUS, J. – MJ11
BAO, J. – TB07
BARABAN, J. H. – TH05, TH06
BARBER, R. J. – MG02, TJ09, RD09
BARKER, B. J. – TD01, TH02, WG06, RA10, FD09
BARTLETT, R. J. – FB05
BAUERECKER, S. – WF15
BAUM, A. – RA06, RA08
BAUMANN, C. A. – MJ01
BAZSO, G. – MJ03
BEAMES, J. M. – TI07, WJ06
BECKLIN, E. E. – RF04, RF05
BEJIANI, M. – MJ08
BELL, T. – FA02
BELLOCHE, A. – TF07
BELLOS, M. A. – MF02
BENNER, D. C. – TE01, TE03, WF17, RB01, RB02
BERDEN, G. – RJ10
BERG, J. E. V. D. – FD04
BERGEMAN, T. H. – TH04
BERGIN, E. A. – FA01, FA02, FA03
BERKE, A. E. – TB09
BERNARD, J. – RF11
BERNATH, P. F. – MG04, TD02, TD03, WA01, RD09, FC01, FC02
BESER, B. – RD03
BETHELM, H. L. – FD02
BEUTHER, H. – TF08
BEČKA, E. – MI03
BHATTA, R. S. – TB10, RE01
BIALKOWSKA-JAWORSKA, E. – WH11
BILLINGHURST, B. E. – RG14
BILLS, B. J. – WH09
BINNS, M. K. L. – RH05
BIRD, R. G. – TG05, RC09
BISWAS, B. – RG11
BLAKE, G. – FA02
BLAKE, T. A. – RH06, RH07, FC06
BLAKE, T. F. – TB02, TB03
BLANCO, S. – RH12
BLANK, L. – RI03
BOBON, M. – TA12
BOCUQUET, R. – RB06, FC05
BONDYBEY, V. E. – TD01, RA10
BORHO, N. – RG08
BORISOV, Y. B. – RG06
BOTTINELLI, S. – WF11
BOUCHEZ, A. – WF11
BOUDON, V. – WF15, RB03
BOURGEIOS, M. T. – RB03

BOWMAN, J. M. – RF08
BRAND, C. – TG06
BRATHWAITE, A. D. – MI04
BRAUER, C. S. – MH09
BRECHIGNAC, P. – WF14, WJ05
BRECKENRIDGE, W. H. – WG08
BREEN, K. J. – RJ12
BRINEY, K. A. – RE04
BROOKS, A. H. – MH05
BROWN, G. G. – MH10
BROWN, K. R. – MI01
BROWN, L. – WF16
BROWN, L. R. – TE01, TE03, TE04, WF15, RB01
BRUMFIELD, B. E. – TA03, FC09
BRÚNKEN, S. – TC04, RF09
BRÉCHIGNAC, P. – RG09
BUCCINO, M. P. – TC10, RH05
BUCHANAN, E. – TD11
BUCHANAN, E. G. – WJ10, WJ11, RG10, RG11
BUCKINGHAM, G. – RE02
BUDARZ, J. – TB06
BURROWS, J. P. – TE11
BUTAEDA, E. V. – RE06
BÜHLER, C. C. – TB07

