<table>
<thead>
<tr>
<th>Time</th>
<th>Room/Location</th>
<th>Topic/Session</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:45AM</td>
<td>AUDITORIUM</td>
<td>MA. PLENARY SESSION</td>
</tr>
<tr>
<td></td>
<td>INDEPENDENCE HALL</td>
<td>AWARDS</td>
</tr>
<tr>
<td>8:30AM</td>
<td>ROOM 160</td>
<td>TA. ATMOSPHERIC SPECIES</td>
</tr>
<tr>
<td></td>
<td>MATH ANNEX*</td>
<td>RA. ELECTRONIC</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FA. ASTRONOMICAL SPECIES &amp; PROCESSES</td>
</tr>
<tr>
<td>8:30AM</td>
<td>ROOM 170</td>
<td>TB. DYNAMICS</td>
</tr>
<tr>
<td></td>
<td>MATH ANNEX*</td>
<td>RB. ATMOSPHERIC SPECIES</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FB. INFRARED/ RAMAN</td>
</tr>
<tr>
<td>8:30AM</td>
<td>ROOM 1000</td>
<td>TC. MICROWAVE</td>
</tr>
<tr>
<td></td>
<td>MCPHERSON LAB</td>
<td>RC. ASTRONOMICAL SPECIES &amp; PROCESSES</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FC. MICROWAVE</td>
</tr>
<tr>
<td>8:30AM</td>
<td>ROOM 1015</td>
<td>TD. MINI-SYMPOSIUM:</td>
</tr>
<tr>
<td></td>
<td>MCPHERSON LAB</td>
<td>PHOTODETACHMENT &amp; PHOTOIONIZATION</td>
</tr>
<tr>
<td></td>
<td></td>
<td>RD. MINI-SYMPOSIUM:</td>
</tr>
<tr>
<td></td>
<td></td>
<td>COLD QUANTUM SYSTEMS</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FD. MINI-SYMPOSIUM:</td>
</tr>
<tr>
<td></td>
<td></td>
<td>COLD QUANTUM SYSTEMS</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8:30AM</td>
<td>ROOM 2015</td>
<td>TE. MINI-SYMPOSIUM: SPECTROSCOPY OF</td>
</tr>
<tr>
<td></td>
<td>MCPHERSON LAB</td>
<td>INTERFACES</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1:30PM</td>
<td>ROOM 160</td>
<td>MF. INFRARED/ RAMAN</td>
</tr>
<tr>
<td></td>
<td>MATH ANNEX*</td>
<td>TF. INFRARED/ RAMAN</td>
</tr>
<tr>
<td></td>
<td></td>
<td>WF. INFRARED/ RAMAN</td>
</tr>
<tr>
<td></td>
<td></td>
<td>RF. ASTRONOMICAL SPECIES &amp; PROCESSES</td>
</tr>
<tr>
<td></td>
<td>ROOM 170</td>
<td>MG. RADICALS AND IONS</td>
</tr>
<tr>
<td></td>
<td>MATH ANNEX*</td>
<td>TG. ELECTRONIC</td>
</tr>
<tr>
<td></td>
<td></td>
<td>WG. ELECTRONIC</td>
</tr>
<tr>
<td></td>
<td>ROOM 1000</td>
<td>MH. MICROWAVE</td>
</tr>
<tr>
<td></td>
<td>MCPHERSON LAB</td>
<td>TH. MICROWAVE</td>
</tr>
<tr>
<td></td>
<td></td>
<td>WH. ASTRONOMICAL SPECIES &amp; PROCESSES</td>
</tr>
<tr>
<td></td>
<td>ROOM 1015</td>
<td>MI. MINI-SYMPOSIUM:</td>
</tr>
<tr>
<td></td>
<td>MCPHERSON LAB</td>
<td>PHOTODETACHMENT &amp; PHOTOIONIZATION</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TI. RADICALS AND IONS</td>
</tr>
<tr>
<td></td>
<td>ROOM 2015</td>
<td>MJ. MATRIX/ CONDENSED PHASE</td>
</tr>
<tr>
<td></td>
<td>MCPHERSON LAB</td>
<td>TJ. MINI-SYMPOSIUM: SPECTROSCOPY OF</td>
</tr>
<tr>
<td></td>
<td></td>
<td>INTERFACES</td>
</tr>
<tr>
<td></td>
<td></td>
<td>WJ. MINI-SYMPOSIUM:</td>
</tr>
<tr>
<td></td>
<td></td>
<td>PHOTODETACHMENT &amp; PHOTOIONIZATION</td>
</tr>
<tr>
<td></td>
<td></td>
<td>RJ. THEORY</td>
</tr>
</tbody>
</table>

* 209 W. 18th Avenue
MA. PLENARY SESSION
MONDAY, JUNE 18, 2012 – 8:45 AM
Room: AUDITORIUM, INDEPENDENCE HALL

Chair: FRANK DE LUCIA, The Ohio State University, Columbus, Ohio

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

MA01 40 min 9:00
A NEW SPECTROSCOPIC WINDOW ON HYDROXYL RADICALS AND THEIR ASSOCIATION REACTIONS OF SIGNIFICANCE IN THE ATMOSPHERE*

MARRSHA I. LESTER, Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323.

*This research was supported by the National Science Foundation and the Office of Basic Science of the Department of Energy.

MA02 40 min 9:45
SPECTROSCOPY OF MOLECULES IN EXTREME ROTATIONAL STATES USING AN OPTICAL CENTRIFUGE

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

Intermission

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

2011 Rao Award Winners
Adam J. Fleisher, University of Pittsburgh
Justin L. Neill, University of Virginia
Thomas J. Preston, University of Wisconsin

COBLENTZ AWARD 11:05
Presentation of Award by Michael L. Myrick, President, Coblentz Society

MA03 40 min 11:10
Coblentz Society Award Lecture
IMAGING EXCITED STATE DYNAMICS WITH 2D ELECTRONIC SPECTROSCOPY

GREGORY S. ENGEL, Department of Chemistry, The University of Chicago, Chicago USA.
MF01 10 min 1:30
TIME RESOLVED FTIR ANALYSIS OF COMBUSTION OF AN ETHANOL/ISOPROPANOL MIXTURE IN A COMMERCIAL INTERNAL COMBUSTION ENGINE

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

MF02 15 min 1:42
SUB-DOPPLER RESOLUTION DIFFERENCE-FREQUENCY-GENERATION INFRARED SPECTROMETER WITH HIGH SENSITIVITY AND WIDE TUNABILITY

S. OKUBO, H. NAKAYAMA, K. IWAKUNI, H. SASADA, Department of Physics, Faculty of Science and Technology, Keio University, Yokohama, Japan; H. INABA, National Metrology Institute of Japan, National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan.

MF03 15 min 1:59
OPTICAL FREQUENCY COMB REFERENCED SUB-DOPPLER RESOLUTION DIFFERENCE-FREQUENCY-GENERATION INFRARED SPECTROMETER

K. IWAKUNI, S. OKUBO, H. NAKAYAMA, and H. SASADA, Department of Physics, Faculty of Science and Technology, Keio University, Yokohama, Japan; H. INABA, National Metrology Institute of Japan, National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan.

MF04 15 min 2:16
DUAL ETALON FREQUENCY COMB (DEFCOM) SPECTROSCOPY

DAVID W. CHANDLER, KEVIN E. STRECKER, Sandia National Laboratory, Livermore, CA 94550.

MF05 15 min 2:33
A MULTI-WATT SINGLE FREQUENCY CW OPO SYSTEM TUNABLE FROM 600NM TO 4600NM

A. HENDERSON, LOCKHEED MARTIN ACULIGHT, 22121 20th Avenue SE, Bothell, WA 98021.

MF06 15 min 2:50
DEVELOPMENT OF A HIGHER RESOLUTION TERAHERTZ TIME-DOMAIN SPECTROMETER

DANIEL B. HOLLAND, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125 (email to D.B.H.: holland@caltech.edu); GEOFFREY A. BLAKE, Division of Geological and Planetary Sciences, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125.
QCL SPECTROSCOPY AT 9 µM CALIBRATED WITH A HIGH-POWER THULIUM-BASED FREQUENCY COMB

ANDREW A. MILLS, JIE JIANG, INGMAR HARTL, MARTIN FERMANN, IMRA America, Ann Arbor, MI; DAVIDE GATTI, MARCO MARANGONI, Campus Point, Dipartimento di Fisica del Politecnico di Milano, Milano, Italy.

Intermission

DIRECT MEASUREMENTS OF COLLISIONALLY BROADENED (CO₂-CO₂) S-BRANCH RAMAN COHERENCE LIFETIMES OF CO₂

JOSEPH R. GORD, Department of Chemistry, Purdue University, West Lafayette, IN 47907; SUKESH ROY, PAUL S. HSU, NAIBO JIANG, WARUNA D. KULATILAKA, and HANS U. STAUFFER, Spectral Ener-gies, LLC, 5100 Springfield Street, Suite 301, Dayton, OH 45431; JAMES R. GORD, Air Force Research Laboratory, Propulsion Directorate, Wright-Patterson AFB, OH 45433.

ANALYSIS OF AN ¹⁸O AND D ENHANCED FT-IBBCEAS WATER SPECTRUM: NEW ASSIGNMENTS FOR HD¹⁸O, HD¹⁶O, D₂¹⁸O AND D₂¹⁶O IN THE NEAR-INFRARED REGION (6000-7000 cm⁻¹).

MICHAEL J. DOWN, JONATHAN TENNYSON, Department of Physics and Astronomy, University College London, London, WC1E 6BT, UK; JOHANNES ORPHAL, Karlsruher Institut für Technologie, IMK-ASF, Postfach 36 40, 76021 Karlsruhe, Germany; PASCALE CHELIN, Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA), Université de Paris-Est, CNRS UMR 7583, Créteil, France; and ALBERT A. RUTH, Physics Department and Environmental Research Institute, University College Cork, Cork, Ireland.

TOWARDS PERFECT WATER LINE INTENSITIES

J. LODI, J. TENNYSON, Department of Physics and Astronomy, University College London, London WC1E 6BT, UK.

HIGH-RESOLUTION INFRARED SPECTROSCOPY OF THE (1, 0, 1) – (0, 0, 0) BAND OF C₃

S. THORWIRTH, J. KRIEG, I. KEPELER, V. LUTTER, S. SCHLEMMER, T. F. GIESEN, I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany; M. E. HARDING, Karlsruher Institut für Technologie, Institut für Nanotechnologie, 76021 Karlsruhe, Germany; J. VÁZQUEZ, Center for Theoretical Chemistry, Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, Texas 78712, U.S.A.

USING PROGRAM ERHAM TO ANALYZE HIGH-RESOLUTION INFRARED SPECTRA OF MOLECULES WITH INTERNAL ROTORS

P. GRONER, Department of Chemistry, University of Missouri-Kansas City, Kansas City, MO 64110-2499; S. ALBERT, M. QUACK, Physical Chemistry, ETH Zürich, CH-8093 Zürich, Switzerland.
COMPARISON OF COMPUTED CONDON LOCI WITH FRANCK–CONDON FACTORS IN DESLANDRES TABLES OF MOLECULAR BAND SYSTEMS

R. HEFFERLIN and B. CLARK, Southern Adventist University, Collegedale, TN 37315; J. TATUM, University of Victoria, Victoria, BC V8W 2Y2, Canada.

VIBRATIONAL SPECTRA OF THE MLCl₂ COMPLEX FROM THEORETICAL CALCULATIONS

BERNA CATIKKAS, Department of Physics, Mustafa Kemal University, Hatay, Turkey, 31034 (email to B.Ç.: berna@mku.edu.tr).
MG. RADICALS AND IONS
MONDAY, JUNE 18, 2012 – 1:30 PM
Room: 170 MATH ANNEX

Chair: TIMOTHY SCHMIDT, The University of Sydney, Sydney, Australia

MG01 15 min 1:30
RENNER-TELLER COUPLING IN H₂S+: PARTITIONING THE ROVIBRONIC AND SPINORBIT COUPLING HAMILTONIAN

G. DUXBURY, Department of Physics, SUPA, John Anderson Building, University of Strathclyde, 107 Rottenrow, Glasgow G4 0NG, Scotland, UK; Ch. JUNGEN, LAC, 1 Laboratoire Aimé Cotton du CNRS, Université de Paris-Sud, 91405 Orsay, France; A. ALIJAH, GSMA, UMR CNRS 6089, Université de Reims Champagne-Ardenne, B.P. 1039, 51687 Reims Cedex 2, France.

MG02 15 min 1:47
RENNER-TELLER COUPLING IN H₂S+: A COMPARISON OF THEORY WITH OPTICAL SPECTRA AND RECENT PFI AND MATI EXPERIMENTAL RESULTS

G. DUXBURY, Department of Physics, SUPA, John Anderson Building, University of Strathclyde, 107 Rottenrow, Glasgow G4 0NG, Scotland, UK; Ch. JUNGEN, LAC, 1 Laboratoire Aimé Cotton du CNRS, Université de Paris-Sud, 91405 Orsay, France; A. ALIJAH, GSMA, UMR CNRS 6089, Université de Reims Champagne-Ardenne, B.P. 1039, 51687 Reims Cedex 2, France.

MG03 15 min 2:04
INFRARED PHOTODISSOCIATION SPECTROSCOPY OF SILICON-CARBONYL CATIONS: EVIDENCE FOR ASYMMETRIC CARBONYL COORDINATION.

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

MG04 15 min 2:21
INITIAL DEVELOPMENT OF HIGH PRECISION, HIGH RESOLUTION ION BEAM SPECTROMETER IN THE NEAR-INFRARED

MICHAEL PORAMBO, BRIAN SILLER, ANDREW MILLS, MANORI PERERA, and HOLGER KRECKEL, 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.

*Present Address: IMRA, Ann Arbor, MI 48105
bPresent Address: Illinois Wesleyan University, Bloomington, IL 61701

MG05 15 min 2:38
MID-IR DIRECT ABSORPTION/DISPERSION SPECTROSCOPY OF A FAST ION BEAM

BRIAN SILLER, 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.
SPONTANEOUS EMISSION BETWEEN ORTHO- AND PARA-LEVELS OF WATER-ION, H$_2$O$^+$

KEIICHI TANAKA, Department of Applied Chemistry, National Chiao Tung University, Hsinchu, 30010, TAIWAN; Department of Chemistry, Faculty of Sciences, Kyushu University, Fukuoka, 812-8581 JAPAN; KENSUKE HARADA, Department of Chemistry, Faculty of Sciences, Kyushu University, Fukuoka, 812-8581 JAPAN; SHINKOH NANBU, Department of Materials and Life Sciences, Faculty of Science and Engineering, Sophia University, Tokyo 102-8554, JAPAN; TAKESHI OKA, Department of Astronomy and Astrophysics and Department of Chemistry, the Enrico Fermi Institute, the University of Chicago, Chicago, Illinois, 60637, USA.

Intermission

INFRARED SPECTROSCOPY OF THE MASS 31 CATION: PROTONATED FORMALDEHYDE VS. THE TRIPLET METHOXY CATION

J. D. MOSLEY, T. C. CHENG, and M. A. DUNCAN, University of Georgia, Dept. of Chemistry, 1001 Cedar St, Athens, GA 30602.

INFRARED SPECTROSCOPY OF PROTONATED CARBONYLS: PROTONATED GLYOXAL

J. D. MOSLEY, T. C. CHENG, and M. A. DUNCAN, University of Georgia, Dept. of Chemistry, 1001 Cedar St, Athens, GA 30602.

TIME-RESOLVED FTIR AND MASS SPECTROSCOPY OF LASER-ABLATED MAGNESIUM.

Y. MIYAMOTO, N. IKEDA, J. TANG, K. KAWAGUCHI, Graduate School of Natural Science and Technology, Okayama University, 3-1-1 Tsushima-naka Okayama 700-8530, Japan; C. MASAKI, Faculty of Science, Okayama University, 3-1-1 Tsushima-naka Okayama 700-8530, Japan.

METAL ION BINDING TO POLYPEPTIDES CHARACTERIZED BY IRMPD SPECTROSCOPY. METAL-AMIDE NITROGEN BINDING AND THE IMINOL TAUTOMERIZATION.

ROBERT C. DUNBAR, Chemistry Department, Case Western Reserve Univ., Cleveland, OH 44106; NICOLAS POLFER, Chemistry Department, University of Florida, Gainesville, FL; GIEL BERDEN, FOM Institute for Plasma Physics, Nieuwegein, Netherlands; JOS OOMENS, FOM Institute for Plasma Physics, Nieuwegein, and University of Amsterdam, Netherlands.

INFRARED SPECTROSCOPIC EVIDENCE FOR ISOTOPOLOGS OF THE HOH OH ANION TRAPPED IN SOLID NEON

MARILYN E. JACOX and WARREN E. THOMPSON, Sensor Science Division, National Institute of Standards and Technology, Gaithersburg, MD 20899-8441.
INFRARED STUDY OF THE WATER-HYDROXYL RADICAL COMPLEX TRAPPED IN SOLID NEON

Marilyn E. Jacox and Warren E. Thompson, Sensor Science Division, National Institute of Standards and Technology, Gaithersburg, MD 20899-8441.

UV/VIS ABSORPTION EXPERIMENTS ON MASS SELECTED CATIONS BY COUNTER-ION INTRODUCTION INTO AN INERT NEON MATRIX

<table>
<thead>
<tr>
<th>Session</th>
<th>Title</th>
<th>Authors</th>
<th>Institution</th>
</tr>
</thead>
<tbody>
<tr>
<td>MH01</td>
<td>BROADBAND ROTATIONAL SPECTRUM AND MOLECULAR GEOMETRY OF OC···AgI</td>
<td>N. R. WALKER, S. L. STEPHENS, W. MIZUKAMI, D. P. TEW AND A. C. LEGON</td>
<td>School of Chemistry, University of Bristol, Bristol, BS8 1TS, U.K.</td>
</tr>
<tr>
<td>MH02</td>
<td>MICROWAVE SPECTRUM AND GEOMETRY OF H₃P···AgI</td>
<td>N. R. WALKER, S. L. STEPHENS, W. MIZUKAMI, D. P. TEW AND A. C. LEGON</td>
<td>School of Chemistry, University of Bristol, Bristol, BS8 1TS, U.K.</td>
</tr>
<tr>
<td>MH03</td>
<td>MICROWAVE SPECTROSCOPY AND INTERNAL DYNAMICS OF THE Ne-NO₂ VAN DER WAALS COMPLEX</td>
<td>BRIAN J. HOWARD, GEORGE ECONOMIDES and LEE DYER</td>
<td>Department of Chemistry, Oxford University, South Parks Road, Oxford, OX1 3QZ, United Kingdom</td>
</tr>
<tr>
<td>MH04</td>
<td>FTMW SPECTROSCOPY AND DETERMINATION OF THE 3-D POTENTIAL ENERGY SURFACE FOR Ar-CS</td>
<td>CHISATO NIIDA, MASAKAZU NAKAJIMA, YASUKI ENDO, CHISATO NIIDA, MASAKAZU NAKAJIMA, YASUKI ENDO</td>
<td>Department of Basic Science, The University of Tokyo, Tokyo 153-8902, Japan; YASUHIRO SUMIYOSHI, Department of Chemical Biology, Gunma University, Maebashi Gunma, 371-8510, Japan; YASUHIRO OHISHIMA, Department of Photo-Molecular Science, Institute for Molecular Science, Okazaki, 444-8585, Japan; HIROSHI KOGUCHI, Department of Chemistry, Hiroshima University, Higashi-Hiroshima, 739-8511, Japan</td>
</tr>
<tr>
<td>MH05</td>
<td>OBSERVATION OF THE PURE ROTATIONAL SPECTRA OF THE H₂O-trans-HOCO COMPLEX</td>
<td>TAKAHIRO OYAMA, MASAKAZU NAKAJIMA, YASUKI ENDO, TAKAHIRO OYAMA, MASAKAZU NAKAJIMA, YASUKI ENDO</td>
<td>Department of Basic Science, Graduate School of Arts and Sciences, The University of Tokyo, Komaba, Meguro-ku, Tokyo, 153-8902, Japan; and YASUHIRO SUMIYOSHI, Department of Chemistry and Chemical Biology, Gunma University, 4-2 Aramaki-machi, Maebashi City, Gunma, 371-8510 Japan</td>
</tr>
<tr>
<td>MH06</td>
<td>STRUCTURE AND INVERSION MOTIONS OF THE WEAKLY BOUND CH₂F₂···CO₂ DIMER</td>
<td>REBECCA A. PEEBLES, AMELIA J. THOMAS, MICHAL M. SERAFIN and SEAN A. PEEBLES</td>
<td>Department of Chemistry, Eastern Illinois University, 600 Lincoln Ave., Charleston, IL 61920</td>
</tr>
</tbody>
</table>
MH07 10 min 3:12
ANALYSIS OF MICROWAVE SPECTRUM, INTERNAL ROTATION AND C–H···F INTERACTIONS OF THE CHF<sub>3</sub>···C<sub>2</sub>H<sub>3</sub>F WEAKLY BOUND COMPLEX

**LENA F. ELMUTI, DANIEL A. OBENCHAIN, REBECCA A. PEEBLES, SEAN A. PEEBLES, Department of Chemistry, Eastern Illinois University, 600 Lincoln Ave., Charleston, IL 61920.**

MH08 15 min 3:24
STRUCTURAL STUDIES OF CH<sub>3</sub>SiF<sub>2</sub>-X (X = NCO, Cl) BY MICROWAVE SPECTROSCOPY

**GAMIL A. GUIRGIS, KORREDA K. GAUSE, Department of Chemistry & Biochemistry, College of Charleston, Charleston, SC 29424 USA; NATHAN A. SEIFERT, DANIEL P. ZALESKI, BROOKS H. PATE, Department of Chemistry, University of Virginia, McCormick Rd., Charlottesville, VA 22904-4319; MICHAEL H. PALMER, School of Chemistry, University of Edinburgh, West Mains Road, Edinburgh EH9 3JJ, UK; REBECCA A. PEEBLES, SEAN A. PEEBLES, LENA F. ELMUTI, DANIEL A. OBENCHAIN, Department of Chemistry, Eastern Illinois University, 600 Lincoln Avenue, Charleston, IL, 61920 USA.**