C
CABEZAS, C. – MH13, MH14, RC05, RC07, RC08
CAMINATI, W. – MI04, WH08
CAMPARGUE, A. – TE09
CARICATO, M. – RI06
CARNEGIE, P. D. – MI05
CAROLLO, R. – MF02
CARPENTIER, Y. – RG09
CARRINGTON JR., T. – RI08, RI09
CASTANO, F. – WH08
CASTO, C. – TE12
CAZZOLI, G. – TC03, RF06
CECCARELLI, C. – WF11
CERNICHARO, J. – FA02
CH'NG, L. C. – TB12
CHAKRAVORTY, T. – MG12, TG08
CHAMAILLÉ, T. – RG09
CHANDRASEKHAR, P. – MF03
CHANG, C. – TD10
CHEN, H. – TA09, TA11
CHEN, J. – RA04, RB09
FRANCISCO, J. S. – RI01
FREEL, K. – TB11, WJ13
FREEMONT, J. – MG01
FREUND, R. W. – WF03
FREY, S. E. – MF09
FRIHA, H. – WF14
FROHMAN, D. J. – MG05, TC11, TC12
FROMMHOLD, L. – FC08
FU, L. – WJ12
FUJIHARA, A. – MG12
FUJII, A. – MG05, MG08
FUJIMORI, R. – TF05
FUJIWARA, T. – TF02, TF03, TF16
FURDAI, H. – WF14
FROHMAN, D. J. – MH05, TC11, TC12
FROMMHOLD, L. – FC08
FU, L. – WJ12
FUJIHARA, A. – MG12
FUJII, A. – MG05, MG08
FUJIMORI, R. – TF05
FUJIWARA, T. – TG12
FAUKE, K. – MI12
FUSSON, H. A. – TF05
FU, L. – WJ12
FUJIWARA, T. – MG05

G

GALILA, H. – WF14
GARAND, E. – RG01, RG02
GARDNER, A. M. – TG01, WG08, RI13
GASTON, B. M. – TA04
GATRONE, E. E. – MJ01
GAUSS, J. – TC03, RH08, FB11
GEBAFFE, T. R. – TF02, TF03, TF16
GEHRZ, R. D. – RF04, RF05
GEORGE, L. – MJ04, MJ05, RE08, RE09
GERARDI, H. K. – RJ11
GERECHT, E. – TC06, RB08, RC06
GERIN, M. – RF01, FA06
GHARAJIBEH, M. A. – MF04, MF05, TH11
GHOSH, D. – FB08
GIESEN, T. F. – MG06
GLOAGUEN, E. – FB07
GOEDERS, J. E. – MJ01
GOLAN, A. – WJ09
GOLDING, P. – FC04
GOULDSMITH, P. F. – RF03
GOLEBOWSKI, D. – TI03
GOLEC, B. – MJ06, MJ09
GONZALEZ, M. A. L. – RB03
GORDON, B. P. – RH01
GORDON, I. E. – TD03, TE08, TE09, FC01, FC02
GORSHELEV, V. – TE11
GOTO, M. – TF02, TF16
GOTTBEHUT, I. – MG06
GOURIET, M. – RF15
GOULD, P. L. – MF02, TH09
GRABOW, J. – MH04, MH08, RA06, RA08, RC02, FD01
GRABOW, J. – U. – TF07, RC07
GRAHAM, W. R. M. – MJ07, MJ08
GRANGER, A. D. – TD05, WG11, WG12
GRAU, M. – TH13
GRAY, T. G. – TG13
GREEN, A. M. – TG01
GRIMMINCK, D. L. A. G. – TC01
GRIMMINGER, R. A. – MF06, WG05
GRONER, P. – MH07, WH09, RH04
GRUBBS II, G. S. – TC11, TC12, WH13, WH14, RH03, RH04, RH13
GRUN, S. A. – FE06, FE07, FE08
GU, Q. – RE10
GUAN, Y. – RD03
GUASCO, T. L. – RG03
GUILLEMIN, J.-C. – WF11, WF12, WF13, FA07, FA09
GUINET, M. – RB06
GUO, C. – RE11
GUPTA, H. – TC05, TF14, WI07, RF10, FA02, FA03
GUPTA, V. – WG13
GUSS, J. S. – TF04
GUTBERLET, A. – RG11
GUTBERLET, A. K. – TG07
GÄRTNER, S. – MI13
GÁMEZ, F. – RH12
H

HAASE, C. – RH01
HABIG, D. – FE06, FE07
HADDAD, M. A. – WF10
HAGA, K. J. – WF17
HAIJIGEOGIU, P. – FC02
HALFEN, D. T. – TC08, TC09, TF06, TH14, RC01, RC03, RC04, RH05
HALONEN, L. – TA05, TJ11, TJ12
HAMASHIMA, T. – MG07
HAMMER, N. I. – TG11, R105
HAN, H. – WJ12
HAN, J. – TB11
HANDLER, K. – WG03
HANKE, K. – FE06, FE07
HARA, M. – FC03
HARADA, K. – WH01, WH02
HARADA, N. – TF10
HARDING, M. E. – MA01, FB10, FB11
HARGREAVES, R. – RD09
HARRISS, B. T. – RC04
HARRIS, B. J. – TC09, RC06
HARRIS, B. T. – RC03
HARTMANN, J. M. – TJ13
HASBROUCK, S. – WC07
HATANO, Y. – FC03
HAVENITH, M. – FE06, FE07, FE08
HAYKAL, I. – WF13, RF15
HAYS, J. – WF17
HEAVEN, M. – RA03
HEAVEN, M. C. – TB04, TB11, TD01, TH02, WG06, WJ13, RA10, FD09
HEID, C. G. – TB13
HENNING, T. – TF08
HERBST, E. – TF01, TF08, TE10, RF07, FA03, FA04, FA10
HERMAN, M. – TI02, TI03, RB03, RD06, RD07, RD08
HEWAGE, D. – RJ03
HEWITT, J. – RF11
HEYDEN, P. V. D. – WF16
HILL, C. – MG02, TJ09
HILL, J. G. – RI01
HANDLE, F. – RB06, FC05
HINDS, E. A. – RA02
HINKLE, C. E. – RI02
HINSEN, C. – FB06
HIROTA, E. – MH03
HOEKSTRA, S. – FD04
HOFFMAN, K. J. – WJ03
HOGAN, S. D. – TH03
HOLKA, F. – MG01
HOLT, J. – TB05
HOPKINS, W. S. – TD05
HOUCHINS, C. – RE05
HOUCK, C. P. – WF17
HOUGEN, J. T. – WG01, WJ04
HRATCHIAN, H. P. – RI07
HSIEH, S. – RB10, FC07
HUANG, X. – TE02, TE04, WF04
HUDSON, T. - RA02
HUENNEKENS, J. – RD03
HUE, T. R. – WF13, RF15, RG12
HUNT, K. L. C. – FC08
HURTMANS, D. – TE06, TE07
I