**Intermission**

MH09 15 min 4:00
INVITED TALK
MICROWAVE SPECTRA AND GEOMETRIES OF H<sub>2</sub>C<sub>2</sub>···AgCl AND H<sub>2</sub>C<sub>2</sub>···CuCl

**N. R. WALKER, S. L. STEPHENS, W. MIZUKAMI, D. P. TEW AND A. C. LEGON, School of Chemistry, University of Bristol, Bristol, BS8 1TS, U.K.**

MH10 15 min 4:17
MICROWAVE SPECTRA, MOLECULAR STRUCTURES AND INTERNAL DYNAMICS OF H<sub>2</sub>S···ICF<sub>3</sub> AND H<sub>2</sub>O···ICF<sub>3</sub> REVEALED BY BROADBAND ROTATIONAL SPECTROSCOPY

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

MH11 15 min 4:34
FOURIER TRANSFORM MICROWAVE SPECTRUM OF CO<sub>2</sub> -(CH<sub>3</sub>)<sub>2</sub> S

**YOSHIYUKI KAWASHIMA and TAKAYUKI MORITANI, 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.**

MH12 15 min 4:51
MICROWAVE SPECTROSCOPY AND PROTON TRANSFER DYNAMICS IN THE FORMIC ACID-ACETIC ACID DIMER

**B.J. HOWARD, E. STEER, F. PAGE, M. TAYLER, B. OUYANG, Department of Chemistry, Oxford University, South Parks Road, Oxford, OX1 3QZ, United Kingdom; H.O. LEUNG, M.D. MARSHALL, Department of Chemistry, Amherst College, Amherst, MA 01002; and J.S. MUENTER, Department of Chemistry, University of Rochester, Rochester, NY 14627.**
MH13

15 min 5:08

STRUCTURE OF THE SEVOFLURANE-BENZENE COMPLEX AS DETERMINED BY CHIRPED-PULSE FTMW SPECTROSCOPY

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

MH14

15 min 5:25

STRUCTURE OF HIGH-ORDER WATER CLUSTERS OF β-PROPIOLACTONE BY BROADBAND MICROWAVE SPECTROSCOPY

JUSTIN L. NEILL, University of Michigan. Department of Astronomy 830 Dennison Bldg. 500 Church St. Ann Arbor, MI 48109-1042; CRISTOBAL PEREZ, MATT T. MUCKLE, BROOKS H. PATE, Department of Chemistry, University of Virginia, McCormick Rd., Charlottesville, VA 22904; ISABEL PENA, JUAN C. LOPEZ, JOSE L. ALONSO, Grupo de Espectroscopía Molecular (GEM), Edificio Quifima, Laboratorios de Espectroscopia y Bioespectroscopía, Parque Científico Uva Universidad de Valladolid, 47011 Valladolid, Spain.
# MI. MINI-SYMPOSIUM: PHOTODETACHMENT AND PHOTOIONIZATION

**MONDAY, JUNE 18, 2012 – 1:30 PM**  
**Room: 1015 MCPHERSON LAB**

**Chair:** CAROLINE JARROLD, Indiana University-Bloomington, Bloomington, Indiana

<table>
<thead>
<tr>
<th>MI01</th>
<th><strong>INVITED TALK</strong></th>
<th>30 min 1:30</th>
</tr>
</thead>
<tbody>
<tr>
<td>SLOW-ELECTRON VELOCITY-MAP IMAGING OF NEGATIVE IONS: APPLICATIONS TO SPECTROSCOPY AND DYNAMICS</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DANIEL NEUMARK, Department of Chemistry, University of California at Berkeley, B64 Hildebrand Hall, Berkeley, CA 94720.</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>MI02</th>
<th>15 min 2:05</th>
</tr>
</thead>
<tbody>
<tr>
<td>STATE-RESOLVED PREDISSOCIATION DYNAMICS OF THE FORMYLOXYL RADICAL BY DISSOCIATIVE PHOTODETACHMENT OF HCO$_2^-$ / DCO$_2^-$</td>
<td></td>
</tr>
<tr>
<td>AMELIA W. RAY, BEN B. SHEN, BERWYCK L. J. POAD and ROBERT E. CONTINETTI*, Department of Chemistry and Biochemistry, University of California, San Diego, La Jolla, CA 92093.</td>
<td></td>
</tr>
</tbody>
</table>

*This work is supported by the US Department of Energy under Grant Number DE-FG03-98ER14879

<table>
<thead>
<tr>
<th>MI03</th>
<th>15 min 2:22</th>
</tr>
</thead>
<tbody>
<tr>
<td>PHOTOELECTRON-PHOTOFRAGMENT COINCIDENCE SPECTROSCOPY OF TERT-BUTOXIDE AND THE CARBANION ISOMER</td>
<td></td>
</tr>
<tr>
<td>BEN B. SHEN, BERWYCK L. J. POAD, AMELIA W. RAY, and ROBERT E. CONTINETTI*, Department of Chemistry and Biochemistry, University of California, San Diego, CA 92093.</td>
<td></td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>MI04</th>
<th>15 min 2:39</th>
</tr>
</thead>
<tbody>
<tr>
<td>VIBRATIONAL AUTODETACHMENT: INTRAMOLECULAR VIBRATIONAL RELAXATION TO ELECTRONIC MOTION</td>
<td></td>
</tr>
<tr>
<td>CHRISTOPHER L. ADAMS, BENJAMIN J. KNURR and J. MATHIAS WEBER, JILA, NIST and Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO 80309.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>MI05</th>
<th>15 min 2:56</th>
</tr>
</thead>
<tbody>
<tr>
<td>PHOTOELECTRON SPECTROSCOPY OF RARE-GAS SOLVATED NUCLEOBASE ANIONS</td>
<td></td>
</tr>
<tr>
<td>ANGELA M. BUONAUGURIO, JING CHEN, AND KIT H. BOWEN, Department of Chemistry, Johns Hopkins University, Baltimore, MD 21218.</td>
<td></td>
</tr>
</tbody>
</table>

**Intermission**
A STUDY OF NbMo AND NbMo\(^-\) BY ANION PHOTOELECTRON SPECTROSCOPY

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

RESONANT TWO-PHOTON DETACHMENT OF WO\(_2^-\)

JENNIFER E. MANN, SARAH E. WALLER, DAVID W. ROTHGEB, AND CAROLINE CHICK JARROLD, Dept. of Chemistry, Indiana University, Bloomington, Indiana, 47405.

ELECTRONIC STRUCTURES OF MoAlO\(_y^-\) (y = 1 – 4) DETERMINED BY PHOTOELECTRON SPECTROSCOPY AND DFT CALCULATIONS

SARAH E. WALLER, JENNIFER E. MANN, EKRAM HOSSIAN, AND CAROLINE CHICK JARROLD, Dept. of Chemistry, Indiana University, Bloomington, Indiana, 47405.

ANION PHOTOELECTRON ANGULAR DISTRIBUTIONS: ELECTRON SCATTERING RESONANCES IN PHOTODETACHMENT

RICHARD MABB, Washington University in St. Louis, St. Louis, Mo, 63130.

C-O AND O-H BOND ACTIVATION OF METHANOLE BY LANTHANUM

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

APPLICATION OF EQUATION-OF-MOTION COUPLED-CLUSTER THEORY TO PHOTODETACHMENT CROSS SECTION CALCULATIONS

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

ELECTRON PROPAGATOR THEORY OF AQUEOUS HALIDE PHOTOELECTRON SPECTRA

J. V. ORTIZ, Department of Chemistry and Biochemistry
Auburn University
Auburn, Alabama 36849-5312.
MJ01 15 min 1:30
IDENTIFICATION OF α- AND β-PROTONATED NAPHTHALENE (C_{10}H_{9}^+) AND THEIR NEUTRAL COUNTER-PARTS ISOLATED IN SOLID PARA-HYDROGEN

MOHAMMED BAHOU, Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu 30010, Taiwan; YU-JONG WU, National Synchrotron Radiation Research Center, 101 Hsin-Ann Road, Hsinchu Science Park, Hsinchu 30076, Taiwan; 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.

MJ02 15 min 1:47
INFRARED SPECTRA OF THE 2-CHLOROPROPYL RADICAL IN SOLID PARA-HYDROGEN

JAY C. AMICANGELO, School of Science, Penn State Erie, Erie, PA 16563; 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.

MJ03 15 min 2:04
DIFFUSION OF HYDROGEN FLUORIDE IN SOLID PARAHYDROGEN.

H. OOE, Y. MIYAMOTO, J. TANG, K. KAWAGUCHI, Graduate School of Natural Science and Technology, Okayama University, 3-1-1 Tsushima-naka Okayama 700-8530, Japan; S. KUMA, K. NAKAJIMA, N. SASAO, T. TANIGUCHI, Research Core for Extreme Quantum World, Okayama University, 3-1-1 Tsushima-naka Okayama 700-8530, Japan; I. NAKANO and M. YOSHIMURA, Faculty of Science, Okayama University, 3-1-1 Tsushima-naka Okayama 700-8530, Japan.

MJ04 15 min 2:21
SPECTROSCOPIC AND COMPUTATIONAL STUDIES OF MATRIX ISOLATED ISO-CXBr_3 (X=F, Cl, Br)

AIMABLE KALUME, LISA GEORGE AND SCOTT A. REID, Department of Chemistry, Marquette University, Milwaukee, WI 53233; BRIAN J. ESSELMAN, ROBERT J. MCMAHON, Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706.

MJ05 15 min 2:38
SPECTROSCOPY OF AND PHOTOINDUCED ELECTRON TRANSFER IN THE COMPLEXES OF C_2H_4 WITH I AND I_2

LISA GEORGE, AIMABLE KALUME AND SCOTT A. REID, Department of Chemistry, Marquette University, Milwaukee, WI 53233.
MJ06 15 min 2:55
CALCULATION OF RAMAN FREQUENCIES AS FUNCTIONS OF TEMPERATURE AND PRESSURE IN PHASES OF SOLID I, II AND III (III') OF BENZENE

H. YURTSEVEN, Department of Physics, Middle East Technical University, 06531 Ankara-Turkey; O. TARI, Department of Mathematics, Istanbul Arel University, Istanbul, Turkey.

Intermission

MJ07 15 min 3:00
HELIUM NANODROPLET ISOLATION OF IONIC LIQUID VAPOR: INRARED LASER SPECTROSCOPY OF [EMIM][Tf₂N]

STEVEN D. FLYNN, GARY E. DOUBERLY, Department of Chemistry, University of Georgia, Athens, Georgia, USA 30602.

MJ08 15 min 3:47
C_{60}^{+} AND C_{60}^{-} IN NEON AND ARGON MATRICES

BASTIAN KERN, DMITRY STRELIKOV, PATRIK WEIS, ARTUR BÖTTCHER and MANFRED M. KAPPES, KIT Karlsruhe Institute for Technology, Division of Physical Chemistry of Microscopic Systems, Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany.

MJ09 10 min 4:04
FTIR OF METHYL PYRUVATE CONFORMERS IN AN ARGON MATRIX

ALLISON B. COMBS, JORDAN L. PRESTON, SARA E. LILLY, COURTNEY D. HATTEN, and LAURA R. MCCUNN, Department of Chemistry, One John Marshall Drive, Huntington, WV 25755.

MJ10 15 min 4:16
FTIR AND DFT STUDY OF THE VIBRATIONAL SPECTRUM OF SiC₅ TRAPPED IN SOLID Ar

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

MJ11 15 min 4:33
VIBRATIONAL SHIFT OF ADSORBED CARBON DIOXIDE WITHIN A METAL-ORGANIC FRAMEWORK

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.

MJ12 5 min 4:50
SYMMETRY PECULIARITIES OF THE INTRACRYSTALLINE FIELDS LAYERED SEMICONDUCTOR CRYSTALS (PbI₂)(1−x) (BiI₃)x

IGOR VERTEGEL, EUGENE CHESNOKOV and ALEKSANDR OVCHARENKO, Institute of Physics National Academy of Sciences of Ukraine 46, Prospect Nauki, 03680 Kiev, Ukraine.
TA01 15 min 8:30
FREQUENCY COMB-REFERENCED MEASUREMENTS OF SELF- AND NITROGEN-PERTURBED LINE SHAPE PARAMETERS IN THE \( \nu_1 + \nu_3 \) BAND OF ACETYLENE

MATTHEW J. CICH, GARY V. LOPEZ, TREVOR J. SEARS\(^a\), 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 HURTMANs, Service de Chimie Quantique et de Photophysique(Atoms, Molecules et Atmospheres), Université Libre de Bruxelles, Bruxelles, Belgium B-10050.

\(^a\)also: Department of Chemistry, Brookhaven National Laboratory, Upton, New York 11973

TA02 15 min 8:47
HIGH ACCURACY MEASUREMENTS OF NEAR-INFRARED CO\(_2\) AND O\(_2\) TRANSITIONS TO SUPPORT ATMOSPHERIC REMOTE SENSING

DAVID A. LONG, JOSEPH T. HODGES, Material Measurement Laboratory, National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, MD 20899, USA; MITCHIO OKUMURA, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125, USA; and CHARLES E. MILLER, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Drive, Pasadena, CA 91109, USA.

TA03 15 min 9:04
TRACE GAS MEASUREMENTS WITH A MULTIPLEXED INTRA-PULSE QUANTUM CASCADE LASER SPECTROMETER

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

TA04 15 min 9:21
ISOTOPICALLY INVARIANT DUNHAM FIT FOR THE \( X^3\Sigma_g^-\), \( a^3\Delta_g \), AND \( b^1\Sigma_g^+ \) STATES 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.

TA05 15 min 9:38
THE ROTATIONAL SPECTRA OF O-17 SUBSTITUTE OXYGEN SINGLET DELTA

BRIAN J. DROUIN, HARSHAL GUPTA, SHANSHAN YU, CHARLES E. MILLER, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109-8099; HOLGER S. P. MÜLLER, I. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, D-50937, Köln, Germany.
LINE MIXING EFFECTS OF O₂ A-BAND WITH PHOTOACOUSTIC SPECTROSCOPY IN SUPPORT OF REMOTE SENSING

THINH Q. BUI, DANIEL HOGAN, PRIYANKA M. RUPASINGHE, MITCHIO OKUMURA, California Institute of Technology, Division of Chemistry, MC 127-72, Pasadena, CA 91125; DAVID A. Long and JOSEPH T. Hodges, NIST, 100 Bureau Drive, Stop 1070, Gaithersburg, MD 20899-1070; CHARLES E. Miller, Jet Propulsion Laboratory, California Institute of Technology, MS 183-901, Pasadena, CA 91109.

aSupport from NSF Graduate Fellowship and NASA OCO Funding are gratefully acknowledged

Intermission

BROADBAND OZONE ABSORPTION CROSS SECTIONS IN NEAR UV - NEAR IR

ANNA SERDYUCHENKO, VICTOR GORSHELEV, MARK WEBER and JOHN P. BURROWS, Institute of Environmental Physics, University of Bremen, Germany.

AIR-BROADENED LINE PARAMETERS FOR THE 2—0 BANDS OF \(^{13}\)C\(^{16}\)O AND \(^{12}\)C\(^{18}\)O AT 2.3 \(\mu\)m


SPEED DEPENDENT LINE SHAPES IN 1.61 \(\mu\)m AND 2.07 \(\mu\)m CO₂ ATMOSPHERIC RETRIEVALS FOR THE OCO-2 MISSION

DAVID R. THOMPSON, LINDA R. BROWN, DAVID CRISP, YIBO JIANG, FABIANO OYAFUSO, KEEYOON SUNG, CHARLES E. MILLER, VIJAY NATRAJ, DEBRA WUNCH, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr., Pasadena, CA 91109, U.S.A.; D. CHRIS BENNER, V. MALATHY DEVI, The College of William and Mary, Williamsburg, VA 23187, U.S.A.

THE \(\nu_3\) AND \(\nu_4\) BANDS OF NITRIC ACID (\(HN\)O₃) AT 7.6 \(\mu\)m FOR ATMOSPHERIC STUDIES

A. PERRIN, J.M. FLAUD, Laboratoire Inter Universitaire des Systemes Atmospheriques, CNRS, Université Paris EST-Créteil, 61 Av du General de Gaulle, 94010 Créteil Cedex France; M. RIDOLFI, M. CARLOTTI, Dipartimento di Chimica Fisica e Inorganica (DCFI), Universisy of Bologna, Viale del Risorgimento, 4 - 40136 - Bologna, Italy.

FIRST HIGH RESOLUTION ANALYSIS OF THE 5\(\nu_3\) BAND OF NITROGEN DIOXIDE NEAR 1.3 \(\mu\)m

D. MONDELAIN, S. KASSI, A. CAMPAVGUE, Laboratoire Interdisciplinaire de Physique (LIPhy), UMR-CNRS 5588, Université Joseph Fourier de Grenoble, B.P. 87, 38402 Saint-Martin-d’Hères Cedex, France; A. PERRIN, Laboratoire Inter Universitaire des Systemes Atmospheriques (LISA), CNRS, Universités Paris Est and Paris 7, 61 Av du Général de Gaulle, 94010 Créteil Cedex France.
TB. DYNAMICS
TUESDAY, JUNE 19, 2012 – 8:30 AM
Room: 170 MATH ANNEX

Chair: SCOTT KABLE, University of Sydney, Sydney, Australia

TB01 15 min 8:30
LIFETIMES OF THE Å STATES OF C₃, C₃-NE, AND C₃-AR

YI-JEN WANG, CHIAO-WEI CHEN, LIUZHU ZHOU, ANTHONY J. MERER, YEN-CHU HSU, Institute of Atomic and Molecular Sciences, Academia Sinica, P. O. Box 23-166, Taipei 10617, Taiwan, R. O. C.

TB02 15 min 8:47
ACTION SPECTROSCOPY AND DISSOCIATION ENERGY OF AMMONIA TRIMER

CORNELIA G. HEID, AMANDA S. CASE, Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706; COLIN M. WESTERN, School of Chemistry, University of Bristol, Bristol, BS8 1TS, U.K.; F. FLEMING CRIM, Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706.

TB03 15 min 9:04
VIBRATIONAL ENERGY RELAXATION OF CHLOROIODOMETHANE IN COLD ARGON

A.JAIN and E.L.SIBERT, Department of Chemistry, University of Wisconsin, Madison, 53706.

TB04 15 min 9:21
ULTRAFAST PHOTOPHYSICS OF SIMPLE AROMATIC CHROMOPHORES

RAUL MONTERO, ALVARO PERALTA CONDE, MARTA FERNÁNDEZ-FERNÁNDEZ, FERNANDO CASTANO and ASIER LONGARTE, Departamento de Química Física, Facultad de Ciencia y Tecnología, Universidad del País Vasco (UPV-EHU), Ap. 644, E-48080 Bilbao, Spain.

TB05 15 min 9:38
FEMTOSECOND TIMESCALE EVOLUTION OF PYRROLE ELECTRONIC EXCITATION

RAUL MONTERO, ALVARO PERALTA CONDE, VIRGINIA OVEJAS, FERNANDO CASTANO and ASIER LONGARTE, Departamento de Química Física, Facultad de Ciencia y Tecnología, Universidad del País Vasco (UPV-EHU), Ap. 644, E-48080 Bilbao, Spain.

TB06 15 min 9:55
DEVELOPMENT OF FEMTOSECOND STIMULATED RAMAN SPECTROSCOPY AS A PROBE OF PHOTOISOMERIZATION DYNAMICS

RYAN D. KIEDA, ADAM D. DUNKELBERGER, JAEOYON SHIN, TRACY OUDENHOVEN, and F. FLEMING CRIM, Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706.

Intermission
PHOTOISOMERIZATION DYNAMICS OF dMe-OMe-NAIP, A MODEL FOR THE RETINAL CHROMOPHORE

ADAM D. DUNKELBERGER, RYAN D. KIEDA, JAEYOOON SHIN, Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706; RICARDO ROSSI PACCA, STEFANIO FUSI, Universitá di Siena, Siena, I-53100, Italy; MASSIMO OLIVUCCI, Università di Siena, Siena, I-53100, Italy and Bowling Green State University, Bowling Green, OH 43403; and F. FLEMING CRIM, Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706.

ELECTRON TUNNELING PATHWAY AND ROLE OF ADENINE IN REPAIR OF DAMAGED DNA BY PHOTOLYASE

ZHEYUN LIU, CHUANG TAN, XUNMIN GUO, YA-TING KAO, JIANG LI, LIUJUAN WANG, and DONGPING ZHONG, Department of Physics, Chemistry, and Biochemistry, The Ohio State University, Columbus, OH 43210.

MOLECULAR UNDERSTANDING OF EFFICIENT DNA REPAIR MACHINERY OF PHOTOLYASE

CHUANG TAN, ZHEYUN LIU, JIANG LI, XUNMIN GUO, LIUJUAN WANG and DONGPING ZHONG, Departments of Physics, Chemistry, and Biochemistry, Programs of Biophysics, Chemical Physics, and Biochemistry, The Ohio State University, Columbus, Ohio, 43210.

TRANSITION METAL ASSISTED DECOMPOSITION KINETICS OF ORGANIC MOLECULES: MODELS FOR CATALYSIS

DARRIN BELLERT, IVANNA LABOREN, and OTSMAR VILLARROEL, Department of Chemistry, Baylor University, Waco, TX 76798.

TRANSIENT ABSORPTION AND TIME-RESOLVED FLUORESCENCE STUDIES OF SOLVATED RUTHENIUM DI-BIPYRIDINE PSEUDO-HALIDE COMPLEXES

R. COMPTON, National Research Council, Postdoctoral Fellow; D. WEIDINGER, Schafer Corporation; J. C. OWRUTSKY, Chemistry Division, Naval Research Laboratory.
TC01 10 min 8:30
PURE ROTATIONAL SPECTROSCOPY OF PANHs I: 1,10-PHENANTHROLINE. IMPLICATIONS OF PANHs IN ASTRONOMICAL ENVIRONMENTS AND OBSERVATIONAL SPECTRA

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

TC02 10 min 8:42
PURE ROTATIONAL SPECTROSCOPY OF PANHs II: ACRIDINE. POSSIBLE APPLICATIONS IN THz COHERENT CONTROL SPECTROSCOPY

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

TC03 10 min 8:54
PURE-ROTATIONAL SPECTROSCOPY OF PANHs III: PHENANTHRIDINE. POSSIBLE APPLICATIONS TO THE SPECTROSCOPY OF PROTONATED AROMATIC SPECIES

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

TC04 15 min 9:06
A PURE ROTATIONAL STUDY OF TWO NEARLY-EQUIVALENT STRUCTURES OF HEXAFLUOROACETONE IMINE

DANIEL A. OBENCHAIN, DANIEL J. FROHMAN, G. S. GRUBBS II, B. E. LONG, WALLACE C. PRINGLE, STEWART E. NOVICK, Department of Chemistry, Wesleyan University, 52 Lawn Avenue, Middletown, CT 06459-0180; S. A. COOKE, School of Natural and Social Sciences, Purchase College SUNY, 735 Anderson Hill Road, Purchase, NY 10577.