IACHELLO, F. – TJ07
LIU, J. – TD04, TJ06
LIU, X. – TI05, TI06, RG08
LIU, Y. – WG09
LOH, H. – TH13
LOIM, N. M. – RG06
LOKSHIN, B. V. – RG06
LONG, B. D. – TG10
LONG, B. E. – WH14, RH03, RH13
LONG, J. – MF08
LONGVAL, Y. – RG09
LOPEZ, G. V. – TD10, TE06, TE07
LORD, S. – FA02
LORENZ, J. – RD04
LOTRICH, V. – FB05
MA, Q. – RB11
MACKIE, J. C. – MF03
MAIER, J. P. – MA03, WG13, WI05
MAKI, A. – FC06
MANN, J. E. – WG14
MANTZ, A. W. – TE03, TE06, TE07, RB01
MARGULES, L. – RF15
MARGULÈS, L. – WF11, WF12, WF13, FA06, FA07, FA08, FA09
MARIS, A. – MH12
MARSH, B. M. – WI10, RG10
MARSHALL, M. D. – WH06, WH07
MARTENS, J. – RD06, RD07
MARTIN, J. P. – RE10
MARTIN-DRUMEL, M. A. – WI05, RF09, RF13
MARTIN-DRUMEL, M.- A. – FA06
MARTINEZ JR., O. – MI08
MARTÍNEZ-HAYA, B. – RH12
MASIELLO, T. – FC06
MATA, M. V. S. – RC08
MATA, S. – MH13, MH14, RC05, RC07
MATSUBA, Y. – MG08
MATTERN, D. L. – TG11
MAWHORTER, R. – RA06, RA08
MCCABE, M. N. – RH01
MCCALL, B. – MI09, MI11
MCCALL, B. J. – MI02, MI03, MI10, TA03, TF02, TF03, TF09, TF16, FC09, FE01
MCCARTHY, M. C. – MI08, WF01, WI05, WJ01, WJ02, RH08
MCCOY, A. B. – MF14, MG03, TJ02, TJ10, RE10, RI02, RI10
MCGUIRE, B. A. – MI03, RF07, RF08, RF14
MIJUNKINS, A. L. – MH10
MCKELLAR, A. R. W. – TI01, TI08, TI09, TI10, TI11
MCMAHON, R. – TB08
MCMAHON, R. J. – RE08, RE09
MCRAVEN, C. P. – TE06, TE07, RA06, RA08
MEDVEDEV, I. R. – MH09, TB05, WF02, RB05, RB07
MEERTS, W. L. – TC01, TD04, TG06, WJ10
MEHTA, D. N. – TG07, RJ04
MELANDRI, S. – MH12
MELNIK, D. G. – TJ06, WJ06
MENTEN, K. M. – TF07
MERER, A. J. – TH05, WJ01, WJ04
MERESHCHENKO, A. S. – RE06, RE07
MERK, F. – TH03, TH07, TH08
MERLONI, A. – MH12
MIKAMI, N. – RD02
MIKHAILOV, V. A. – MH01
MILLER, C. E. – TE01, TE10
MILLER, E. M. – MF14
MILLER, S. J. – RG02
MILLER, T. A. – TD04, TD06, TD07, TJ06, WJ06, WJ10, WJ11
MILLS, A. – MI09, MI10, MI11
MIN, J. – RC01, RC03, RC04, RH05
MINEI, A. J. – MH05
MINITTI, M. P. – TB06, TB07
MITRUSHCHENKOV, A. – RI01
MIVIEVAR, F. – TI12
MIZUSE, K. – MG07
MOAZZEN-AHMADI, N. – TI01, TI04, TI08, TI10, TI11, TI12
MOLLNER, A. K. – TB12
MOMOSE, T. – FE01
MONJE, R. R. – RF03
MONS, M. – FB07
MOORE-FURNEAUX, J. – RA07
MORONG, C. P. – TF16
MORRISON, A. M. – MG09, MJ02, TA08, WJ08
MORSE, M. D. – WG08
MOSLEY, J. – WJ07
MOSYAGIN, N. S. – FD08
MOTIYENKO, R. – WF13
MOTIYENKO, R. A. – WF11, WF12, FA07, FA08, FA09
MOURAD, R. – RJ08, RJ09
MOURET, G. – RB06, FC05
MUCKLE, M. T. – WJ01, WH09, WJ09, RC10
MUEATER, J. S. – TC07
MUKHERJEE, M. – TG08
MUKHOPADHYAY, A. – MG12
MURAMOTO, Y. – RD02
MURPHY, B. – RA06
MURPHY, B. – RA08
MUZANGWA, L. – TH12
MÁDER, H. – TC04
MUČK, L. A. – RH08
MÜLLER, H. S. P. – TC04, TE10, TF07, WJ09, RF09
NAGARAJAN, R. – MF07
NAGESH, J. – TJ04, TJ05
NAHAR, S. N. – FB01
NAKANE, A. – WF06
NAKANO, T. – MI12
NAKAYAMA, Y. – MG08
NAMAL, M. – RD02
NEESE, C. – MH09
NEESE, C. F. – TB05, WF02, RB05, RB07
NEILL, J. L. – WF01, WH09, WH10, WH11, WJ01, RC06, RC09, RC10, RC11, RC12, RF14
NEMCHICK, D. J. – TG02, TG03
NESBITT, D. – FE09
NESBITT, D. – MG03, RE02
NEUFELD, D. A. – RF03
NEZ, M. N. – WF09
NG, Y. W. – MF10, WG10
NIBLER, J. W. – FC06
NIETO, P. – MF11, MF12
NIMLOS, M. A. – RC08
NITSCHE, M. – TG02, TG03
NISHIMIYAMA, N. – MF11, MF12
NOLAN, A. – TB08
VAQUERO, V. – MH11, RC09
VARADWAJ, A. – FB03
VARADWAJ, P. R. – FB03
VARELA, M. – RC07
VASA, S. K. – TC01
VASILIOU, A. – TC07
VASILIOU, A. J. – WJ09
VASQUEZ, R. – RG09
VASYUNIN, A. I. – FA10
VASYUNINA, T. – TF08
VERBRAAK, H. – TF04
VERVLOET, M. – WJ05, RF09, RF13
VISWANATHAN, K. S. – MG10, MG11
VOGT, R. A. – TG13
VOLK, A. – WI12
VORONKOV, M. – TF08
VÁZQUEZ, J. – FB10, FB11