TC05 15 min 9:23
A ROTATIONAL STUDY OF 2H–3H–PERFLUOROPENTANE AND ITS ISOTOPOLOGUES

CHINH H. DUONG, DANIEL A. OBENCHAIN, STEWART E. NOVICK, Department of Chemistry, Wesleyan University, 52 Lawn Avenue, Middletown, CT 06459-0180; S. A. COOKE, School of Natural and Social Sciences, Purchase College SUNY, 735 Anderson Hill Road, Purchase, NY 10577.
CONFORMATIONS AND BARRIERS TO METHYL GROUP INTERNAL ROTATION IN TWO ASYMMETRIC ETHERS: PROPYL METHYL ETHER AND BUTYL METHYL ETHER

B. E. LONG, Department of Chemistry, Wesleyan University, Hall-Atwater Laboratories, 52 Lawn Ave, Middletown, CT 06459-0180; F. DeCHIRICO, S. A. COOKE, School of Natural and Social Sciences, Purchase College SUNY, 735 Anderson Hill Road, Purchase, NY 10577.

MW SPECTROSCOPY COUPLED WITH ULTRAFAST UV LASER VAPORIZATION: RIBOSE FOUND IN THE GAS PHASE

EMILIO J. COCINERO, PATRICIA ECJIA, FRANCISCO J. BASTERRETXEA, JOSÉ A. FERNÁNDEZ, FERNANDO CASTANO, Departamento de Química Física, Facultad de Ciencia y Tecnología, Universidad del País Vasco (UPV-EHU), Ap. 644, E-48080 Bilbao, Spain; ALBERTO LESARRI, Departamento de Química-Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, E-47011 Spain; JENS-UWE GRABOW, Institut für Physikalische Chemie, Lehrgebiet A, Universität Hannover, Callinstrasse, 3A, D-30167 Hannover, Germany.

FOURIER TRANSFORM MICROWAVE STUDIES OF BI-MOLECULES OF CARBOXYLIC ACIDS

LUCA EVANGELISTI, GANG FENG, GOU QIAN, ASSIMO MARIS 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; EMILIO COCINERO, PATRICIA EJICA, JOSE’ A. FERNANDEZ and FERNANDO CASTANO, Departamento de Química Física, Facultad de Ciencia y Tecnología, Universidad del País Vasco, E-48080 Bilbao, Spain; ALBERTO LESARRI, Departamento de Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, E-47011 Spain; ROLF MEYER, Sonnenbergstrasse 18, CH-5621 Zufikon, Switzerland.

THE ROTATIONAL SPECTRA OF PERFLUOROPROPIONIC ACID AND ITS HYDRATES

WEI LIN, AGAPITO SERRATO III, Department of Chemistry and Environmental Sciences, University of Texas at Brownsville, 80 Fort Brown, Brownsville, TX 78520; DANIEL A. OBENCHAIN, G. S. GRUBBS II, STEWART E. NOVICK, Department of Chemistry, Wesleyan University, 52 Lawn Avenue, Middletown, CT 06459-0180; S. A. COOKE, School of Natural and Social Sciences, Purchase College SUNY, 735 Anderson Hill Road, Purchase, NY 10577.

THE MILLIMETER WAVE SPECTRUM OF LINALOOL

COREY J EVANS, STEPHANIE M ALLPRESS, Department of Chemistry, University of Leicester, Leicester, LE17RH, United Kingdom; PETER D GODFREY, DON MCNAUGHTON, School of Chemistry, Monash University, 3800, Victoria, Australia.
THE CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE (CP-FTMW) SPECTRUM AND POTENTIAL ENERGY CALCULATIONS FOR AN AROMATIC CLAISEN REARRANGEMENT MOLECULE, ALLYL PHENYL ETHER

G. S. GRUBBS II, Department of Chemistry, Wesleyan University, 52 Lawn Ave., Middletown, CT 06459-0180; S. A. COOKE, School of Natural and Social Sciences, Purchase College SUNY, 735 Anderson Hill Road, Purchase, NY 10577; and STEWART E. NOVICK, Department of Chemistry, Wesleyan University, 52 Lawn Ave., Middletown, CT 06459-0180.

ROTATIONAL SPECTRUM AND LARGE AMPLITUDE MOTIONS OF 3,4-, 2,5- and 3,5-DIMETHYL-BENZALDEHYDE

J. KLEINER, Laboratoire Interuniversitaire des Systèmes Atmosphériques, CNRS et Universités Paris Diderot et Paris Est, 61 av. Général de Gaulle, 94010, Créteil, France; M. TUDORIE, Service de Chimie Quantique et Photophysique, Université Libre de Bruxelles, 50 av. F.-D. Roosevelt, 1050 Bruxelles, Belgique; M. JAHN, J.-U. GRABOW, Gottfried-Wilhelm-Leibniz-Universität, Institut für Physikalische Chemie und Elektrochemie, Lehrgebiet A, Callinstrasse 3A, D-30167 Hannover, Germany; M. GOUBET, Laboratoire PhLAM, UMR 8523 CNRS, Bât. P5, Université des Sciences et Technologies de Lille 1, F-59655 Villeneuve d’Ascq, France.

SEMIEXPERIMENTAL EQUILIBRIUM STRUCTURES FOR THE EQUATORIAL CONFORMERS OF N-METHYLPIPERIDONE AND TROPINONE BY THE MIXED ESTIMATION METHOD

JEAN DEMAISON, Laboratoire de Physique des Lasers, Atomes et Molécules, Université de Lille I, 59655 Villeneuve d’Ascq Cedex, France; NORMAN C. CRAIG, Department of Chemistry and Biochemistry, Oberlin College, Oberlin, OH 44074; 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, Lehrgebiet A, Gottfried-Wilhelm-Leibniz Universität, Callinstrasse 3A, D-30167 Hannover, Germany; ALBERTO LESARRI, Departamento de Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, E-47011 Valladolid, Spain; H. D. RUDOLPH, Department of Chemistry, University of Ulm, D-89069 Ulm, Germany.
TD. MINI-SYMPOSIUM: PHOTODETACHMENT AND PHOTOIONIZATION

TUESDAY, JUNE 19, 2012 – 8:30 AM
Room: 1015 MCPHERSON LAB

Chair: RICHARD MABBS, Washington University in St. Louis, St. Louis, Missouri

**TD01 30 min 8:30**
TRANSITION-METAL-DOPED PLANAR BORON CLUSTERS: A NEW CLASS OF AROMATIC COMPOUNDS WITH HIGH COORDINATION

LAI-SHENG WANG, Department of Chemistry, Brown University, Providence, Rhode Island.

**TD02 15 min 9:05**
ELECTRON SPIN STATES AND STRUCTURES OF LANTHANIDE (Ce, Pr, and Nd) COMPLEXES OF CYCLOOC-TATERAENE

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

**TD03 15 min 9:22**
Cyclopolymerization of acetylene to benzyne and naphthalene

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

**TD04 15 min 9:39**
ELECTRONIC RELAXATION OF THE PHENYLALANINE RESIDUE IN GAS PHASE PEPTIDES: ROLE OF THE NEIGHBOURING AMIDE GROUPS IN THE PHOTOPHYSICS

Y. LOQUAIS, H.S. BISWAL, B. TARDIVEL, V. BRENNER, M. MONS, CEA, IRAMIS, SPAM, Lab. Francis Perrin, URA 2453, Gif-sur-Yvette, F-91191, France; E. GLOAGUEN, CNRS, INC & INP, Lab. Francis Perrin, URA 2453, Gif-sur-Yvette, F-91191, France; C. JOUVET, M. BROQUIER, CNRS, INP, ISMO, CLUPS, UMR 8214, Orsay, F-91405, France; M. MALIS, I. LJUBIC and N. DOSLIC, Ruder Bošković Institute, Department of Physical Chemistry, Zagreb, 10000, Croatia.

**TD05 15 min 9:56**
PROTON TRANSFER IN NEUTRAL PEPTIDES EXAMINED BY CONFORMATIONAL SPECIFIC IR AND UV SPECTROSCOPY

SANDER JAEQX, JOS OOMENS, FOM institute Rijnhuizen, Edisonbaan 14, 3439 MN Nieuwegein, The Netherlands; ANOUK M. RIJS, Radboud University Nijmegen, Institute of Molecules and Materials (molecular & biophysics), Toernooiveld 7, 6525 ED Nijmegen, the Netherlands.

Intermission
TD06 15 min 10:30
SURPRISING COMPLEXITY OF A SMALL MOLECULE: PHOTOFragmentation dynamics of ICN, ICN·Arₙ, and ICN·(CO₂)ₙ

ANNE B. McCoy, Department of Chemistry, The Ohio State University, Columbus, OH 43210; AMANDA S CASE, JOSHUA P. MARTIN, and W. CARL LINEBERGER, JILA and Department of Chemistry and Biochemistry University of Colorado, Boulder, CO 80309.

TD07 15 min 10:47
NONRADIATIVE DECAY DYNAMICS OF METHYL-4-HYDROXYCINNAMATE AND ITS MONOHYDRATED COMPLEX REVEALED BY PICosecond PUMP-PROBE SPECTROSCOPY

T. EBATA, D. SHIMADA, R. KUSAKA, and Y. INOKUCHI, Department of Chemistry, Graduate School of Science, Hiroshima University, Higashi-Hiroshima 739-8526, Japan; M. EHARA, Institute for Molecular Science, 38 Myodaiji, Okazaki 444-8585, Japan.

TD08 15 min 11:04
DEUTERATION EFFECT STUDY ON THE VIBRATIONAL DYNAMICS OF PHENOL AND PHENOL-WATER COMPLEX BY PICosecond TIME-RESOLVED IR-UV PUMP-PROBE SPECTROSCOPY IN A SUPersonic MOLECULAR BEAM

YASUNORI MIYAZAKI, YOSHIYA INOKUCHI, and TAKAYUKI EBATA, Department of Chemistry, Graduate School of Science, Hiroshima University, Japan.

TD09 15 min 11:21
PICosecond TIME-RESOLVED IR-UV PUMP-PROBE SPECTROSCOPIC STUDY ON VIBRATIONAL ENERGY RELAXATION OF BENZENE DIMER AND TRIMER IN THE CH STRETCHING REGION

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

TD10 15 min 11:38
PHOTOELECTRON SPECTROSCOPY OF ALUMINUM DOPED BORON CLUSTERS

WEI-LI LI, CONSTANTIN ROMANESCU, LAI-SHENG WANG, Brown University, Chemistry Department, 324 Brook Street, Providence, RI 02912, USA.
TE  MINI-SYMPOSIUM:  SPECTROSCOPY  OF  INTERFACES  
TUESDAY, JUNE 19, 2012  –  8:30 AM  
Room: 2015 MCPHERSON LAB  

Chair: MICHAEL DUNCAN, University of Georgia, Athens, Georgia

TE01  
INVITED TALK  
30 min  8:30  
SELECTIVE ADSORPTION OF IONS TO AQUEOUS INTERFACES AND ITS EFFECTS ON EVAPORATION RATES  

RICHARD J. SAYKALLY, Department of Chemistry, University of California and Chemical Sciences Division, Lawrence Berkeley National Laboratory Berkeley, CA 94720-1460.

TE02  
10 min  9:05  
BISULFATE (HSO$_4^-$) DEHYDRATION AT THE VAPOR/SOLUTION INTERFACE PROBED BY VIBRATIONAL SUM FREQUENCY GENERATION SPECTROSCOPY  

AARON M. JUBB and HEATHER C. ALLEN, Department of Chemistry and Biochemistry, The Ohio State University, 100 W. 18th Ave., Columbus, OH, 43210.

TE03  
10 min  9:17  
INTERFACIAL WATER STRUCTURE AND CATION BINDING WITH THE DPPC PHOSPHATE AT AIR/AQUEOUS INTERFACES STUDIED BY VIBRATIONAL SUM FREQUENCY GENERATION SPECTROSCOPY  

WEI HUA, HEATHER C. ALLEN, Department of Chemistry and Biochemistry, The Ohio State University, 100 W. 18th Ave., Columbus, OH, 43210.

TE04  
15 min  9:29  
The spectroscopic study of estrogen and its hydrated clusters in a super sonic jet  

FUMIYA MORISHIMA, YOSHIYA INOKUCHI and TAKAYUKI EBATA, Department of Chemistry, Graduate School of Science, Hiroshima University, Higashi-hiroshima, 739-8526, Japan.

Intermission

TE05  
15 min  10:15  
INFRARED SPECTROSCOPY OF LARGE-SIZED NEUTRAL AND PROTONATED METHANOL CLUSTERS  

TOMOHIRO KOBAYASHI, RYUNOSUKE SHISHIDO, ASUKA FUJII, Department of Chemistry, Graduate School of Science, Tohoku University, Sendai 980-8578, Japan; JER-LAI KUO, Institute of Atomic and Molecular Science, Academia Sinica, Taipei 10617, Taiwan.

TE06  
10 min 10:32  
INFRARED SPECTROSCOPY OF (CH$_3$)$_3$N-H$^+$-(H$_2$O)$_n$ (n = 1-22)  

RYUNOSUKE SHISHIDO, ASUKA FUJII, Department of Chemistry, Graduate School of Science, Tohoku University, Sendai 980-8578, Japan; and KUO JER-LAI, Institute of Atomic and Molecular Sciences Academia Sinica, Taipei, Taiwan.
TE07 15 min 10:44
INVESTIGATING ELECTRONIC PROPERTIES OF IONIZED PAH CLUSTERS

C. JOBLIN, D. KOKKIN, A. BONNAMY, D. TOUBLANC, IRAP; Université de Toulouse, UPS; CNRS; 9 Av. colonel Roche, BP 44346, F-31028 Toulouse Cedex 4, France; M. RAPACIOLI, A. SIMON, L. DONTOT, A. GAMBOA, F. SPIEGELMAN, LCPQ, Université de Toulouse, UPS; CNRS; 118 Route de Narbonne, 31062 Toulouse Cedex 09, France; P. PARNEIX, T. PINO, O. PIRALI, G. FÉRAUD, H. FRIHA, C. FALVO, P. BRÉCHIGNAC, ISMO; Université Paris-Sud 11; CNRS; Bât. 210, 91405 Orsay Cedex, France; G. GARCIA, L. NAHON, Synchrotron SOLEIL, L’Orme des Merisiers, St Aubin, B.P. 48, 91192 Gif sur Yvette, France; G. MULAS, INAF; Osservatorio Astronomico di Cagliari, Strada n. 54, Loc. Poggio dei Pini, 09012 Capoterra, CA, Italy.

TE08 15 min 11:01
QUANTUM STATE-RESOLVED REACTIVE AND INELASTIC SCATTERING AT GAS-LIQUID AND GAS-SOLID INTERFACES

MONIKA GRÜTTER, DANIEL J. NELSON AND DAVID J. NESBITT, JILA, University of Colorado and National Institute of Standards and Technology, and Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO 80309, U.S.A.

TE09 15 min 11:18
PROBING THE STRUCTURE OF IONIC LIQUID SURFACES BY ROTATIONALLY AND ELECTRONICALLY INELASTIC SCATTERING OF NO

M. P. ZIEMKIEWICZ, A. ZUTZ, and D. J. NESBITT, JILA, University of Colorado and National Institute of Standards and Technology, Boulder, Colorado, USA.

TE10 10 min 11:35
PHOTOELECTRON SPECTROSCOPY OF SOLVATED ELECTRONS IN LIQUID MICROJETS

MADELINE ELKINS, ALEXANDER STREVE, and DANIEL NEUMARK, Department of Chemistry, University of California - Berkeley, Berkeley, CA 94720.
THE HIGH-RESOLUTION FAR-INFRARED SPECTRA OF SULFUR DI-CYANIDE, S(CN)₂ AND THE PURSUIT OF THAT OF CYANOGEN ISO-THIOCYANATE, NCNCS

MANFRED WINNEWISSER, BRENDA P. WINNEWISSER, FRANK C. DE LUCIA, Department of Physics, The Ohio State University, Columbus Ohio, 43210-1106, USA; DENNIS W. TOKARYK, DAMIEN FORTHOMME, SEPHEN C. ROSS, Department of Physics and Centre for Laser, Atomic, and Molecular Sciences, University of New Brunswick, P. O. Box 4400, Fredericton NB E3B 5A3, Canada; BRANT E. BILLINGHURST, Canadian Light Source, Inc., University of Saskatchewan, Saskatoon, SK, Canada.

COMBINATION BANDS OF THE NONPOLAR OCS DIMER INVOLVING INTERMOLECULAR MODES

M. REZAEI, J. NOROOZ OLLAEE, 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.

PHOTOIONIZATION INDUCED WATER MIGRATION OF 4-AMINOBENZONITRILE-(H₂O)₁ CLUSTER

TAKASHI NAKAMURA, Chemical Resources Laboratory, Tokyo Tech, 4259 Nagatsuta-machi, Midori-ku, Yokohama-shi, Kanagawa, 226-8503, Japan; MITSUHIKO MIYAZAKI, MASAAKI FUJII, Chemical Resources Laboratory, Tokyo Tech, 4259 Nagatsuta-machi, Midori-ku, Yokohama-shi, Kanagawa, 226-8503, Japan; and KOICHI TSUKIYAMA, Department of Chemistry, Faculty of Science Division I, Tokyo University of Science, 1-3 Kagurazaka, Shinjuku-ku, Tokyo, 162-8601, Japan.

ISOLATION OF ION-DRIVEN CONFORMATIONS IN DIPHENYLACETYLENE MOLECULAR SWITCHES USING CRYOGENIC INFRARED SPECTROSCOPY

ARRON B. WOLK, Yale University, 225 Prospect Street, New Haven, CT 06520; ETIENNE GARAND, Yale University, 225 Prospect Street, New Haven, CT 06520; IAN M. JONES, Yale University, 225 Prospect Street, New Haven, CT 06520; MICHAEL Z. KAMRATH, Yale University, 225 Prospect Street, New Haven, CT 06520; ANDREW HAMILTON, University of Oxford, 12 Mansfield Road, Oxford, OX1 3TA; and MARK A. JOHNSON, Yale University, 225 Prospect Street, New Haven, CT 06520.

INFRARED SPECTROSCOPY OF COLD, HYDRATED ALKALINE EARTH-HYDROXIDE CLUSTERS

CHRISTOPHER JOHNSON, CHRISTOPHER LEAVITT, JOSEPH FOURNIER, MARK JOHNSON, Department of Chemistry, Yale University, New Haven, CT 06520.
TF06 15 min 2:55
A HIGH RESOLUTION FAR INFRARED STUDY OF LOW LYING VIBRATIONAL BANDS OF 3-OXETANONE

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

Intermission

TF07 15 min 3:30
GAS-PHASE SPECTROSCOPY OF TYROSINE BY LASER DESORPTION SUPersonic JET TECHNIQUE - STABILIZATION MECHANISM OF THE MOST STABLE CONFORMER

YOKO SHIMOZONO, SHUN-ICHI ISHIUCHI, MASAAKI FUJII, Chemical Resources Laboratory, Tokyo Institute of Technology, 4259, Nagatsuta-cho, Midori-ku, Yokohama 226-8503 Japan; and KOICHI TSUKIYAMA, Department of Chemistry, Faculty of Science, Tokyo University of Science, 1-3 Kagurazaka, Shinjuku, Tokyo 162-8601 Japan.

TF08 15 min 3:47
POLARIZED MATRIX INFRARED SPECTRA OF CYCLOPENTADIENONE

THOMAS K. ORMOND, ADAM M. SCHEER, G. BARNEY ELLISON, Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO 80309-0215; MARK R. NIMLOS, Center for Renewable Chemical Technologies & Materials, NREL, 1617 Cole Blvd., Golden, CO 80401; JOHN W. DAILY, Department of Mechanical Engineering, University of Colorado, Boulder, CO 80309-0427; JOHN F. STANTON, Institute for Theoretical Chemistry, Department of Chemistry, University of Texas, Austin, TX 78712.

TF09 15 min 4:04
MIXED HELICES IN THE GAS PHASE: CONFORMATION-SPECIFIC UV AND IR SPECTROSCOPY OF POLYGLYCINE Z-(GLY)ₙ (n=1,3,5)

JACOB C. DEAN and TIMOTHY S. ZWIER, Department of Chemistry, Purdue University, West Lafayette, IN 47907.

TF10 15 min 4:21
UTILIZING FORCE FIELD METHODS TO EXPLORE POTENTIAL ENERGY LANDSCAPES OF FLEXIBLE BIOMOLECULES

ZACHARY S. DAVIS, Department of Chemistry, Purdue University, West Lafayette, Indiana 47907; JOANNE M. CARR, IVAN Y. W. TAN, DAVID J. WALES, Cambridge University Center for Computational Chemistry, Lensfield, Cambridge, United Kingdom CB2 1EW; TIMOTHY S. ZWIER, Department of Chemistry, Purdue University, West Lafayette, Indiana 47907.

TF11 10 min 4:38
BINDING OF Na⁺ AND K⁺ TO THE HEADGROUP OF PALMITIC ACID MONOLAYERS STUDIED BY VIBRATIONAL SUM FREQUENCY GENERATION SPECTROSCOPY

ZISHUAI HUANG and HEATHER C. ALLEN, Department of Chemistry and Biochemistry, The Ohio State University, 100 W. 18th Ave., Columbus, OH, 43210.
CONFORMATIONAL AND STRUCTURAL STUDIES OF ISOPROPYLAMINE FROM TEMPERATURE DEPENDENT RAMAN SPECTRA OF XENON SOLUTIONS AND AB INITIO CALCULATIONS

JOSHUA J. KLAASSEN, IKHLAS D. DARKHALIL, JAMES R. DURIG, Department of Chemistry, University of Missouri-Kansas City, Kansas City, MO 64110, USA.
TG. ELECTRONIC
TUESDAY, JUNE 19, 2012 – 1:30 PM
Room: 170 MATH ANNEX

Chair: JOSH BARABAN, Massachusetts Institute of Technology, Cambridge, Massachusetts

TG01 15 min 1:30
LASER INDUCED FLUORESCENCE SPECTROSCOPY SiCN : ROTATIONAL ANALYSIS OF THE A 2∆ – X 2Π TRANSITION

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

TG02 10 min 1:47
IMPROVED EXPERIMENTAL LINE POSITIONS FOR THE (1,1) BAND OF THE b1Σ+ - X3Σ− TRANSITION OF O2 BY INTRACAVITY LASER ABSORPTION SPECTROSCOPY

LEAH C. O’BRIEN, Department of Chemistry, Southern Illinois University, Edwardsville, IL 62026-1652; EMILY C. O’BRIEN, JAMES J. O’BRIEN, Department of Chemistry & Biochemistry and Center for NanoScience, University of Missouri, St. Louis, MO 63121-4400.

TG03 15 min 1:59
SPECTROSCOPY OF CuN IN THE NEAR INFRARED BY INTRACAVITY LASER ABSORPTION SPECTROSCOPY

LEAH C. O’BRIEN, KAITLIN A. WOMACK, Department of Chemistry, Southern Illinois University, Edwardsville, IL 62026-1652; JAMES J. O’BRIEN, Department of Chemistry & Biochemistry and Center for NanoScience, University of Missouri, St. Louis, MO 63121-4400.

TG04 15 min 2:16
THE SOLUTION TO THE ELECTRONIC SPECTRUM OF THE CHLORINE CATION (Cl2⁺)

MOHAMMED A. GHARAIBEH and DENNIS J. CLOUTHIER, Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055; APOSTOLOS KALEMOS, National and Kapodistrian University of Athens, School of Natural Sciences, Department of Chemistry, Laboratory of Physical Chemistry, P.O. Box 64 004, 157 10 Zografou, Athens, Greece; ROBERT W. FIELD, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139.

TG05 15 min 2:33
THE VISIBLE SPECTRUM of NICKEL DIOXIDE, NiO2

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

Intermission
TG06

CAVITY RINGDOWN ABSORPTION SPECTRUM OF THE $T_1 (n, \pi^*) \leftarrow S_0$ TRANSITION OF ACROLEIN: ANALYSIS OF THE $0_0^+$ BAND ROTATIONAL CONTOUR

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

TG07

COMPUTATIONAL APPROACHES TO THE DETERMINATION OF THE MOLECULAR GEOMETRY OF ACROLEIN IN ITS $T_1 (n, \pi^*)$ STATE

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

TG08

CONSISTENT ASSIGNMENTS OF THE VIBRATIONS OF SUBSTITUTED BENZENES

ADRIAN M. GARDNER and TIMOTHY G. WRIGHT, School of Chemistry, University of Nottingham, University Park, Nottingham, NG7 2RD, UK.

TG09

ELECTRONIC AND PHOTOELECTRON SPECTROSCOPY OF TOLUENE

ADRIAN M. GARDNER, ALISTAIR M. GREEN, VICTOR TAMÉ-REYES and TIMOTHY G. WRIGHT, School of Chemistry, University of Nottingham, University Park, Nottingham, NG7 2RD, UK.

TG10

RESONANCE ENHANCED MULTIPHOTON IONIZATION (REMPI) SPECTROSCOPY OF WEAKLY BOUND COMPLEXES

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

TG11

CONFORMATION-SPECIFIC INFRARED AND ULTRAVIOLET SPECTROSCOPY OF $\alpha$-METHYLBENZYL RADICAL: PROBING THE STATE-DEPENDENT EFFECTS OF METHYL ROCKING AGAINST A RADICAL SITE

NATHANIEL M. KIDWELL, DEEPALE N. MEHTA, and TIMOTHY S. ZWIER, Department of Chemistry, Purdue University, West Lafayette, IN 47907-2084; NEIL J. REILLY, DAMIAN L. KOKKIN, and MICHAEL C. McCARTHY, Harvard-Smithsonian Center for Astrophysics, 60 Garden St., Cambridge, MA 02138, and School of Engineering & Applied Sciences, Harvard University, 29 Oxford St., Cambridge, MA 02138.

TG12

VIBRONIC SPECTROSCOPY OF PHENYLVINYLNITRILE

DEEPALE N. MEHTA, POLINA NAVOTNAYA, ALEX PAROBEK, RACHEL CLAYTON, VANESA VAQUERO VARA, and TIMOTHY S. ZWIER, Department of Chemistry, Purdue University, West Lafayette, IN 47907-2084 U.S.A.
<table>
<thead>
<tr>
<th>Session</th>
<th>Time</th>
<th>Title</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>TH01</td>
<td>15 min 1:30</td>
<td>PROTIC ACID HYDROGEN BONDING IN CHLOROFLUOROETHYLENES: THE HYDROGEN FLUORIDE-VINYL CHLORIDE COMPLEX</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>TH02</td>
<td>15 min 1:47</td>
<td>BROADBAND CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE SPECTROSCOPY AND MOLECULAR STRUCTURE OF THE ARGON-(Z)-1-CHLORO-2-FLUOROETHYLENE COMPLEX</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>TH03</td>
<td>15 min 2:04</td>
<td>ROTATIONAL SPECTRUM OF Ar...PROPARGYL ALCOHOL COMPLEX</td>
<td>DEVENDRA MANI, ABHISHEK SHAHI and E. ARUNAN, Department of Inorganic and Physical Chemistry, Indian Institute of Science Bangalore, India-560012.</td>
</tr>
<tr>
<td>TH04</td>
<td>15 min 2:21</td>
<td>ROTATIONALLY-RESOLVED SPECTRA OF 2-METHYLFURAN FROM THE CM-WAVE TO THE FAR INFRARED</td>
<td>STEVEN T. SHIPMAN and IAN A. FINNERAN, Division of Natural Sciences, New College of Florida, Sarasota, FL 34243; SUSANNA L. WIDICUS WEAVER, Department of Chemistry, Emory University, Atlanta, GA 30322; JENNIFER VAN WIJNGAARDEN, Department of Chemistry, University of Manitoba, Winnipeg MB R3T 2N2 Canada.</td>
</tr>
<tr>
<td>TH05</td>
<td>15 min 2:38</td>
<td>THE FOURIER TRANSFORM MICROWAVE (FTMW) SPECTRA OF CYCLOHEXENE OXIDE AND ITS ARGON COMPLEX</td>
<td>DANIEL J. FROHMAN, STEWART E. NOVICK, and WALLACE C. PRINGLE, Department of Chemistry, Wesleyan University, 52 Lawn Ave., Middletown, CT 06459-0180.</td>
</tr>
<tr>
<td>TH06</td>
<td>15 min 2:55</td>
<td>MICROWAVE SPECTRA OF DEUTERIUM ISOTOPOLOGUES OF cis-HEXATRIENE</td>
<td>NORMAN C. CRAIG, HANNAH A. FUSON, HENGFENG TIAN, and HERMAN VAN BESIEN, Department of Chemistry and Biochemistry, Oberlin College, Oberlin, OH 44074; ANDREW A. CONRAD AND MICHAEL J. TUBERGEN, Department of Chemistry, Kent State University, Kent, OH 44242.</td>
</tr>
</tbody>
</table>
TH07 15 min 3:12
THE CONFORMATIONS AND STRUCTURES OF 1H-NONAFLUOROBUTANE

JOSEPH A. FOURNIER, ROBERT K. BOHN, Dept. of Chemistry, Univ. of Connecticut, Storrs, CT 06269-3060; JOHN A. MONTGOMERY, JR., Dept. of Physics, Univ. of Connecticut, Storrs, CT 06269-3046.

TH08 15 min 3:29
ROTATIONAL SPECTRA AND STRUCTURES OF THE MONO- AND DI-FLUORINATED PYRIDINES

CODY W. VAN DIJK, MING SUN AND JENNIFER VAN WIJNGAARDEN, Department of Chemistry, University of Manitoba, Winnipeg MB R3T 2N2 Canada.

Intermission

TH09 15 min 4:00
MILLIMETER AND SUBMILLIMETER-WAVE SPECTRUM OF AMINOACETONITRILE (NH₂CH₂CN)

YUTA MOTOKI, YUKARI TSUNODA, HIROYUKI OZEKI, Department of Environmental Science, Toho University, 2-2-1 Miyama, Funabashi, 274-8510, Japan; KAORI KOBAYASHI, Department of Physics, University of Toyama, 3190 Gofuku, Toyama, 930-8555, Japan.

TH10 15 min 4:17
PERTURBATIONS AND VIBRATIONAL ENERGIES IN ACRYLONITRILE FROM GLOBAL ANALYSIS OF ITS MM-WAVE TO THz ROTATIONAL SPECTRUM

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.

TH11 15 min 4:34
STRUCTURE AND ROTATIONAL DYNAMICS OF ISOAMYL ACETATE AND METHYL PROPIONATE STUDIED BY MICROWAVE SPECTROSCOPY


TH12 15 min 4:51
ROTATIONAL ENERGIES IN VARIOUS TORSIONAL LEVELS OF CH₂DOH²

L. H. COUDERT, A. EL HILALI, LISA, CNRS/Universités Paris Est et Paris Diderot, 61 Avenue du Général de Gaulle, 94010 Créteil, France; L. MARGULES, R. A. MOTIYENKO, Laboratoire PhLAM, UMR 8523 CNRS, Bât. P5, Université des Sciences et Technologies de Lille 1, 59655 Villeneuve d’Ascq Cedex, France; and S. KLEE, Physikalisch-Chemisches Institut, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany.

²Work supported by the CNES, the INSU program PCMI, and the ANR-08-BLAN-0225 and ANR-08-BLAN-0054 contracts.
TH13
15 min 5:08

INTENSITIES IN THE ROTATIONAL-TORSIONAL SPECTRUM OF METHANOL

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

TH14
15 min 5:25

ROTATIONAL SPECTRUM OF NEOPENTYL ALCOHOL, (CH₃)₃CCH₂OH

ZBIGNIEW KISIEL, LECH PSZCZÓŁKOWSKI, Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warszawa, Poland; ZHIFENG XUE, MARTIN A. SUHM, Institut für Physikalische Chemie, Universität Göttingen, Tammannstr. 6, 37077 Göttingen, Germany.
TI01 15 min 1:30
MODERATE RESOLUTION JET COOLED CAVITY RINGDOWN SPECTRA OF THE $\tilde{A}$ STATE OF NO$_3$ RADICAL

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

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

TI02 15 min 1:47
HIGH RESOLUTION JET COOLED CAVITY RINGDOWN SPECTROSCOPY OF THE $\tilde{A}$ STATE $3\tilde{0}$ BAND OF THE NO$_3$ RADICAL

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

TI03 10 min 2:04
FTIR SPECTROSCOPY OF THE $\nu_4$ BANDS OF $^{14}$NO$_3$ and $^{15}$NO$_3$

R. FUJIMORI, N. SHIMIZU, J. TANG, K. KAWAGUCHI, Department of Chemistry, Faculty of Science, Okayama University, 3-1-1, Tsushima-Naka, Okayama 700-8530, Japan; T. ISHIWATA, Graduate School of Information Sciences, Hiroshima City University, 3-4-1 Otsuka-Higashi, Hiroshima 731-3194, Japan.

TI04 15 min 2:16
FTIR SPECTRUM AND PERTURBATION ANALYSIS OF THE $\nu_2$ BAND OF $^{15}$NO$_3$

N. SHIMIZU, R. FUJIMORI, J. TANG, K. KAWAGUCHI, Department of Chemistry, Faculty of Science, Okayama University, 3-1-1, Tsushima-Naka, Okayama 700-8530, Japan; T. ISHIWATA, Graduate School of Information Sciences, Hiroshima City University, 3-4-1 Otsuka-Higashi, Hiroshima 731-3194, Japan.

TI05 15 min 2:33
DISPERSED FLUORESCENCE SPECTROSCOPY OF THE $\tilde{B} 2E' - \tilde{X} 2A_2$ TRANSITION OF NO$_3$

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

TI06 15 min 2:50
ENERGY LEVELS OF THE NITRATE RADICAL BELOW 2000 CM$^{-1}$

J.F. STANTON AND C.S. SIMMONS, Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, TX 78712.
OXYGEN-18 STUDIES OF HOCO AND HONO FORMATION

Oscar Martínez, Jr., 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.

A UV+VUV MULTIPHOTON IONIZATION SCHEME FOR OH RADICALS

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

A UV+VUV MULTIPHOTON IONIZATION SCHEME FOR OH RADICALS

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

This research was supported by the Office of Basic Science of the Department of Energy.

CONFIRMED ASSIGNMENTS OF ISOMERIC DIMETHYLBENZYL RADICALS GENERATED BY CORONA DISCHARGE

Young Wook Yoon, Sang Kuk Lee, Department of Chemistry, Pusan National University, Pusan 609-735, Korea.

CAVITY-RINGDOWN SPECTROSCOPY OF THE VIBRONICALLY MIXED $^2A_2 - ^2B_2$ EXCITED STATES OF THE BENZYL RADICAL AND THE $^12A_2 \leftrightarrow ^2B_1$ TRANSITION OF THE PHENOXY RADICAL IN A SUPERSONIC JET EXPANSION

Michael N. Sullivan, Keith Freel, J. Park, M.C. Lin, and Michael C. Heaven, Department of Chemistry, Emory University, Atlanta, GA 30322.

THE CYCLOPENTADIENYL RADICAL REVISITED: THE EFFECTS OF ASYMMETRIC DEUTERATION OF JAHN-TELLER MOLECULES

Samantha Strom, Jinjun Liu, University of Louisville, Department of Chemistry, Louisville, KY 40292.

THE PHENALENYL FREE RADICAL - A JAHN-TELLER-HERZBERG-TELLER D3H PAH

G. D. O’Connor, T. P. Troy, D. A. Roberts, N. Chalyavi, B. Fü克莱, M. J. Crossley, K. Nauta, Tw Schmidt, School of Chemistry, The University of Sydney, NSW 2006, Australia; and J. F. Stanton, Department of Chemistry and Biochemistry, The University of Texas at Austin, 1 University Station A5300, Austin, Texas 78712-0165, United States.

LASER INDUCED FLUORESCENCE STUDY OF $^2B - ^2\tilde{A}$ TRANSITION OF ISOPROPOXY RADICAL

Rabi Chhantyal-Pun, Jinjun Liu, and Terry A. Miller, Laser Spectroscopy Facility, Department of Chemistry, The Ohio State University, 120 W. 18th Avenue, Columbus OH 43210.

Present address: Department of Chemistry, University of Louisville, 2320 South Brook Street, Louisville, Kentucky 40292.
ANALYSIS OF THE ROTATIONALLY-RESOLVED SPECTRA OF ISOPROPOXY RADICAL USING MULTIMODE VIBRONIC CALCULATIONS

DMITRY G. MELNIK, and TERRY A. MILLER, Laser Spectroscopy Facility, Department of Chemistry, The Ohio State University, 120 W. 18th Avenue, Columbus, Ohio 43210; JINJUN LIU, Department of Chemistry, University of Louisville, 2320 South Brook Street, Louisville, Kentucky 40292.
TJ. MINI-SYMPOSIUM: SPECTROSCOPY OF INTERFACES
TUESDAY, JUNE 19, 2012 – 1:30 PM
Room: 2015 MCPHERSON LAB

Chair: ASUKA FUJII, Tohoku University, Sendai, Japan

TJ01  INVITED TALK  30 min  1:30
ION ORGANIZATION AND REVERSED ELECTRIC FIELD AT AIR/AQUEOUS INTERFACES REVEALED BY HETERODYNE-DETECTED SUM FREQUENCY GENERATION SPECTROCOPY

WEI HUA, ZISHUAI HUANG, AARON M. JUBB, HEATHER C. ALLEN, Department of Chemistry, The Ohio State University, 100 W. 18th Ave., Columbus, OH, 43210.

TJ02  15 min  2:05
BROADBAND SUM-FREQUENCY GENERATION SPECTROSCOPY OF HIGH-FREQUENCY VIBRATIONS OF WATER MOLECULES AT SILICA SURFACES

OLEKSANDR ISAIENKO, SATOSHI NIHONYANAGI, DEVIKA SIL and ERIC BORGUET, 1901 North 13th Street, Philadelphia, Pennsylvania, 19122 USA.

TJ03  15 min  2:22
STRUCTURE, ENERGETICS AND FINITE TEMPERATURE OH- STRETCH SPECTROSCOPY OF THE WATER HEXAMER

C. J. TAINTER, J. L. SKINNER, Theoretical Chemistry Institute and Department of Chemistry, University of Wisconsin, Madison, WI 53706.

TJ04  15 min  2:39
INFRARED SPECTROSCOPY OF PROTONATED BENZENE-WATER NANOCLUSTERS: HYDRONIUM, ZUNDEL AND EIGEN AT A HYDROPHOBIC INTERFACE

T. C. CHENG, B. BANDYOPADHYAY, and M. A. DUNCAN, University of Georgia, Dept. of Chemistry, 1001 Cedar St, Athens, GA 30602.

TJ05  15 min  2:56
INFRARED PHOTODISSOCIATION SPECTROSCOPY OF VANADIUM-CARBON DIOXIDE CATIONS: EVIDENCE FOR AN INTRACLUSTER REACTION.

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

Intermission
UV AND IR SPECTROSCOPIC STUDIES OF COLD ALKALI METAL ION-BENZO CROWN ETHER COMPLEXES IN THE GAS PHASE

YOSHIYA INOKUCHI, Department of Chemistry, Faculty of Science, Hiroshima University, Hiroshi-Hiroshima 739-8526, Japan; OLEG V. BOYarkin, Laboratoire de Chimie Physique Moléculaire, École Polytechnique Fédérale de Lausanne, Lausanne CH-1015, Switzerland; RYOJI KUSAKA, Department of Chemistry, Faculty of Science, Hiroshima University, Hiroshi-Hiroshima 739-8526, Japan; TAKEHARU HAINO, Department of Chemistry, Faculty of Science, Hiroshima University, Hiroshi-Hiroshima 739-8526, Japan; TAKAYUKI EBATA, Department of Chemistry, Faculty of Science, Hiroshima University, Hiroshi-Hiroshima 739-8526, Japan; and THOMAS R. RIZZO, Laboratoire de Chimie Physique Moléculaire, École Polytechnique Fédérale de Lausanne, Lausanne CH-1015, Switzerland.

GAS PHASE HYDRATION OF MODEL PEPTIDE CHAINS: FAR/MID INFRARED SIGNATURE OF WATER INTERMOLECULAR MOTIONS IN THE MONOHYDRATE

M. CIRTOG, Y. LOQUAIS, V. BRENNER, B. TARDIVEL, M. MONS, CEA, IRAMIS, SPAM, Lab. Francis Perrin, URA 2453, F-91191, Gif-sur-Yvette, France; E. GLOAGUEN, CNRS, INC & INP, Lab. Francis Perrin, URA 2453, F-91191, Gif-sur-Yvette, France; A. M. RIJS, Institute for Molecules and Materials, Radboud University Nijmegen, Toernooiveld 7, 6525 ED Nijmegen, the Netherlands.

IR SPECTROSCOPY OF Au--(CO)₉ CLUSTERS: STRONG CLUSTER SIZE DEPENDENCE OF METAL-LIGAND INTERACTION

BENJAMIN J. KNURR and J. MATTHIAS WEBER, JILA, NIST and Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO 80309.

THE THZ SPECTRUM OF LANTHANIDE AND TRANSITION METAL HALIDES - EFFECTS ON THE WATER SPECTRUM

G. SCHWAAB, VINAY SHARMA AND MARTINA HAVENITH, Physical Chemistry II, Department of Chemistry and Biochemistry, Ruhr University Bochum, D-44780 Bochum, Germany.
WA. PLENARY SESSION
WEDNESDAY, JUNE 20, 2012 – 8:30 AM
Room: AUDITORIUM, INDEPENDENCE HALL

Chair: ANNE B. MCCOY, The Ohio State University, Columbus, Ohio

WA01  40 min  8:30
THE ATACAMA LARGE MILLIMETER/SUBMILLIMETER ARRAY (ALMA): EARLY RESULTS

ALWYN WOOTTON, National Radio Astronomy Obsy, 520 Edgemont Rd, Charlottesville, Va 22903.

WA02  40 min  9:15
TERAHERTZ SPECTROSCOPY OF MOLECULES, RADICALS AND IONS USING EVENSON-TYPE TUNABLE FIR SPECTROMETER

FUSAKAZU MATSUSHIMA, Department of Physics, University of Toyama, Gofuku 3190, Toyama 930-8555, Japan.

Intermission

WA03  40 min  10:20
FEMTOSECOND ROTATIONAL RAMAN FOUR-WAVE MIXING SPECTROSCOPY

SAMUEL LEUTWYLER and HANS-MARTIN FREY, Departement für Chemie und Biochemie, Freiestrasse 3, CH-3012 Bern, Switzerland.

WA04  40 min  11:05
CALCULATING RO-VIBRATIONAL SPECTRA USING AN ECKART FRAME

XIAOGANG WANG and TUCKER CARRINGTON, JR., Chemistry Department, Queen’s University, Kingston, Canada.
WF01 15 min 1:30
HIGH RESOLUTION INFRARED SPECTRA OF AR-WATER AND NE-WATER AT 6 µm

X. LIU and Y. XU, Department of Chemistry, University of Alberta, Edmonton, AB T6G 2G2.

WF02 15 min 1:47
DIODE LASER SPECTROSCOPY OF N₂–D₂O COMPLEX IN THE V₂ BEND REGION OF D₂O

SONG LI, RUI ZHENG, YU ZHU, YU YANG, and CHUANXI DUAN, College of Physical Science and Technology, Central China Normal University, Wuhan 430079, China.