W
WALKER, K. A. – TD03
WALKER, N. R. – MH01, MH02, WH04, WH05
WALLER, S. E. – WG14
WALTERS, A. – TF07, WF09, WF11
WANG, D. – TH09
WANG, F. – RA03
WANG, H. – MF08
WANG, S. – FA02
WANG, X. – WI09
WANG, Y. – RF08
WANG, Z. – RD05
WATSON, T. – FB05
WEAVER, S. L. W. – WF07, RF07, RF08, RF12, RF14, FA05
WEBER, A. – FC06
WEBER, J. M. – MI06, MI07
WEBER, M. – TE11
WEBER, P. M. – TB06, TB07
WEEKS, D. E. – RI03
WEIDINGER, D. – RE05
WELLEN, B. A. – TJ10
WEN, C. – TG14
WENGER, C. – WF15
WHITE, A. R. – TA01, TA02
WIBERG, K. B. – TG10
WIESENFELD, L. – TF13
WIJNGAARDEN, J. A. V. – RG14
WIJNGAARDEN, J. V. – RG13, RH09
WILCOX, D. S. – RH11
WILLIAMS, O. L. – RH11
WILLIAMS, S. R. – FD07
WITHERS, C. D. – WG08
WLODARCZAK, G. – FA06
WOLFE, C. M. – RD03
WOLFF, J. E. – TG02, TG03
WOLK, A. B. – RG01, RG02, RJ13
WOLLENHAUPT, M. – TG06
WOMACK, K. – WG04
WOOLF, N. J. – TF11, TF12
WOON, D. E. – MF01, TF15, WG07, RJ04, RI11, RJ12, FB02
WRIGHT, A. M. – RI05
WRIGHT, T. G. – TG01, WG08, RI13
WU, L. – WG09, RJ08, RJ09

X
XANTHEAS, S. S. – MA02, MG09
XIA, Z. – MH04
XU, L. – WI03, WI09, RI04
XU, Y. – TI05, TI06, WH12, RG04, RG08

Y
YAHN, T. – TH13
YAMADA, K. M. T. – RG05
YAMADA, Y. – FC03
YAMANAKA, R. – WH01
YANG, D. – WG09, RJ01, RJ02, RJ03
YANG, D. S. – RJ08, RJ09
YANG, G. – RG04
YANG, J. – MF07, TJ14, TJ15, FB06
YANG, S. L. – RB02
YANG, T. – RA09
YANG, T. Z. – RA06, RA08
YE, J. – WA04, FD06
YI, J. T. – TG06
YIMER, Y. – RE01
YOON, Y. W. – RJ05
YOUNG, J. W. – TG09, WI02
YU, S. – MH09, TC04, TC05, TE09, TE10, WI07, RF09, RF10, FA02, FA03
YURIYA, T. – MF11, MF12
YURCHENKO, S. N. – MG02, TJ09, RD09

Z
ZACK, L. N. – TF06
ZALESKI, D. P. – WF01, WH10, WH11, RC10, RC11, RF14
ZENG, T. – TJ16
ZGIERSKI, M. – TB08, TD11
ZGIERSKI, M. Z. – TG12
ZHANG, C. – WG09
ZHANG, Y. – TB06
ZHAO, D. – WF10
ZHAO, W. – TA06
ZHELDAKOV, I. L. – RE06
ZHUANG, X. – WI05, RD05
ZIMKIEWICZ, M. – FE09
ZINCHENKO, I. – TF08
ZIURYS, L. M. – TC08, TC09, TC10, TF06, TF11, TF12, TH14, WF03, RC01, RC03, RC04, RH05
ZOBOV, N. F. – RD09
ZWIER, T. S. – TB08, TD11, TG07, WI10, WI11, RG10, RG11, RJ04