WF03 15 min 2:04
ANALYSIS OF THE HIGH-RESOLUTION MID-INFRARED SPECTRUM OF DEUTERATED WATER CLUSTERS

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

WF04 15 min 2:21
OVERTONE VIBRATIONAL SPECTROSCOPY AND DYNAMICS IN H₂–H₂O COMPLEXES: A COMBINED THEORETICAL AND EXPERIMENTAL STUDY

MICHAEL P. ZIEMKIEWICZ, CHRISTIAN PLUETZER, DAVID J. NESBITT, JILA, University of Colorado and National Institute of Standards and Technology, Boulder, Colorado; YOHANN SCRIBANO, CNRS-Université de Bourgogne, Dijon, France; ALEXANDRE FAUROE, CNRS, Institut de Planétologie et d’Astrophysique de Grenoble(IPAG), France; AD VAN DER AVOIRD, Radboud University, 6525 AJ Nijmegen, The Netherlands.

WF05 15 min 2:38
OVERTONE VIBRATIONAL SPECTROSCOPY AND DYNAMICS IN H₂–H₂O COMPLEXES: A COMBINED THEORETICAL AND EXPERIMENTAL STUDY

MICHAEL P. ZIEMKIEWICZ, CHRISTIAN PLUETZER and DAVID J. NESBITT, JILA, University of Colorado and National Institute of Standards and Technology, Boulder, Colorado, USA; YOHANN SCRIBANO, CNRS-Université de Bourgogne, Dijon, France; ALEXANDRE FAUROE, CNRS, Institut de Planétologie et d’Astrophysique de Grenoble(IPAG), France; and AD VAN DER AVOIRD, Radboud University, Nijmegen, The Netherlands.

Intermission
WF06 15 min 3:10
INFRARED SPECTRA OF He-, Ne-, AND Ar-C$_2$D$_2$ COMPLEXES

M. REZAI, 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; BERTA FERNÁNDEZ, Department of Physical Chemistry and Center for Research in Biological Chemistry and Molecular Materials (CIQUS), University of Santiago de Compostela, E-15782 Santiago de Compostela, Spain; DAVID FARRELLY, Department of Chemistry and Biochemistry, Utah State University, Logan, UT 84322-0300.

WF07 15 min 3:27
COMBINATION BANDS OF THE NONPOLAR N$_2$O DIMER AND INFRARED SPECTRA OF (C$_2$D$_4$)$_2$ AND (C$_2$D$_4$)$_3$ USING A QUANTUM CASCADE LASER

M. REZAEI, 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; K.H. MICHAELIAN, Natural Resources Canada, CANMET Western Research Center, 1 Oil Patch Drive, Suite A202 Devon Alberta T9G 1A8, Canada.

WF08 15 min 3:44
HIGH RESOLUTION OVERTONE SPECTROSCOPY OF ACETYLENE-WATER VAN DER WAALS COMPLEXES


WF09 10 min 4:01
HIGH RESOLUTION INFRARED SPECTRA OF JET-COOLED FORMAMIDE AND FORMAMIDE DIMER IN THE C=O STRETCH REGION

FUMIE X. SUNAHORI, YUNJIE XU, Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada, T6G 2G2.

WF10 15 min 4:13
ANALYSIS OF AB INITIO NORMAL-MODE DISPLACEMENT VECTORS ALONG THE INTERNAL ROTATION PATH FOR THE THREE C-H STRETCHING VIBRATIONS IN METHANOL

LI-HONG XU, RONALD M. LEES, Centre for Laser, Atomic and Molecular Sciences (CLAMS) Physics Department University of New Brunswick, 100 Tucker Park Road, Saint John, NB, Canada E2L 4L5; JON T. HOUGEN, Sensor Sciences Division, National Institute of Standards and Technology, Gaithersburg, MD 20899-8441.

WF11 15 min 4:30
TWO MODEL HAMILTONIANS FOR TORSION-INVERSION TUNNELING IN THE CH-STRETCH VIBRATIONALLY EXCITED STATES OF METHYLAMINE

MAHESH B DAWADI, AND DAVID S PERRY, Department of Chemistry, The University of Akron, OH 44325-3601.

WF12 15 min 4:47
ELUCIDATING THE COUPLING IN THE CH STRETCH SPECTRAL REGION

EVAN G. BUCHANAN and TIMOTHY S. ZWIER, Department of Chemistry, Purdue University, West Lafayette, IN 47907-2804; EDWIN L. SIBERT, Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706-1322.
WG01 15 min 1:30
UNGERADE POLYADS IN THE 45800 – 46500 CM\(^{-1}\) REGION OF THE S\(_1\) STATE OF C\(_2\)H\(_2\)


WG02 15 min 1:47
IDENTIFICATION OF NEW CIS VIBRATIONAL LEVELS IN THE S\(_1\) STATE OF C\(_2\)H\(_2\)

J. H. BARABAN, P. B. CHANGALA, R. G. SHAVER, 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.

WG03 15 min 2:04
UNUSUAL ANHARMONICITIES IN ISOMERIZING SYSTEMS: THE S\(_1\) STATE OF C\(_2\)H\(_2\)

J. H. BARABAN, R. W. FIELD, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139, USA; J. F. STANTON, Institute for Theoretical Chemistry, Departments of Chemistry and Biochemistry, The University of Texas at Austin, Austin, Texas 78712; A. J. MERER, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan.

WG04 15 min 2:21
UNKNOWN BANDS OBSERVED IN THE 266 NM PHOTOLYSIS OF IODOMETHANES

JIA-JEN DU, CHIA-HSIN CHEN, and BOR-CHEN CHANG, Department of Chemistry, National Central University, 300 Jhongda Road, Jhongli 32001, Taiwan.

WG05 15 min 2:38
UV AND 532 NM PHOTODISSOCIATION OF O-NITROTOLUENE: DETECTION OF ELECTRONICALLY EXCITED NITRIC OXIDE IN NITROGEN AND ARGON

HELENA DIEZ-Y-RIEGA and HERGEN EILERS, Applied Sciences Laboratory, Institute for Shock Physics, Washington State University, Spokane, WA 99210-1495, USA.

WG06 15 min 2:55
FLUORESCENCE EMISSION AND EXCITATION SPECTRA OF PHOTO-FRAGMENTED NITROBENZENE.

CHRISTOPHER J. LUE, CHAKREE TANJAROON, J. BRUCE JOHNSON, SUSAN D. ALLEN, SCOTT W. REEVE, Arkansas Center for Laser Applications and Science and Department of Chemistry and Physics, P.O. Box 419 State University, AR 72467.
MIMICKING TRIMERIC INTERACTIONS IN THE AROMATIC SIDE CHAINS OF THE PROTEINS: A GAS PHASE STUDY OF INDOLE...(PYRROLE)$_2$ HETEROTRIMER

ALOKE DAS and SUMIT KUMAR, Indian Institute of Science Education and Research, 900 NCL Innovation Park, Dr. Homi Bhabha Road, Pune-411008, Maharashtra, India.

Intermission

VIBRONIC COUPLING IN A FLEXIBLE BICHROMOPHORE: 1,2-DIPHENOXYETHANE

EVAN G. BUCHANAN and TIMOTHY S. ZWIER, Department of Chemistry, Purdue University, West Lafayette, IN 47907-2804; DAVID F. PLUSQUELLIC, National Institute of Standards and Technology, Radiation and Biomolecular Physics Division, Gaithersburg, MD 20899-8443.

COMPREHENSIVE SPECTROSCOPIC CHARACTERIZATION OF MODEL AROMATIC SUBSTITUENTS OF LIGNIN

JACOB C. DEAN, VANESA VAQUERO VARA, KELLY M HOTOPP, BRIAN C. DIAN and TIMOTHY S. ZWIER, Department of Chemistry, Purdue University, West Lafayette, IN 47907.

SPECTROSCOPIC INVESTIGATION OF LIGNIN LINKAGES: UV AND IR SIGNATURES OF PRIMARY DILIGNOLS

JACOB C. DEAN, PATRICK S. WALSH, JOSEPH R. GORD, BIDYUT BISWAS, P. V. RAMACHANDRAN, and TIMOTHY S. ZWIER, Department of Chemistry, Purdue University, West Lafayette, IN 47907.

SYNERGISTIC TWO-PHOTON ABSORPTION ENHANCEMENT IN PHOTOSYNTHETIC LIGHT HARVESTING

KUO-MEI CHEN, YU-WEI CHEN and TING-FONG GAO, National Sun Yat-sen University, Kaohsiung, Taiwan, Republic of China.

EMISSION AND fs/ns-TRANSIENT ABSORPTION OF ORGANOMETALLIC COMPLEXES BOUND TO A DINUCLEAR METAL CENTER

CHRISTOPHER B. DURR, SAMANTHA E. BROWN-XU and MALCOLM H. CHISHOLM, The Ohio State University, Department of Chemistry and Biochemistry, Columbus, Ohio 43210.

TUNING FÖRESTER RESONANCE ENERGY TRANSFER (FRET) IN DNA-FLUOROPHORE CONSTRUCTS

MARVIN POLLUM and CARLOS E. CRESPO HERNÁNDEZ, Department of Chemistry and Center for Chemical Dynamics, Case Western Reserve University, Cleveland, OH 44106.
WH01 15 min 1:30

A CONFUSION LIMITED SPECTRAL SURVEY OF ORION


WH02 15 min 1:47

HERSCHEL OBSERVATIONS OF EXTRAORDINARY SOURCES (HEXOS).

J. L. NEILL, N. R. CROCKETT, E. A. BERGIN, Department of Astronomy, University of Michigan, 500 Church St, Ann Arbor, MI 48109, USA; and THE HEXOS TEAM, http://www.hexos.org/team.php/.

WH03 15 min 2:04

UNRAVELING THE MYSTERIES OF COMPLEX INTERSTELLAR ORGANIC CHEMISTRY USING HERSCHEL/HIFI SPECTRAL LINE SURVEYS

SHIYA WANG, MARY L. RADHUBER, JACOB C. LAAS, JAY A. KROLL, JAMES L. SANDERS, AND SUSANNA L. WIDICUS WEAVER, Department of Chemistry, Emory University, Atlanta, GA 30322; DARIUSZ C. LIS, Division of Physics, Mathematics, and Astronomy, California Institute of Technology, Pasadena, CA 91125; ERIC HERBST, Departments of Chemistry, Physics, and Astronomy, University of Virginia, Charlottesville, VA 22904.

WH04 15 min 2:21

ANALYSIS OF OH⁺, H₂O⁺, AND H₃⁺ IN A DIFFUSE MOLECULAR CLOUD TOWARD W51

NICK INDRIOLO, DAVID A. NEUFELD, Department of Physics & Astronomy, Johns Hopkins University, Baltimore, MD 21218; MARYVONNE GERIN, LERMA, CNRS UMR 8112, 24 rue Lhomond, 75231 Paris Cedex 05, France; THOMAS R. GEBALLE, Gemini Observatory, Hilo, HI 96720.

WH05 15 min 2:38

OBSERVATIONS OF OH⁺ AND H₂O⁺ ACROSS THE GALAXY WITH HERSCHEL

NICK INDRIOLO, DAVID A. NEUFELD, Department of Physics & Astronomy, Johns Hopkins University, Baltimore, MD 21218; MARYVONNE GERIN, LERMA, CNRS UMR 8112, 24 rue Lhomond, 75231 Paris Cedex 05, France; THE PRISMAS CONSORTIUM..

WH06 15 min 2:55

MORPHOLOGY OF GAS IN THE GALACTIC CENTER FROM SPECTROSCOPY OF H₃⁺

TA KESH I OKA, Department of Astronomy and Astrophysics and Department of Chemistry, University of Chicago, Chicago, IL 60637; THOMAS R. GEBALLE, Gemini Observatory, Hilo, HI 96720; NICK INDRIOLO, Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD 21218; MIWA GOTO, Universitäts-Sternwarte München, Müßlījenchen Germany 81679.
Intermission

**WH07**  
15 min 3:30  
SPECTRUM AND DIFFUSE INTERSTELLAR BANDS TOWARD HERSCHEL 36 EXCITED BY DUST EMIS- 
SION  
JULIE DAHLSTROM, Carthage College; TAKESHI OKA, Department of Astronomy and Astrophysics and 
Department of Chemistry, University of Chicago, Chicago, IL 60637; SEAN JOHNSON, DANIEL E. WELTY, 
LEW M. HOBBS, and DONALD G. YORK, Department of Astronomy and Astrophysics, University of 
Chicago, Chicago, IL 60637.

**WH08**  
15 min 3:47  
MOLECULAR CONTENT OF THE HELIX NEBULA  
L.N. ZACK, N. R. ZEIGLER, and L.M. ZIURYS, Department of Chemistry, Department of Astronomy, and 
Steward Observatory, University of Arizona, Tucson, AZ 85721.

**WH09**  
15 min 4:04  
THE MOLECULAR CONTENT OF PLANETARY NEBULAE: THE DUMBBELL AND THE RED SPIDER  
JESSICA L. EDWARDS, LUCY M. ZIURYS, ERIN G. COX, NEVILLE J. WOOLF, Department of Chem-
istry and Biochemistry, Department of Astronomy, Steward Observatory, The University of Arizona, Tucson, 
AZ 85721.

**WH10**  
15 min 4:21  
SPECTRAL LINE SURVEYS OF YOUNG STELLAR OBJECTS USING THE CALTECH SUBMILLIMETER OBSER-
VATORY  
JAMES L. SANDERS III, MARY L. RADHUBER, JACOB C. LAAS, JAY A. KROLL and SUSANNA L. WIDICUS WEAVER, Emory University, Department of Chemistry, Atlanta, Georgia 30322.

**WH11**  
15 min 4:38  
IDENTIFYING LOCAL CHEMICAL ENVIRONMENTS IN ORION KL BY BROADBAND DATA CUBE ANALYSIS  
BRENT J. HARRIS, CLARE YANG, KEVIN K. LEHMANN, BROOKS H. PATE, Department of Chemistry, 
University of Virginia, Charlottesville, VA 22904; ANTHONY J. REMIJAN, CRYSTAL L. BROGAN, Na-
tional Radio Astronomy Observatory, Charlottesville, VA 22904.

**WH12**  
15 min 4:55  
THE ROTATIONAL SPECTRUM OF HCl+  
HARSHAL GUPTA, B. J. DROUIN, J. C. PEARSON, Jet Propulsion Laboratory, California Institute of 
Technology, 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 2012 © California Institute of Technology. All rights reserved.*
WH13  15 min  5:12

**HERSCHEL/HIFI IDENTIFICATION OF HCl⁺ IN THE INTERSTELLAR MEDIUM**

M. DE LUCA, M. GERIN, E. FALGARONE, LERMA-LRA, UMR 8112 du CNRS, Observatoire de Paris, École Normale Supérieure, UPMC & UCP, 24 rue Lhomond, 75231, Paris Cedex 05, France; HARSHAL GUPTA, B. J. DROUIN, J. C. PEARSON, Jet Propulsion Laboratory, California Institute of Technology*, Pasadena, CA 91109; D. A. NEUFELD, The Johns Hopkins University, Baltimore, MD 21218; D. C. LIS, R. MONJE, T. G. PHILLIPS, California Institute of Technology, Pasadena, CA 91125; D. TEYSSIER, European Space Astronomy Centre, ESA, Madrid, Spain; J. R. GOICOECHEA, B. GODARD, T. A. BELL, Centro de Astrobiología (CSIC/INTA), Madrid, Spain; A. COUTENS, Université de Toulouse, UPS-OMP, IRAP, Toulouse, France.

*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 2012 © California Institute of Technology. All rights reserved.

WH14  15 min  5:29

**INTEGRAL FIELD SPECTROSCOPY OF THE RED RECTANGLE: UNRAVELING THE CARRIER OF THE RRBs IN 2D**

D. L. KOKKIN, IRAP; Université de Toulouse, UPS; CNRS; 9 Av. Colonel Roche, BP 44346, F-31028 Toulouse Cedex 4, France; R. G. SHARP, Research School of Astronomy & Astrophysics, Mount Stromlo Observatory, Cotter Road, Weston Creek, ACT 2611, Australia; M. NAKAJIMA, Department of Chemical System Engineering, School of Engineering, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan; T. W. SCHMIDT, School of Chemistry, The University of Sydney, New South Wales, 2006, Australia.
WI. RADICALS AND IONS
WEDNESDAY, JUNE 20, 2012 – 1:30 PM
Room: 1015 MCPHERSON LAB

Chair: KENTAROU KAWAGUCHI, Okayama University, Okayama, Japan

WI01 15 min 1:30
THE PREDICTED INFRARED SPECTRUM OF THE HYPERMETALLIC MOLECULE CaOCa IN ITS LOWEST TWO ELECTRONIC STATES \( \tilde{X}^1\Sigma^+ \) AND \( \tilde{a}^3\Sigma^+ \)

B. OSTOJIĆ, Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Studentski trg 14-16, 11 000 Belgrade, Serbia; P. R. BUNKER, P. SCHWERDTFEGER, Centre for Theoretical Chemistry and Physics (CTCP), The New Zealand Institute for Advanced Study(NZIAS), Massey University Auckland, Private Bag 102904, North Shore City, 0745 Auckland, New Zealand; ARTUR GERTYCH, PER JENSEN, FB C – Physikalische und Theoretische Chemie, Bergische Universität, D-42097 Wuppertal, Germany.

WI02 15 min 1:47
INTERMOLECULAR INTERACTIONS BETWEEN THE SUPEROXIDE RADICAL AND HYDROGEN FLUORIDE

WAFAQ M. FAWZY, YUCHENG ZHANG, and MAHMOUD ELSAYED, Department of Chemistry, Murray State University, Murray, KY 42071.

WI03 15 min 2:04
INTERMOLECULAR INTERACTIONS BETWEEN URACIL AND REACTIVE SPECIES

SIJIN REN and WAFAQ M. FAWZY, Department of Chemistry, Murray State University, Murray, KY 42071.

WI04 15 min 2:21
A NEW APPROACH TO INVESTIGATE PAH DERIVED CATIONS AS DIB CARRIERS

D. L. KOKKIN, C. MARSHALL, A. BONNAMY, and C. JOBLIN, IRAP; Université de Toulouse, UPS; CNRS; 9 Av. colonel Roche, BP 44346, F-31028 Toulouse cedex 4, France; A. SIMON, LCPQ, Université de Toulouse, UPS; CNRS; 118 Route de Narbonne, 31062 Toulouse Cedex 09, France.

WI05 15 min 2:38
HIGH-RESOLUTION PHOTOELECTRON SPECTROSCOPIC STUDY OF CYCLOPROPENE (c-C_3H_4)

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

WI06 15 min 2:55
SUB-DOPPLER SPECTROSCOPY OF MOLECULAR IONS IN THE MID-INFRARED

JAMES N. HODGES, KYLE N. CRABTREE, Department of Chemistry, University of Illinois, Urbana, IL 61801; BENJAMIN J. McCALL, Departments of Chemistry, Astronomy, and Physics, University of Illinois, Urbana, IL 61801.
THE INFRARED SPECTRUM OF CH$_5^+$ REVISITED

KYLE N. CRABTREE, JAMES N. HODGES, Department of Chemistry, University of Illinois, Urbana, IL 61801; BENJAMIN J. McCALL, Departments of Chemistry, Astronomy, and Physics, University of Illinois, Urbana, IL 61801.

INTERMISSION

INFRARED PHOTODISSOCIATION SPECTROSCOPY OF ALUMINUM BENZENE CATION COMPLEXES

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

STRUCTURES AND SPECTROSCOPIC PROPERTIES CALCULATED FOR C$_6$H$_7^+$ AND ITS COMPLEXES WITH Ne, Ar, N$_2$, OR CO$_2$

P. BOTSCHWINA and R. OSWALD, Institute of Physical Chemistry, University of Göttingen, Tammannstr. 6, D-37077 Göttingen, Germany.

ROVIBRATIONAL STATES OF CIHCl$^{-}$ ISOTOPOMERS: A JOINT THEORETICAL AND SPECTROSCOPIC INVESTIGATION

P. BOTSCHWINA, P. SEBALD, and R. OSWALD, Institute of Physical Chemistry, University of Göttingen, Tammannstr. 6, D-37077 Göttingen, Germany; K. KAWAGUCHI, Department of Chemistry, Okayama University, Tsushimanaka 3-1-1, Okayama 700-8530, Japan.

VIBRONIC SPECTROSCOPY OF JET-COOLED 2-FLUORO-$m$-XYLYL AND 2-CHLORO-$m$-XYLYL RADICALS GENERATED BY CORONA DISCHARGE

YOUNG WOOK YOON, CHANG SOON HUH, SANG KUK LEE, Department of Chemistry, Pusan National University, Pusan 609-735, Korea.

SPECTROSCOPY IDENTIFICATION OF BENZYL-TYPE RADICALS GENERATED BY CORONA DISCHARGE OF PRECURSORS OF MIXED SUBSTITUENTS

YOUNG WOOK YOON, CHANG SOON HUH, SANG KUK LEE, Department of Chemistry, Pusan National University, Pusan 609-735, Korea.

JET-COOLED, BROAD RANGE NEAR-IR SCAN OF REACTIVE INTERMEDIATES USING CAVITY RINGDOWN SPECTROSCOPY

NEAL D. KLINE, TERRANCE J. CODD, MING-WEI CHEN*, And TERRY A. MILLER, Laser Spectroscopy Facility, Department of Chemistry, The Ohio State University, 120 W. 18th Avenue, Columbus, Ohio 43210.

*Present Address: Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL, 61801
SPECTROSCOPIC AND KINETIC MEASUREMENTS OF ORGANIC PEROXY RADICALS BY DUAL-WAVELENGTH CAVITY RING DOWN SPECTROSCOPY

DMITRY G. MELNIK, and TERRY A. MILLER, Laser Spectroscopy Facility, Department of Chemistry, The Ohio State University, 120 W. 18th Avenue, Columbus, Ohio 43210.
**WJ. MINI-SYMPOSIUM: PHOTODETACHMENT AND PHOTOIONIZATION**

**WEDNESDAY, JUNE 20, 2012 – 1:30 PM**

**Room: 2015 MCPHERSON LAB**

**Chair: DONG-SHENG YANG, University of Kentucky, Lexington, Kentucky**

<table>
<thead>
<tr>
<th>WJ01</th>
<th><strong>INVITED TALK</strong></th>
<th>30 min 1:30</th>
</tr>
</thead>
<tbody>
<tr>
<td>HIGH-RESOLUTION PHOTOELECTRON AND PHOTOIONIZATION SPECTROSCOPY</td>
<td></td>
<td></td>
</tr>
<tr>
<td>F. MERKT, Laboratorium für Physikalische Chemie, ETH Zurich, CH 8093 Zurich, Switzerland.</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>WJ02</th>
<th>15 min 2:05</th>
</tr>
</thead>
<tbody>
<tr>
<td>THE GAS-PHASE SPECTROSCOPY STUDY OF ThN and ThN⁺</td>
<td></td>
</tr>
<tr>
<td>I. O. ANTONOV, B. J. BARKER, M. C. HEAVEN, Department of Chemistry, Emory University, Atlanta, GA 30322.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>WJ03</th>
<th>15 min 2:22</th>
</tr>
</thead>
<tbody>
<tr>
<td>MASS-ANALYZED THRESHOLD IONIZATION OF M₂O₂ (M = Ce and Pr)</td>
<td></td>
</tr>
<tr>
<td>LU WU, BENI DANGI, MOURAD ROUJANE, and DONG-SHENG YANG, Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>WJ04</th>
<th>15 min 2:39</th>
</tr>
</thead>
<tbody>
<tr>
<td>PREFERRED METAL BINDING SITE OF ANILINE</td>
<td></td>
</tr>
<tr>
<td>SUDESH KUMARI, BRAD SOHNLEIN AND DONG-SHENG YANG, Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055.</td>
<td></td>
</tr>
</tbody>
</table>

**Intermission**

<table>
<thead>
<tr>
<th>WJ05</th>
<th>15 min 3:10</th>
</tr>
</thead>
<tbody>
<tr>
<td>PHOTOIONIZATION OF ALKALI-DOPED HELIUM NANODROPLETS</td>
<td></td>
</tr>
<tr>
<td>MORITZ THEISEN, FLORIAN LACKNER, GÜNTER KROIS, MARKUS KOCH and WOLFGANG E. ERNST, Institute of Experimental Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>WJ06</th>
<th>15 min 3:27</th>
</tr>
</thead>
<tbody>
<tr>
<td>PHOTOIONIZATION SPECTROSCOPY OF ISOLATED Cr ATOMS IN ULTRACOLD HELIUM NANODROPLETS</td>
<td></td>
</tr>
<tr>
<td>ANDREAS KAUTSCH, MATTHIAS HASEWEND, MARTIN RATSCHEK, MARKUS KOCH, and WOLFGANG E. ERNST, Institute of Experimental Physics, TU Graz, Petersgasse 16, 8010 Graz, Austria.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>WJ07</th>
<th>15 min 3:44</th>
</tr>
</thead>
<tbody>
<tr>
<td>PHOTOIONIZATION OF HIGHLY CHARGED ARGON IONS AND THEIR DIAGNOSTIC LINES</td>
<td></td>
</tr>
<tr>
<td>SULTANA N. NAHAR, Department of Astronomy, The Ohio State University, Columbus, OH 43210.</td>
<td></td>
</tr>
</tbody>
</table>
HIGH-RESOLUTION PFI-ZEKE PHOTOELECTRON SPECTROSCOPY OF Cl₂: THE GROUND (Xᵢ+ 2Πguns) AND FIRST EXCITED (Aᵢ⁺ 2Πguns) ELECTRONIC STATES OF Cl₂⁺

SANDRO MOLLET, and FRÉDÉRIC MERKT, ETH Zürich, Laboratorium für Physikalische Chemie, Wolfgang Pauli-Strasse 10, 8093 Zürich, Switzerland.

ROTATIONALLY RESOLVED PHOTOELECTRON SPECTROSCOPY OF ArXe AND KrXe

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

PROBING THE ADSORPTION OF CARBON MONOXIDE ON TRANSITION METAL CLUSTERS USING IR ACTION SPECTROSCOPY

VIVIKE J. F. LAPOUTRE, JOS OOMENS and JOOST M. BAKKER, FOM Institute Rijnhuizen, Edisonbaan 14, 3439MN Nieuwegein, The Netherlands.
RA01
15 min 8:30
ELECTRONIC TRANSITIONS OF PALLADIUM MONOBORIDE AND PLATINUM MONOBORIDE

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

RA02
15 min 8:47
THE OPTICAL STARK SPECTRUM OF THE $[^{11.9}\Omega=3/2−X^{3}\Pi_{3/2}]$ BAND SYSTEM OF PLATINUM MONOFLUORIDE, PtF

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

RA03
15 min 9:04
X-RAY RESONANT IRRADIATION AND HIGH-Z RADIOSENSITIZATION IN CANCER THERAPY USING PLATINUM NANO-REAGENTS

SULTANA N. NAHAR, Department of Astronomy, The Ohio State University, Columbus, OH 43210; S. LIM, Biophysics Program, The Ohio State University, Columbus, OH 43210; M. MONTENEGRO, Catholic University of Chile; A.K. PRADHAN, Department of Astronomy, Biophysics Program, Chemical Physics, The Ohio State University, Columbus, OH 43210; R. BARTH, Pathology Department, The Ohio State University, Columbus, OH 43210; E. BELL, Radiation Oncology, The Ohio State University, Columbus, OH 43210; C. TURRO, R. PITZER, Department of Chemistry, The Ohio State University, Columbus, OH 43210.

RA04
15 min 9:21
LASER INDUCED FLUORESCENCE SPECTROSCOPY OF SCANDIUM MONOIODIDE

ZHENWU LIAO, MEI YANG, MAN-CHOR CHAN, Department of Chemistry, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong; YE XIA, A. S.-C. CHEUNG, Department of Chemistry, The University of Hong Kong, Pokfulam Road, Hong Kong.

RA05
15 min 9:38
THE SPECTROSCOPY STUDY OF UF AND UF$^+$

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

RA06
15 min 9:55
THE OPTICAL STARK SPECTRUM OF THE $[^{17.8}\Omega^+=X^{3}\Sigma^+]$ BAND OF GOLD MONOFLUORIDE, AuF

RUOHAN ZHANG, CHENGBING QIN, AND TIMOTHY C. STEIMLE, Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287; THOMAS VARBERG, Department of Chemistry, Macalaster College, 1600 Grand Avenue, St. Paul, MN 55105.
Intermission

RA07 15 min 10:30
LASER-INDUCED FLUORESCENCE SPECTROSCOPY OF JET-COOLED NiF: AN INVESTIGATION OF THE \( \Omega \)-TYPE DOUBLING IN THE \( \Omega=1/2 \) STATES OF THE \( 3d^9 \) GROUND ELECTRONIC CONFIGURATION

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

RA08 10 min 10:47
EXOMOL: MOLECULAR LINE LISTS FOR ASTROPHYSICAL APPLICATIONS. A THEORETICAL LINE LIST FOR NICKEL HYDRIDE.

S. N. YURCHENKO, L. LODI, A. KERRIDGE and J. TENNYSON, University College London, Department of Physics and Astronomy, London WC1E 6BT, UK.

RA09 15 min 10:59
LABORATORY MEASUREMENTS OF THE ZEEMAN EFFECT IN THE F–X SYSTEM OF IRON MONOHYDRIDE

PATRICK CROZET, GUILLAUME TOURASSE, AMANDA J. ROSS, LASIM, Université Lyon 1 & CNRS, 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; FRÉDÉRIC PALETOU, Observatoire Midi-Pyrénées (CNRS) 14 Av Edouard Belin, 31400 Toulouse, France; ARTURO LÓPEZ ARISTE, THEMIS Telescope, CNRS UPS 853, C/Vía Lactea s/n, 38200 La Laguna, Tenerife, Spain.

RA10 15 min 11:16
FOURIER TRANSFORM EMISSION SPECTROSCOPY OF THE \( E^2\Pi-X^2\Sigma^+ \) TRANSITIONS OF SrH, SrD AND BaH.

R.S. RAM, Department of Chemistry, University of York, Heslington, York, YO10 5DD, UK; Department of Chemistry, University of Arizona, Tucson, AZ 85721, USA; K. TERESZCHUK, Department of Chemistry, University of York, Heslington, York, YO10 5DD, UK; P.F. BERNATH, Department of Chemistry and Biochemistry, Old Dominion University, Norfolk, VA 23529 USA; Department of Chemistry, University of York, Heslington, York, YO10 5DD, UK; and K.A. WALKER, Department of Physics, University of Toronto, Toronto, Ont., M5S 1A7, Canada.

RA11 15 min 11:33
NEAR INFRARED LASER SPECTROSCOPY OF SCANDIUM MONOBROMIDE

YE XIA, A. S.-C. CHEUNG, Department of Chemistry, The University of Hong Kong, Pokfulam Road, Hong Kong.; ZHENWU LIAO, MEI YANG, MAN-CHOR CHAN, Department of Chemistry, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong.
MEASUREMENT OF HYPERFINE STRUCTURE AND PERMANENT ELECTRIC DIPOLE MOMENTS IN THE ELECTRONIC SPECTRUM OF IRIUM MONOHYDRIDE AND DEUTERIDE

C. LINTON, Physics Department and Centre for Laser, Atomic and Molecular Sciences, University of New Brunswick, Fredericton, NB, Canada E3B 5A3; A. D. GRANGER and A. G. ADAM, Chemistry Department and Centre for Laser, Atomic and Molecular Sciences, University of New Brunswick, Fredericton, NB, Canada E3B 5A3; S. E. FREY, A. LE and T. C. STEIMLE, Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287, USA.
RB. ATMOSPHERIC SPECIES
THURSDAY, JUNE 21, 2012 – 8:30 AM
Room: 170 MATH ANNEX

Chair: V. MALATHY DEVI, College of William and Mary, Williamsburg, Virginia

RB01  15 min  8:30
MULTISPECTRUM FITTING OF FTS AND CRDS SPECTRA SIMULTANEOUSLY

D. CHRIS BENNER, V. MALATHY DEVI, Department of Physics, College of William and Mary, Williamsburg, VA; KEEYON SUNG, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109, U.S.A.; JOSEPH T. HODGES, National Institute of Standards and Technology, Gaithersburg, MD 20899.

RB02  15 min  8:47
CAUSAL CORRELATION FUNCTIONS AND FOURIER TRANSFORMS: APPLICATION IN CALCULATING PRESSURE INDUCED SHIFTS

Q. MA, NASA/Goddard Institute for Space Studies and Department of Applied Physics and Applied Mathematics, Columbia University, 2880 Broadway, New York, NY 10025, USA; R. H. TIPPING, Department of Physics and Astronomy, University of Alabama, Tuscaloosa, AL 35487, USA; N. N. LAVRENTIEVA, V. E. Zuev Institute of Atmospheric Optics SB RAS, 1, Akademichesky Zuev square, Tomsk 634021, Russia.

RB03  15 min  9:04
EVALUATION OF THE EXPERIMENTAL AND THEORETICAL INTENSITIES OF WATER-VAPOR LINES IN THE $2 \mu m$ REGION USING SOLAR-POINTING FTS SPECTRA

I. E. GORDON, L. S. ROTHMAN, Harvard-Smithsonian Center for Astrophysics, Atomic and Molecular Physics Division, Cambridge MA 02138, USA; L. LODI, J. TENNYSON, University College London, Department of Physics and Astronomy, London, UK; G. C. TOON, L. R. BROWN, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109, USA.

RB04  15 min  9:21
THE COF$_2$ HOT BANDS IN THE $\nu_0$ REGION AND THE $2\nu_0$ OVERTONE$^a$

E. A. COHEN, B. J. DROUIN, and L. R. BROWN, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109-8099.

$^a$This work was done at the Jet Propulsion Laboratory, California Institute of Technology under contract with the National Aeronautics and Space Administration.

RB05  15 min  9:38
PHOTO-TAUTOMERIZATION OF ACETALDEHYDE TO VINYL ALCOHOL: A NEW MECHANISM FOR ORGANIC ACID FORMATION IN THE TROPOSPHERE

HIGH RESOLUTION STIMULATED RAMAN SPECTROSCOPY OF CARBON TETRAFLUORIDE CF₄

V. BOUDON, Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR 6303 CNRS-Université de Bourgogne, 9. Av. A. Savary, BP 47870, F-21078 Dijon Cedex, France; D. BERMEJO, R. Z. MARTÍNEZ, Instituto de Estructura de la Materia, CSIC Serrano 123, E-28006 Madrid, Spain.

Intermission

PRELIMINARY MODELING OF CH₃D FROM 4000 TO 4550 cm⁻¹

A. V. NIKITIN, Laboratory of Theoretical Spectroscopy, Institute of Atmospheric Optics, Russian Academy of Sciences, 634055 Tomsk, Russian Federation; LINDA R. BROWN, K. SUNG, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109; M. REY; VI. G. TYUTEREV, Groupe de Spectrométrie Moléculaire et Atmosphérique, UMR CNRS 6089, Université de Reims, U.F.R. Sciences, B.P. 1039, 51687 Reims Cedex 2, France; M. A. H. SMITH, Science Directorate, NASA Langley Research Center, Hampton, VA 23681, USA; A. W. MANTZ, Dept. of Physics, Astronomy and Geophysics, Connecticut College, New London, CT 06320, USA.

SUBMILLIMETER SPECTRUM OF METHYL CHLORIDE: ANALYSIS OF THE ν₃=1 EXCITED STATE

ALISSA P. FISHER, Auburn University; DANE J. PHILLIPS, Kratos Defense and Security Solutions Digital Fusion, 4904 Research Dr., Huntsville, Al, 35805; DENNIS G. WILSON, Massachusetts Institute of Technology; ELIZABETH RHODES, University of Alabama Tuscaloosa; HENRY O. EVERITT, Army Aviation and Missile RD&E Center, Weapon Sciences Directorate, Redstone Arsenal, AL, 35898.

IMPROVED LINE PARAMETERS FOR CH₄ AROUND 1.6 MICRONS

VICTOR GORSHLEV, ANNA SERDYUCHENKO, M. BUCHWITZ, J. BURROWS, University of Bremen, Germany; N. HUMPAGE, J. REMEDIOS, University of Leicester, UK.

ANALYTICAL CHEMICAL SENSING IN THE SUBMILLIMETER/TERAHERTZ SPECTRAL RANGE

BENJAMIN L. MORAN, ALYSSA M. FOSNIGHT, IVAN R. MEDVEDEV, Department of Physics, Wright State University, 3640 Colonel Glenn Highway, Dayton, OH 45435, USA; CHRISTOPHER F. NEESE, Department of Physics, Ohio State University, 191 West Woodruff Ave., Columbus, OH 43210, USA.
RC01 15 min 8:30
CDMS AND JPL MOLECULAR SPECTROSCOPY CATALOGUES IN A COMMON INFRASTRUCTURE: VAMDC

S. SCHLEMMER, C. P. ENDRES, I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany; B.J. DROUIN, S. YU, J.C. PEARSON, Jet Propulsion Laboratory, 4800 Oak Grove Drive, Pasadena, CA 91109; H. S. P. MÜLLER, P. SCHILKE, J. STUTZKI, I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany.

RC02 15 min 8:47
CDMS 2012: A DATABASE WITHIN THE FRAMEWORK OF THE VIRTUAL ATOMIC AND MOLECULAR DATA CENTRE – RECENT DEVELOPMENTS

HOLGER S. P. MÜLLER, C. P. ENDRES, J. STUTZKI, S. SCHLEMMER, I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany.

RC03 15 min 9:04
OBSERVING MOLECULES IN THE INTERSTELLAR MEDIA: THEORETICAL AND EXPERIMENTAL STUDIES OF ENERGY TRANSFER.

LAURENT WIESENFELD, ALEXANDRE FAURE, UJF-Grenoble l/CNRS, Institut de Planétologie et d’Astrophysique de Grenoble (IPAG) UMR 5274, Grenoble, France; FRANÇOIS LIQUE, LOMC – CNRS, Le Havre University, 76058 Le Havre France; and NICOLE FEAUTRIER, LERMA and UMR 8112 of CNRS, Observatoire de Paris-Meudon, 92195 Meudon Cedex, France.

RC04 15 min 9:21
COMPUTATION OF COLLISION-INDUCED ABSORPTION BY SIMPLE MOLECULAR COMPLEXES, FOR ASTROPHYSICAL APPLICATIONS

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.

RC05 15 min 9:38
METHANOL PHOTODISSOCIATION STUDIES USING MILLIMETER AND SUBMILLIMETER SPECTROSCOPY

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

Intermission
TIME-SLICE VELOCITY-MAP ION IMAGING STUDIES OF THE PHOTODISASSOCIATION OF ASTROPHYSICALLY IMPORTANT SMALL MOLECULES IN THE VACUUM ULTRAVIOLET REGION BY RESONANT SUM/DIFFERENCE FOUR-WAVE MIXING

HONG GAO, YU SONG, LEI YANG, JINGANG ZHOU, C. Y. NG, WILLIAM M. JACKSON, Department of Chemistry, University of California, Davis, Davis, CA 95616, USA; YANG PAN, National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, Anhui 230029, P. R. China.

OSCILLATOR STRENGTHS AND PREDISSOCIATION RATES FOR RYDBERG COMPLEXES IN $^{12}$C$^{16}$O BETWEEN 92.9 AND 93.4 NM

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

THE ANALYSIS OF ASTROPHYSICAL ‘WEEDS’ USING 3-D SUBMILLIMETER SPECTROSCOPY

SARAH M. FORTMAN, JAMES P. MCMILLAN, CHRISTOPHER F. NEESE, and FRANK C. DE LUCIA, Department of Physics, 191 W. Woodruff Ave., Ohio State University, Columbus, OH 43210, USA.

COMPUTATIONAL STUDY AND LABORATORY SPECTROSCOPY OF PREBIOTIC MOLECULES PRODUCED BY O($^1$D) INSERTION REACTIONS

BRIAN M. HAYS, BRIDGET A. DEPRINCE, SUSANNA L. WIDICUS WEAVER, Emory University, Department of Chemistry, Atlanta, GA 30322.

HIGH RESOLUTION SPECTROSCOPY OF HEXAMETHYLENETETRAMINE (HMT) $\text{C}_6\text{N}_4\text{H}_{12}$

V. BOUDON, Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR 6303 CNRS-Université de Bourgogne, 9 Av. A. Savary, BP 47870, F-21078 Dijon Cedex, France; O. PIRAL1, Ligne AILES – Synchrotron SOLEIL, L’Orme des Merisiers, F-91192 Gif-sur-Yvette, France.

NUCLEAR SPIN OF H$_3^+$ AND H$_2$ IN DENSE MOLECULAR CLOUDS

KYLE N. CRABTREE, Department of Chemistry, University of Illinois, Urbana, IL 61801; BENJAMIN J. McCALL, Departments of Chemistry, Astronomy, and Physics, University of Illinois, Urbana, IL 61801.

GAS-GRAIN MODELING OF O$_2$ IN INTERSTELLAR CLOUDS

DONGHUI QUAN, Department of Chemistry, Eastern Kentucky University, Richmond, KY 40475; ERIC HERBST, Department of Chemistry, University of Virginia, Charlottesville, VA 22904.
RD. MINI-SYMPOSIUM: COLD QUANTUM SYSTEMS
THURSDAY, JUNE 21, 2012 – 8:30 AM
Room: 1015 MCPHERSON LAB

Chair: GARY DOUBERLY, University of Georgia, Athens, Georgia

**RD01**
PROBING MOLECULES WITH LASER-COOLED ATOMIC IONS

KENNETH R. BROWN, Schools of Chemistry and Biochemistry; Computational Science and Engineering; and Physics
Georgia Institute of Technology, Atlanta, GA 30332-0400.

**RD02**
SPECTROSCOPIC APPLICATIONS OF STATE-SELECTED SYMPATHETICALLY-COOLED MOLECULAR IONS

XIN TONG, MATTHIAS GERMANN and STEFAN WILLITSCH, Department of Chemistry, University of Basel, Klingelbergstrasse 80, CH-4056 Basel, Switzerland.

**RD03**
DETECTING HYDROGEN ATOMS IN SOLID PARAHYDROGEN USING FTIR SPECTROSCOPY

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

**RD04**
PHOTOCHEMICAL STUDIES OF CH$_3$OH ISOLATED IN SOLID PARAHYDROGEN

DAVID T. ANDERSON, KYLIE A. KUFELD, DOMINIQUE SCHOECH, ROBERT B. SLIPP, AND FARAJ M. ALMARRI, Department of Chemistry, University of Wyoming, Laramie, WY 82071-3838.

**RD05**
FTIR STUDIES OF AMMONIA PHOTOCHEMISTRY IN SOLID PARAHYDROGEN

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

**Intermission**

**RD06**
HOW CHLORINE ATOM REACTS WITH H$_2$ IN IR-IRRADIATED SOLID PARA-HYDROGEN

JEN-YU WU, MOHAMMED BAHOU, Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu 30010, Taiwan; 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.
THEORETICAL SPIN-ORBIT SPECTROSCOPY OF CI DOPANTS IN SOLID PARAHYDROGEN

ROBERT HINDE, Department of Chemistry, University of Tennessee, Knoxville, TN 37996 USA.

INFRARED SPECTROSCOPY OF 1-CHLOOROMETHYLLALLYL AND 1-METHYLLALLYL RADICALS PRODUCED IN A SOLID PARA-HYDROGEN MATRIX.

MOHAMMED BAHOU, JEN-YU WU, KEIICHI TANAKA, Dept of Applied Chemistry, National Chiao Tung University, Hsinchu, 30010, TAIWAN ; YUAN-PERN LEE, Dept of Applied Chemistry, National Chiao Tung University, and Institute of Atomic & Molecular Sciences, Academia Sinica, Taipei 10617, TAIWAN.

IR-IR DOUBLE RESONANCE EXPERIMENT OF CH$_3$F-(ortho-H$_2$)$_n$ CLUSTERS IN SOLID para-H$_2$

Y. MIYAMOTO, Graduate School of Natural Science and Technology, Okayama University, 3-1-1 Tsushima-naka Okayama 700-8530 JAPAN; A. MIZOGUCHI, and H. KANAMORI, Department of Physics, Tokyo Institute of Technology, Tokyo, 152-8551 JAPAN.

LINESHAPE ANALYSIS OF CH$_3$F-(ortho-H$_2$)$_n$ ABSORPTION SPECTRA IN 3000 cm$^{-1}$ REGION IN SOLID para-H$_2$

Y. MIYAMOTO, Graduate School of Natural Science and Technology, Okayama University, 3-1-1 Tsushima-naka Okayama 700-8530, Japan; T. MOMOSE, Department of Chemistry, The University of British Columbia, 2036 Main Mall, Vancouver, British Columbia V6T 1Z1, Canada; H. KANAMORI, Department of Physics, Tokyo Institute of Technology, Ohokayama 2-12-1, Tokyo 152-8551, Japan.
RE. DYNAMICS
THURSDAY, JUNE 21, 2012 – 8:30 AM
Room: 2015 MCPHERSON LAB

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

RE01 15 min 8:30
GAIN AND LASING OF OPTICALLY PUMPED METASTABLE RARE GAS ATOMS

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

RE02 15 min 8:47
COOPERATIVE EFFECTS IN A RYDBERG GAS

YAN ZHOU, DAVID GRIMES, ANTHONY COLOMBO, and ROBERT FIELD, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02319.

RE03 15 min 9:04
USING A HIGH RESOLUTION MID-IR OPO FOR CHEMICAL DYNAMICS STUDIES OF HIGHLY EXCITED MOLECULES

GERALDINE O. ECHEBIRI, MATTHEW D. SMARTE, WENDELL W. WALTERS and AMY S. MULLIN, Department of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742.

RE04 10 min 9:21
OPTICAL PROBING OF OCS IN EXTREME ROTATIONAL STATES

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

RE05 15 min 9:33
POLARIZATION DEPENDENT DYNAMICS OF CO2 TRAPPED IN AN OPTICAL CENTRIFUGE

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

RE06 15 min 9:50
IR/THZ DOUBLE RESONANCE SPECTROSCOPY OF METHYL FLUORIDE AND COLLISION PARTNERS SELF, N2, Ar, He, CO2, AND AIR

DANE J. PHILLIPS, Kratos Defense and Security Solutions Digital Fusion, 4904 Research Dr., Huntsville, Al, 35805; FRANK C. DE LUCIA, Department of Physics, 191 Woodruff Ave. Ohio State University, Columbus, OH 43210; HENRY O. EVERITT, Army Aviation and Missile RD&E Center, Weapon Sciences Directorate, Redstone Arsenal, AL, 35898.

Intermission
ULTRAVIOLET PHOTODISSOCIA TION DYNAMICS OF THE 1-PROPENYL RADICAL

MICHAEL LUCAS, Department of Chemistry, University of California at Riverside, Riverside, CA 92521; YU SONG, Department of Chemistry, University of California at Davis, Davis, CA 95616; JINGSONG ZHANG, Department of Chemistry, University of California at Riverside, Riverside, CA 92521; CHRISTOPHER BRAZIER, Department of Chemistry and Biochemistry, California State University, Long Beach, Long Beach, CA 90840.

OBSERVATION OF VIBRATIONALLY HOT CH₂CHO IN THE 351NM PHOTODISSOCIA TION OF XCH₂CH₂ONO (X=F,Cl,Br,OH)

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

PRODUCT STATE AND SPEED DISTRIBUTIONS IN PHOTOCHEMICAL TRIPLE FRAGMENTATIONS

M.S. QUINN, G. DE WIT, B.R. HEAZLEWOOD, K. NAUTA, S.H. KABLE, and M.J.T. JORDAN, School of Chemistry, University of Sydney, Sydney, NSW, 2006, Australia; S.A. REID, Department of Chemistry, Marquette University, Milwaukee, WI, 53233, USA; A.T. MACCARONE, Department of Chemistry, University of Wollongong, Wollongong, NSW, 2522, Australia.

HYDROGEN ABSTRACTION FROM CH₃D BY CHLORINE RADICALS WITH VARYING KINECTIC ENERGY DISTRIBUTIONS

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

VIBRATIONALLY DRIVEN HYDROGEN ABSTRACTION BY THE BROMINE ATOM FROM CYCLOHEXANE

THOMAS J. PRESTON, MICHAEL A. SHALOSKI, and F. FLEMING CRIM, Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706.

THE MARRIAGE OF SPECTROSCOPY AND DYNAMICS: CHIRPED-PULSE FOURIER-TRANSFORM MM-WAVE (CP-FT-MMW) SPECTROSCOPY IN PULSED UNIFORM SUPersonic FLOWS

CHAMARA ABYESEKERA, JAMES M. OLDHAM, ARTHUR G. SUITS, Department of Chemistry, Wayne State University, Detroit, MI 48202; G. BARRATT PARK, ROBERT W. FIELD, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139.
RF. ASTRONOMICAL SPECIES AND PROCESSES
THURSDAY, JUNE 21, 2012 – 1:30 PM
Room: 160 MATH ANNEX
Chair: NICHOLAS INDRIOLO, Johns Hopkins University, Baltimore, Maryland

RF01 15 min 1:30
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.

RF02 15 min 1:47
INFRARED SPECTROSCOPIC STUDIES WITH THE STRATOSPHERIC OBSERVATORY FOR INFRARED ASTRONOMY (SOFIA)

R. D. GEHRZ, Minnesota Institute for Astrophysics, 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.

RF03 15 min 2:04
ROTATIONAL SPECTRA OF VIBRATIONALLY EXCITED HCL

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

RF04 15 min 2:21
THE ROTATIONAL SPECTRA OF OH DOUBLET PI ISOPOLOGUES

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

RF05 15 min 2:38
MICROWAVE STUDY OF METHYL FORMATE IN THE NEW VIBRATIONAL EXCITED STATES

YUSUKE SAKAI, KAORI KOBAYASHI, Department of Physics, University of Toyama, 3190 Gofuku, Toyama, 930-8555 Japan; MASAHIRO TSUKAMOTO, MASAHARU FUJITAKE, and NOBUKIMI OHASHI, Kanazawa University, Japan.

RF06 15 min 2:55
LABORATORY STUDY OF THE ROTATIONAL SPECTRUM OF 2-BUTANONE

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.

Intermission
USING HOT EMISSION SPECTRA IN GENERATING LINE LISTS OF MOLECULES (NH₃, CH₄) FOR ASTROPHYSICAL APPLICATIONS

R.J. HARGREAVES, L. MICHAUX, Department of Chemistry, University of York, Heslington, York, YO10 5DD, UK; G. LI, Harvard-Smithsonian Center for Astrophysics, Atomic and Molecular Physics Division, MS#50, 60 Garden St., Cambridge, MA, 02138, USA; C. BEALE, Department of Chemistry & Biochemistry, Old Dominion University, 4541 Hampton Boulevard, Norfolk, VA, 23529-0126, USA; M. IRFAN, School of Physics and Astronomy, The University of Manchester, Oxford Road, Manchester, M13 9PL, UK; and P.F. BERNAH, Department of Chemistry & Biochemistry, Old Dominion University, 4541 Hampton Boulevard, Norfolk, VA, 23529-0126, USA; and University of York, Dept. of Chemistry, Heslington, York, YO10 5DD, UK.

BROADBAND SCREENING FOR INTERSTELLAR SPECIES: ADDITIONAL LABORATORY MEASUREMENTS AND INTERSTELLAR DETECTION OF ETHANIMINE (CH₃CHNH) IN SGR B2(N)

RYAN A. LOOMIS, DANIEL P. ZALESKI, AMANDA L. STEBER, JUSTIN L. NEILL, MATT T. MUCKLE, NATHAN A. SEIFERT, and BROOKS H. PATE, Department of Chemistry, University of Virginia, McCormick Rd., P.O. Box 400319, Charlottesville, VA 22904; VALERIO LATTANZI, OSCAR MARTINEZ, JR., 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.

UNRAVELING THE COMPLEX NEAR-UV SPECTRUM OF Si₂C

N. J. REILLY and M. C. McCARTHY, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 02138, and School of Engineering & Applied Sciences, Harvard University, 29 Oxford St., Cambridge, MA 02138; D. L. KOKKIN, IRAP; Université de Toulouse, UPS; CNRS; 9 Av. colonel Roche, BP 44346, F-31028 Toulouse cedex 4, France; R. C. FORTENBERRY, and T. D. CRAWFORD, Department of Chemistry, Virginia Tech, Blacksburg, VA 24061.

LABORATORY DETECTIONS OF CYANOTHIOFORMALDEHYDE (HCSCN) AND MERCAPTOACETONITRILE (HSCH₂CN) BY CP-FTMW SPECTROSCOPY

DANIEL P. ZALESKI, JUSTIN L. NEILL, MATT T. MUCKLE, NATHAN A. SEIFERT, AMANDA A. STEBER, BRENT J. HARRIS, and BROOKS H. PATE, Department of Chemistry, University of Virginia, McCormick Rd., P.O. Box 400319, Charlottesville, VA 22904; VALERIO LATTANZI and MICHAEL 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.

HIGH RESOLUTION SPECTRUM OF THE $^{13}$C$^{12}$C$^{12}$C LOWEST BENDING MODE

C. P. ENDRES, V. LUTTER, J. KÖTTING, J. KRIEG, S. THORWIRTH, S. SCHLEMMER, T. F. GIESEN, I. Physikalisches Institut. Universität zu Köln, 50937 Köln, Germany; M. E. HARDING, Karlsruher Institut für Technologie, Institut für Nanotechnologie, 76021 Karlsruhe, Germany; J. VÁZQUEZ, Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, Texas 78712, USA.
ASSIGNMENTS, PERTURBATIONS, PATHOLOGIES AND A ROTATIONAL ANALYSIS OF THE SPECTRUM OF CH$_2$DOH

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

THZ AND LONG PATH FOURIER TRANSFORM SPECTROSCOPY OF METHANOL; TORSIONALLY COUPLED HIGH-K LEVELS

JOHN C. PEARSON, SHANSHAN YU, BRIAN J. DROUIN, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr., Pasadena, CA 91109; RONALD M. LEES, LI-HONG XU, Centre for Laser, Atomic and Molecular Sciences (CLAMS) Physics Department University of New Brunswick, 100 Tucker Park Road, Saint John, NB, Canada E2L 4L5; BRANT E. BILLINGHURST, Canadian Light Source Inc, University of Saskatchewan, 100 Perimeter Drive, Saskatchewan, SK, Canada S7N 0X4.

ON THE ELECTRONIC SPECTROSCOPY OF CLOSED SHELL CATIONS DERIVED FROM RESONANCE STABILIZED RADICALS: INSIGHTS FROM THEORY AND FRANCK-CONDON ANALYSIS

TYLER P. TROY, SCOTT H. KABLE, TIMOTHY W. SCHMIDT, School of Chemistry, The University of Sydney, NSW 2006, Australia; SCOTT A. REID, Department of Chemistry, Marquette University, Milwaukee, WI 53233.
<table>
<thead>
<tr>
<th>RG01</th>
<th>10 min 1:30</th>
</tr>
</thead>
<tbody>
<tr>
<td>DIRECT POTENTIAL FITTING FOR THE $A^3\Pi_{1u}$ and $X^1\Sigma^+_g$ STATES OF Br$_2$</td>
<td></td>
</tr>
<tr>
<td>Tokio Yukiya, Nobuo Nishimiya, Masao Suzuki, Department of Electronics and Information Technology, Tokyo Polytechnic University, Iyama 1583, Atsugi City, Kanagawa 243-0297, Japan; Robert J. Le Roy, Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>RG02</th>
<th>15 min 1:42</th>
</tr>
</thead>
<tbody>
<tr>
<td>ANALYSIS OF THE VISIBLE ABSORPTION SPECTRUM OF I$_2$ IN INERT SOLVENTS USING A PHYSICAL MODEL</td>
<td></td>
</tr>
<tr>
<td>J. Tellinghuisen, Department of Chemistry, Vanderbilt University, Nashville, TN 37235.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>RG03</th>
<th>5 min 1:59</th>
</tr>
</thead>
<tbody>
<tr>
<td>WAVELENGTH ANOMALIES IN UV-Vis SPECTROPHOTOMETRY</td>
<td></td>
</tr>
<tr>
<td>J. Tellinghuisen, Department of Chemistry, Vanderbilt University, Nashville, TN 37235.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>RG04</th>
<th>15 min 2:06</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEPERTURBATION STUDIES OF AiO : INTERACTIONS IN THE $A^2\Pi \sim X^2\Sigma^+$ STATES</td>
<td></td>
</tr>
<tr>
<td>K. Sunanda, M. D. Saksena, and B. N. Jagatap, Atomic and Molecular Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400 085, India; M. N. Deo, High Pressure Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400 085, India; N. Mhaske and S. H. Behere, Department of Physics, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad, India.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>RG05</th>
<th>15 min 2:23</th>
</tr>
</thead>
<tbody>
<tr>
<td>FOURIER TRANSFORM EMISSION SPECTROSCOPY OF THE $A^2\Pi-X^2\Sigma^+$ (RED) SYSTEM OF $^{13}$C$^{14}$N.</td>
<td></td>
</tr>
<tr>
<td>R. S. Ram, Department of Chemistry, University of York, Heslington, York, YO10 5DD, UK; Department of Chemistry, University of Arizona, Tucson, AZ 85721, USA; and P. F. Bernath, Department of Chemistry and Biochemistry, Old Dominion University, Norfolk, VA 23529 USA; Department of Chemistry, University of York, Heslington, York, YO10 5DD, UK.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>RG06</th>
<th>15 min 2:40</th>
</tr>
</thead>
<tbody>
<tr>
<td>HYPERFINE-RESOLVED SATURATION SPECTROSCOPY OF METASTABLE N$_2$ IN THE (1-0) BAND OF THE $B^3\Pi_u - A^3\Sigma^+_g$ ELECTRONIC TRANSITION</td>
<td></td>
</tr>
<tr>
<td>D. Forthomme, C. McRaven, G. E. Hall, T. J. Sears, Chemistry Department, Brookhaven National Laboratory, Bldg. 555A, P.O. Box 5000, Upton, NY 11973, USA.</td>
<td></td>
</tr>
</tbody>
</table>
PRODUCTION OF A BEAM OF HIGHLY VIBRATIONALLY EXCITED CO USING PERTURBATIONS

N. BARTELS, T. SCHÄFER, J. HÜHNERT, A. M. WODTKE, Georg August Universität Göttingen, Institut für Physikalische Chemie, Tammanstrasse 6, 37075 Göttingen, Germany; and R. W. FIELD, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139, USA.

OBSERVATION OF BLUE-DETUNED PHOTOASSOCIATION TO THE 2 \( (0^+ \) STATE OF \(^{85}\)Rb\(_2\) VIA REMPI


Intermission

IS THE EQUILIBRIUM STRUCTURE OF BeOH LINEAR OR BENT?

KYLE J. MASCARITOTOLO, JEREMY M. MERRITT, and MICHAEL C. HEAVEN, Department of Chemistry, Emory University, Atlanta, GA 30322.

AN EXPERIMENTAL AND QUANTUM CHEMICAL STUDY OF THE ELECTRONIC SPECTRUM OF THE HBCI FREE RADICAL

MOHAMMED A. GHARAIBEH, RAMYA NAGARAJAN and DENNIS J. CLOUTHIER, Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055; RICARDO TARRONI, Dipartimento di Chimica Fisica ed Inorganica, Università di Bologna, Viale Risorgimento 4, 40136 Bologna, Italy.

GAS PHASE SPECTROSCOPIC INVESTIGATION OF CHROMATE-ESTERS

SYDNEY H. KAUFMAN and J. MATHIAS WEBER, JILA, NIST and Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO 80309.

ELECTRONIC SPECTROSCOPY OF THE NO-X (X = RARE GAS, ALKANE) COMPLEXES

ADRIAN M. GARDNER, VICTOR TAMÉ-REYES, JOE HARRIS, JODIE McDaniel and TIMOTHY G. WRIGHT, School of Chemistry, University of Nottingham, University Park, Nottingham, NG7 2RD, UK.

GAS PHASE ELECTRONIC PHOTODISSOCIATION SPECTRA OF COPPER NITRATE CLUSTER IONS

SYDNEY H. KAUFMAN, CASEY R. CHRISTOPHER and J. MATHIAS WEBER, JILA, NIST and Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO 80309.
THE OPTICAL SPECTRUM OF THE SILICON TERMINATED CARBON CHAINS SiCnH

D. L. Kokkin, IRAP; Université de Toulouse, UPS; CNRS; 9 Av. colonel Roche, BP 44346, F-31028 Toulouse cedex 4, France and Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 02138, and School of Engineering & Applied Sciences, Harvard University, 29 Oxford St., Cambridge, MA 02138; N. J. Reilly, and M. C. McCarthy, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 02138, and School of Engineering & Applied Sciences, Harvard University, 29 Oxford St., Cambridge, MA 02138; R. C. Fortenberry, and T. D. Crawford, Department of Chemistry, Virginia Tech, Blacksburg, VA 24061.
THE ROTATIONAL SPECTRUM OF D$_2^{17}$O: ACCURATE SPECTROSCOPIC AND HYPERFINE PARAMETERS

Cristina Puzzarini, Gabriele Cazzoli, Dipartimento di Chimica "G. Ciamician", Università di Bologna, I-40126 Bologna, Italy; Juana Vázquez, Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, Texas 78712, USA; Michael E. Harding, Karlsruher Institut für Technologie, Institut für Nanotechnologie, 76021, Karlsruhe, Germany; Jürgen Gauss, Institut für Physikalische Chemie, Universität Mainz, D-55099 Mainz, Germany.

IDENTIFICATION OF THE CAGE, PRISM, AND BOOK ISOMERS OF WATER HEXAMER AND THE PREDICTED LOWEST ENERGY HEPTAMER AND NONAMER CLUSTERS BY BROADBAND ROTATIONAL SPECTROSCOPY

Cristobal Perez, Matt T. Muckle, Daniel P. Zaleski, Nathan Seifert, Brooks H. Pate, Department of Chemistry, University of Virginia, McCormick Rd., Charlottesville, VA 22904; Zbigniew Kisiel, Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warszawa, Poland; Berhane Temelso, George C. Shields, Dean’s Office, College of Arts and Sciences, and Department of Chemistry, Bucknell University, Lewisburg, PA 17837.

WATER CLUSTERS OBSERVED BY CHIRPED-PULSE ROTATIONAL SPECTROSCOPY: STRUCTURES AND HYDROGEN BONDING

Zbigniew Kisiel, Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warszawa, Poland; Cristobal Perez, Matt T. Muckle, Daniel P. Zaleski, Nathan Seifert, Brooks H. Pate, Department of Chemistry, University of Virginia, McCormick Rd., Charlottesville, VA 22904-4319; Berhane Temelso, George C. Shields, Dean’s Office, College of Arts and Sciences, and Department of Chemistry, Bucknell University, Lewisburg, PA 17837.

FTMW SPECTROSCOPY OF SILYL MERCAPTAN, H$_3$SiSH

S. Thorwirth, I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany; V. Lattanzi, Oscar Martinez, Jr., Michael C. McCarthy, Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, U.S.A. and School of Engineering and Applied Sciences, Harvard University, 29 Oxford Street, Cambridge, MA 02138, U.S.A.; 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.

FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF SCS (X$^2\Sigma$), YS (X$^2\Sigma$) AND VS (X$^4\Sigma$)

L. M. Ziurys, G. R. Adande, D. T. Halfen, Department of Chemistry and Steward Observatory, University of Arizona, Tucson, AZ 85721.
THE CCN ($X^2\Pi_{1/2}$) RADICAL REVISITED: NEW FOURIER TRANSFORM MICROWAVE MEASUREMENTS

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

FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF ALKALI METAL HYDROSULFIDES: DETECTION OF KSH

P. M. SHERIDAN, M. K. L. BINNS, J. P. YOUNG, Department of Chemistry and Biochemistry, Canisius College, Buffalo, NY 14208; M. P. BUCCHINO, and L. M. ZIURYS, Department of Chemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, AZ 85721.

Intermission

MICROWAVE SPECTRUM OF HEXAFLUOROISOPROPANOL

ABHISHEK SHAHI, DEVENDRA MANI and E. ARUNAN, Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore-560012, India.

MILLIMETER-WAVE SPECTROSCOPY OF ETHYLMERCUry HYDRIDE

M. GOUBET, R. A. MOTIYENKO, L. MARGULÈS, Laboratoire PhLAM, UMR 8523 CNRS - Université Lille 1, 59655 Villeneuve d'Ascq Cedex, France; J.-C. GUILLEMIN, Sciences Chimiques de Rennes, UMR 6226 CNRS - ENSCR, 35708 Rennes Cedex 7, France.

CHIRPED-PULSE AND CAVITY BASED FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF THE METHYL LACTATE-AMMONIA ADDUCT

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

HALOGEN BOND AND INTERNAL MOTIONS: THE LOW-BARRIER CASE OF CF$_3$Cl-DIMETHYLETHER

LUCA EVANGELISTI, GANG FENG, QIAN GOU and WALTHER CAMINATI, Dipartimento di Chimica "G. Cianiian" dell’Università, Via Selmi 2, I-40126 Bologna, Italy; JENS-UWE GRABOW, Lehrgebiet Physikalische Chemie A, Institut für Physikalische Chemie und Elektrochemie, Universität Hannover, Callinstr. 3A, D-30167 Hannover, Germany.

THE COMMON CHLORINE NUCLEAR ELECTRIC QUADRUPOLE COUPLING TENSOR FOR ACYL CHLORIDES

R. A. POWOSKI, Glori Energy, Inc., 4315 South Dr, Houston, Texas 77053; S. A. COOKE, School of Natural and Social Sciences, Purchase College SUNY, 735 Anderson Hill Road, Purchase, NY 10577.
THE MILLIMETER WAVE SPECTRUM OF ESTRAGOLE AND VERBENONE

COREY J EVANS, STEPHANIE M ALLPRESS, Department of Chemistry, University of Leicester, Leicester, LE1 7RH, United Kingdom; PETER D GODFREY, DON MCNAUGHTON, School of Chemistry, Monash University, 3800, Victoria, Australia.
RI. MINI-SYMPOSIUM: COLD QUANTUM SYSTEMS
THURSDAY, JUNE 21, 2012 – 1:30 PM
Room: 1015 MCPHERSON LAB
Chair: TAKAMASA MOMOSE, The University of British Columbia, Vancouver, BC, Canada

RI01
INVITED TALK
SPECTRA OF COLD MOLECULAR IONS FROM HOT HELIUM NANODROPLETS

MARCEL DRABBELS, Laboratoire de Chimie Physique Moléculaire, Ecole polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland.

RI02
15 min 2:05
HOT MOLECULES IN HELIUM NANODROPLETS: A NEW ROUTE TO OPTICAL SPECTRA

BENJAMIN SHEPPERSO, ADRIAN BOATWRIGHT, CHENG FENG, DANIEL SPENCE, SHENGFU YANG, and ANDREW M. ELLIS, Department of Chemistry, University of Leicester, University Road, Leicester, LE1 7RH, UK.

RI03
15 min 2:22
HELIUM NANODROPLET ISOLATION SPECTROSCOPY OF NO₂ AND VAN DER WAALS COMPLEXES

ROBERT R. FEHNEL, KEVIN K. LEHMANN, Department of Chemistry, University of Virginia, Charlottesville VA, 22904-4319.

RI04
15 min 2:39
SATURATION OF THE NO₂ ν₁ + ν₃ AND THE CH₄ ν₃ TRANSITIONS IN HELIUM NANODROPLETS

ROBERT R. FEHNEL, KEVIN K. LEHMANN, Department of Chemistry, University of Virginia, Charlottesville VA, 22904-4319.

RI05
15 min 2:56
INFRARED SPECTROSCOPY OF OH AND OH-C₂H₂ EMBEDDED IN HELIUM NANODROPLETS

PAUL RASTON, TAO LIANG, STEVEN D. FLYNN, ALEXANDER M. MORRISON, AND GARY E. DOUBERY, Department of Chemistry, University of Georgia, Athens, GA 30602-2556.

Intermission

RI06
INVITED TALK
DOPANT ROTATION IN MOLECULAR SUPERFLUID CLUSTERS

PIERRE-NICOLAS ROY, Department of Chemistry, University of Waterloo, Waterloo, Ontario, Canada, N2L 3G1.
RI07  10 min  4:05

OBSERVATION OF VORTICES IN SUPERFLUID He DROPLETS

LUIS F. GOMEZ, EVGENY LOGINOV, ANDREY F. VILESOV, Department of Chemistry, University of Southern California, Los Angeles, CA 90089-0482.

RI08  15 min  4:17

PYRIDINE AGGREGATION IN HELIUM NANODROPLETS

PABLO NIETO, TORSTEN POERSCHKE, DANIEL HABIG, GERHARD SCHWAAB and MARTINA HAVENITH, Department of Physical Chemistry II, Ruhr-Universität Bochum, Germany.

RI09  15 min  4:34

PROBING TRANS-HOOO/DOOO AND HOOO-(O\textsubscript{2})\textsubscript{n} CLUSTERS: A HENDI APPROACH

T. LIANG, P. RASTON, and G. E. DOUBERLY, Department of Chemistry, University of Georgia, Athens, Georgia 30602-2556.

RI10  15 min  4:51

ON THE OUTCOME OF THE REACTIONS BETWEEN HYDROCARBON RADICALS AND O\textsubscript{2} IN HELIUM NANODROPLETS

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

RI11  15 min  5:08

INFRARED SPECTROSCOPY OF HOCl EMBEDDED IN HELIUM NANODROPLETS

PAUL RASTON, DONALD KELLOWAY, AND WOLFGANG JÄGER, Department of Chemistry, University of Alberta, Edmonton, Alberta T6G-2G2, Canada.

RI12  15 min  5:25

ASYMMETRIC TOP ROTORS IN SUPERFLUID PARA-HYDROGEN NANO-CLUSTERS

TAO ZENG, Department of Chemistry, University of Waterloo, Waterloo, ON, Canada, N2L 3G1; HUI LI, Institute of Theoretical Chemistry, State Key Laboratory of Theoretical and Computational Chemistry, Jilin University, 2519 Jiefang Road, Changchun 130023, People’s Republic of China; and PIERRE-NICHOLAS ROY, Department of Chemistry, University of Waterloo, Waterloo, ON, Canada, N2L 3G1.

RI13  15 min  5:42

MOLECULAR DYNAMICS SIMULATIONS ON VARIOUS WEAKLY BOUND WATER-PARAHYDROGEN SYSTEMS AT ULTRACOLD TEMPERATURE

MATTHEW SCHMIDT, Department of Chemistry, University of Waterloo, Waterloo, ON, Canada, N2L 3G1; CHRISTOPHER ING, Department of Biochemistry, University of Toronto, 27 King’s College Circle, Toronto, Ontario, Canada MSS 1A1; STEPHEN CONSTABLE, TAO ZENG, JING YANG, MICHAEL NYMAN and PIERRE-NICHOLAS ROY, Department of Chemistry, University of Waterloo, Waterloo, ON, Canada, N2L 3G1.
RJ. THEORY
THURSDAY, JUNE 21, 2012 – 1:30 PM
Room: 2015 MCPHERSON LAB
Chair: PETER BOTSCHWINA, University of Goettingen, Goettingen, Germany

RJ01 30 min 1:30
INVITED TALK
INTENSITIES OF FUNDAMENTAL AND OVERTONE VIBRATIONAL TRANSITIONS
HENRIK G. KJAERGAARD, Department of Chemistry, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen Ø, Denmark.

RJ02 15 min 2:05
HIGH-ACCURACY POTENTIALS FOR VAN DER WAALS SYSTEMS
RICHARD DAWES, Missouri University of Science and Technology, Rolla, MO 65409, USA; XIAO-GANG Wang, JAMES BROWN, TUCKER CARRINGTON, JR., Queen’s University, Kingston, Ontario, K7L 3N6 Canada.

RJ03 15 min 2:22
THE AMMONIA DIMER REVISITED
RICHARD DAWES, Missouri University of Science and Technology, Rolla, MO 65409-0010; AD VAN DER AVOIRD, Radboud University, 6525 AJ Nijmegen, The Netherlands.

RJ04 15 min 2:39
RESONANCE AND REVIVALS I. QUANTUM ROTOR AND INFINITE-WELL DYNAMICS
WILLIAM G. HARTER, Department of Physics, University of Arkansas, Fayetteville, AR 72701; ALVASON ZHENHUA LI, Microelectronics-Photonics, University of Arkansas, Fayetteville, AR 72701.

RJ05 15 min 2:56
RESONANCE AND REVIVALS II. MORSE OSCILLATOR AND DOUBLE MORSE WELL DYNAMICS
ALVASON ZHENHUA LI, Microelectronics-Photonics Program, University of Arkansas, Fayetteville, AR 72701; WILLIAM G. HARTER, Department of Physics, University of Arkansas, Fayetteville, AR 72701.

Intermission

RJ06 15 min 3:30
MULTI-VALUED VERSUS SINGLE-VALUED LARGE-AMPLITUDE BENDING-TORSIONAL-ROTATIONAL COORDINATE SYSTEMS FOR SIMULTANEOUSLY TREATING TRANS-BENT AND CIS-BENT ACETYLENE IN ITS S1 EXCITED ELECTRONIC STATE
JON T. HOUGEN, Sensor Sciences Division, National Institute of Standards and Technology, Gaithersburg, MD 20899-8441, USA.
RJ07 15 min 3:47

USING FIXED-NODE DIFFUSION MONTE CARLO TO PROBE ROTATION-VIBRATION COUPLING IN HIGHLY FLUXIONAL ASYMMETRIC TOP MOLECULES

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

RJ08 15 min 4:04

EXTENSIONS OF FIXED-NODE DIFFUSION MONTE CARLO TO THE STUDY OF THE ROTATIONALLY EXCITED STATES OF H₂D⁺

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

RJ09 15 min 4:21

EXPLORING ROTATION-VIBRATION COUPLING IN HIGHLY FLUXIONAL MOLECULES USING SURFACE HOPPING DIFFUSION MONTE CARLO

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

RJ10 10 min 4:38

BOUND AND SCATTERING STATE SOLUTIONS OF SCHRODINGER EQUATION FOR ASYMMETRIC WOODS SAXON POTENTIAL

N. CANDEMIR, Physics Department, Science Faculty, Anadolu University, Eskişehir, 26470, Turkey.
THEORETICAL AND EXPERIMENTAL WATER COLLISIONS WITH NORMAL AND PARAHYDROGEN

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

ROTATIONAL SPECTROSCOPY OF ISOCYANIC MOLECULES: ALLYL ISOCYANIDE AND DIISOCYANOMETHANE

R. A. MOTIYENKO, L. MARGULES, I. HAYKAL, T. R. HUET, Laboratoire PhLAM, UMR 8523 CNRS - Université Lille 1, 59655 Villeneuve d'Ascq Cedex, France; E. J. COCINERO, P. ECIJA, J. A. FERNANDEZ, F. CASTANO, Dpto. Química Física, Facultad de Ciencia y Tecnología, Universidad del País Vasco, Barrio Sarriena s/n, 48940, Leioa, Spain; A. LESARRI, Dpto. Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, Prado de la Magdalena s/n, 47005, Valladolid, Spain; J.-C. GUILLEMIN, Sciences Chimiques de Rennes, UMR 6226 CNRS - ENSCR, 35708 Rennes Cedex 7, France.

TERAHertz SPECTROSCOPY OF METHYLAMINE

R. A. MOTIYENKO, L. MARGULÈS, Laboratoire PhLAM, UMR 8523 CNRS - Université Lille 1, 59655 Villeneuve d’Ascq Cedex, France; V. V. ILYUSHIN, E. A. ALEKSEEV, Institute of Radio Astronomy of NASU, Chervonoproporna 4, 61002 Kharkov, Ukraine; B. DROUIN, S. YU, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California 91109, USA; J. CERNICHARO, B. TERCERO, Centro de Astrobiología (CSIC-INTA), Laboratory of Molecular Astrophysics. Department of Astrophysics. Ctra de Ajalvir, Km 4, 28850 Torrejón de Ardoz, Madrid, Spain.

THZ SPECTROSCOPY OF ACETALDEHYDE AND SEARCH OF $^{13}$C SPECIES IN ORION

L. MARGULÈS, R. A. MOTIYENKO, Laboratoire PhLAM, CNRS UMR 8523, Université de Lille 1, 59655 Villeneuve d’Ascq Cedex, France; V. V. ILYUSHIN, Institute of Radio Astronomy of NASU, Chervonoproporna Str., 4, 61002 Kharkov, Ukraine; B. TERCERO, J. CERNICHARO, Centro de Astrobiología (CSIC-INTA), Laboratory of Molecular Astrophysics. Department of Astrophysics. Ctra de Ajalvir, Km 4, 28850 Torrejón de Ardoz, Madrid, Spain; and J.-C. GUILLEMIN, Sciences Chimiques de Rennes, UMR 6226 CNRS-ENSCR, Avenue du Général Leclerc, CS 50837, 35708 Rennes Cedex 7, France.
SPECTROSCOPY OF A MAJOR COMPLEX ORGANIC MOLECULE: MONO-DEUTERATED DIMETHYL ETHER

C. RICHARD, L. MARGULÉS, R. A. MOTIYENKO, Laboratoire PhLAM, UMR 8523 CNRS, Bât. P5, Université des Sciences et Technologies de Lille 1, 59655 Villeneuve d’Ascq Cedex, France; P. GRONER, Department of Chemistry, University of Missouri-Kansas City, Kansas City, MO 64110-2499; L. H. COUDERT, LISA, CNRS/Universités Paris Est et Paris Diderot, 61 Avenue du Général de Gaulle, 94010 Créteil, France; J.-C. GUILLEMIN, Sciences Chimiques de Rennes, UMR 6226 CNRS-ENSCR, Avenue du Général Leclerc, CS 50837, 35708 Rennes Cedex 7, France.

Intermission

TOWARDS AN ACCURATE INFRARED LINELIST FOR SO₂

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; TIMOTHY J. LEE, MS 245-1, NASA Ames Research Center, Moffett Field, CA, 94035.

THEORETICAL NH₃ SPECTRA IN 5800-7000 CM⁻¹ REGION AND CO₂ IR INTENSITY: UPDATES

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; TIMOTHY J. LEE, MS 245-1, NASA Ames Research Center, Moffett Field, CA, 94035; KEEYOUN SUNG, LINDA R. BROWN, Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr., Pasadena, CA 91109; and SERGEY A. TASHKUN, Laboratory of Theoretical Spectroscopy, V.E. Zuev Institute of Atmospheric Optics, SB, Russian Academy of Science, 634055, Tomsk, Russia.

LINE PARAMETERS OF THE PH₃ PENTAD IN THE 4 – 5µm REGION

V. MALATHY DEVI, D. CHRIS BENNER, The College of William and Mary, Williamsburg, VA 23187; I. KLEINER, Laboratoire Interuniversitaire des Systemes Atmospheriques (LISA), UMR 7583 CNRS/IPSL-Universités Paris-ESst and Diderot, 94010 Creteil Cedex, France; R. L. SAMS, T. A. BLAKE, Pacific Northwest National Laboratory, Richland, WA 99352; LINDA R. BROWN, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109; L. N. FLETCHER, Department of Physics, University of Oxford, Clarendon Laboratory, Oxford, OX1 3PU, UK.

LINE BY LINE SPECTRAL PARAMETERS IN THE 4ν₁₃ SPECTRAL REGION OF METHANE

D. CHRIS BENNER, V. MALATHY DEVI, Department of Physics, College of William and Mary, Williamsburg, VA 23187-8795; J. J. O’BRIEN, S. SHAJI, Department of Chemistry, University of Missouri - St. Louis, St. Louis, MO 63121-4400; P. T. SPICKLER, C. P. HOUCK, J. A. COAKLEY, J. DOLPH, K. RANKIN, Department of Physics, Bridgewater College, Bridgewater, VA 22812.
FA10 15 min 11:18
A GLOBAL FREQUENCY ANALYSIS OF $^{13}$CH$_3$CH$_3$ INCLUDING DATA FROM THE LOWEST FOUR VIBRATIONAL STATES

N. MOAZZEN-AHMADI, Department of Physics and Astronomy, University of Calgary, Calgary, AB T2N 1N4, Canada; V.-H. HORNEMAN, Department of Physical Sciences, University of Oulu, PO Box 3000, Finland-90014, Oulu, Finland.

FA11 Post-deadline Abstract 15 min 11:35
DIRECT FREQUENCY COMB SPECTROSCOPY FOR THE STUDY OF MOLECULAR DYNAMICS IN THE INFRARED FINGERPRINT REGION.$^a$

ADAM J. FLEISHER, BRYCE BJORK, KEVIN C. COSSEL, JUN YE, JILA, National Institute of Standards and Technology and University of Colorado, Boulder, Colorado 80309-0440, USA; LORA NUGENT-GLANDORF, FLORIAN ADLER, TYLER NEELY, and SCOTT DIDDAMS, National Institute of Standards and Technology, Boulder, Colorado 80305-3337, USA.

$^a$This research is supported by AFOSR, DTRA, NSF, NRC, and NIST

FA12 Post-deadline Abstract 15 min 11:52
MILLIMETRE-WAVE SPECTRUM OF ANTI-$^{13}$C$_1$ AND $^{13}$C$_2$ ISOTOPOLOGUES OF ETHANOL AND APPLICATIONS TO RADIO ASTRONOMY

AURELIA BOUCHEZ, ADAM WALTERS, SANDRINE BOTTINELLI, IRAP, Université de Toulouse, UPS-OMP, CNRS, 9 Av. colonel Roche, BP 44346, 31028 Toulouse Cedex 4, France; HOLGER S. P. MÜLLER, MATTHIAS H. ORDU, FRANK LEWEN, MONICA KOEBER, CHRISTIAN P. ENDRES, STEPHAN SCHLEMMER, I. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany.
FB01 15 min 8:30
HIGH RESOLUTION EMISSION SPECTROSCOPY OF THE VIBRATION-ROTATION BANDS OF HBO AND HBS.

G. Li\textsuperscript{a}, R.S. Ram, R.J. Hargreaves, Department of Chemistry, University of York, Heslington, York, YO10 5DD, UK; P.F. Bernath, Department of Chemistry and Biochemistry, Old Dominion University, Norfolk, VA 23529 USA; Department of Chemistry, University of York, Heslington, York, YO10 5DD, UK; and H. Li, State Key Lab of Theoretical and Computational Chemistry, Jilin University, Changchun City, China, 130023.

\textsuperscript{a}Current address: Harvard-Smithsonian Center for Astrophysics, Atomic and Molecular Physics Division, MS#50, 60 Garden St., Cambridge, MA, 02138, USA.

FB02 15 min 8:47
FIRST INFRARED SPECTRA OF NITROUS OXIDE PENTAMER

M. Rezaei, 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.

FB03 15 min 9:04
“PROTON SPONGES”: A RIGID ORGANIC SCAFFOLD TO REVEAL THE QUANTUM STRUCTURE OF THE INTRAMOLECULAR PROTON BOND

Andrew F. Deblase, Mark A. Johnson, Yale University, P. O. Box 208107, New Haven, CT, 06520; Michael T. Scerba, Steven Bloom, and Thomas Lectka, Johns Hopkins University, 3400 North Charles Street, Baltimore, MD, 21218; Travis Dudding, Brock University, St. Catharines, ON, Canada L2S 3A1.

FB04 15 min 9:21
OBSERVATION OF SINGLE AND DOUBLE IONIC H-BONDS IN PROTONATED DIPEPTIDE IONS USING IR-IR DOUBLE RESONANCE SPECTROSCOPY

Christopher M. Leavitt, Arron B. Wolk, Joseph A. Fournier, Michael Z. Kamrath, Etienne Garand and Mark A. Johnson, Sterling Chemistry Laboratory, Yale University, PO Box 208107, New Haven, CT 06520; Michael J. Van Stipdonk, Department of Chemistry, Wichita State University, 1845 Fairmont Ave, Wichita, KS 67208.

FB05 15 min 9:38
VIBRATIONAL COOLING OF LARGE MOLECULES IN SUPERSONIC EXPANSIONS: THE CASE OF C\textsubscript{60} AND PYRENE

Jacob T. Stewart, Brian E. Brumfield,\textsuperscript{a} Bradley M. Gibson, Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801; Benjamin J. McCall, Departments of Chemistry and Astronomy, University of Illinois at Urbana-Champaign, Urbana, IL 61801.

\textsuperscript{a}Present Address: Department of Electrical Engineering, Princeton University, Princeton, NJ 08544
Intermission

FB06 15 min 10:10
SUB-TERRAHERTZ SPECTROSCOPY OF E.COLI DNA: EXPERIMENT, STATISTICAL MODEL, AND MD SIMULATIONS

I. SIZOV, T. DOROFEEVA, T. KHROMOVA, B. GELMONT, and T. GLOBUS, Department of Electrical and Computer Engineering, University of Virginia, Charlottesville, VA 22904.

FB07 15 min 10:27
ISOMER-SPECIFIC INFRARED SPECTROSCOPY AS A DIAGNOSTIC TOOL FOR REACTIVE INTERMEDIATES TOWARDS NAPHTHALENE

NATHANIEL M. KIDWELL, DEEPAI N. MEHTA, JOSEPH A. KORN, and TIMOTHY S. ZWIER, Department of Chemistry, Purdue University, West Lafayette, IN 47907-2084; JOSHUA A. SEBREE, NASA Goddard Space Flight Center, Greenbelt, MD 20771.

FB08 15 min 10:44
SINGLE CONFORMATION SPECTROSCOPY OF SUBEROYLANILIDE HYDROXAMIC ACID: A MOLECULE BITES ITS TAIL

DI ZHANG, JACOB DEAN and TIMOTHY S. ZWIER, Department of chemistry, Purdue University, West Lafayette, IN 47906.

FB09 10 min 11:01
DFT STUDY OF SOLVENT EFFECTS ON CONFORMATIONAL EQUILIBRIA AND VIBRATIONAL SPECTRA OF 4-(1-PYRROLIDINYL)PIPERAZINE

O. BAGLAYAN, Physics Department, Science Faculty, Anadolu University, Eskisehir, 26470, Turkey; G. KEŞAN, Faculty of Science, University of South Bohemia, Czech Republic; C. PARLAK, Department of Physics, Dumlupınar University, Kütahya, 43100, Turkey; and M. SENYEL, Physics Department, Science Faculty, Anadolu University, Eskisehir, 26470, Turkey.

FB10 10 min 11:13
DFT, FT-RAMAN AND FT-IR INVESTIGATIONS OF 1-CYCLOPENTYLPIPERAZINE

O. BAGLAYAN, Physics Department, Science Faculty, Anadolu University, Eskisehir, 26470, Turkey; M. FATIH KAYA, Department of Physics, Dumlupınar University, Kütahya, 43100, Turkey; C. PARLAK, Department of Physics, Dumlupınar University, Kütahya, 43100, Turkey; O. ALVER, Physics Department, Science Faculty, Anadolu University, Eskisehir, 26470, Turkey; M. SENYEL, Physics Department, Science Faculty, Anadolu University, Eskisehir, 26470, Turkey.

FB11 15 min 11:25
FEMTOSECOND TIME-RESOLVED INFRARED SPECTRA OF ORGANO METALLIC COMPLEXES BOUND TO A DINUCLEAR METAL CENTER

SAMANTHA E. BROWN-XU and CHRISTOPHER B. DURR, The Ohio State University, Department of Chemistry and Biochemistry, Columbus, Ohio 43210.
## FC. MICROWAVE

**FRIDAY, JUNE 22, 2012 – 8:30 AM**  
**Room: 1000 MCPHERSON LAB**

<table>
<thead>
<tr>
<th>Title</th>
<th>Speaker(s)</th>
<th>Room/Address</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>FC01</strong> A NEW U-BAND (40 - 60 GHz) FOURIER TRANSFORM MICROWAVE SPECTROMETER</td>
<td>D. T. Halfen, J. Min, and L. M. Ziurys, Department of Chemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, AZ 85721.</td>
<td></td>
</tr>
<tr>
<td><strong>FC02</strong> FOURIER TRANSFORM MICROWAVE SPECTRUM OF THE AlC$_2$ ($\tilde{X}^2\text{A}_1$) RADICAL</td>
<td>D. T. Halfen, J. Min, and L. M. Ziurys, Department of Chemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, AZ 85721.</td>
<td></td>
</tr>
<tr>
<td><strong>FC03</strong> THE FOURIER TRANSFORM MICROWAVE SPECTRUM OF YOH AND YOD ($\tilde{X}^1\Sigma^+$)</td>
<td>D. T. Halfen and L. M. Ziurys, Department of Chemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, AZ 85721.</td>
<td></td>
</tr>
<tr>
<td><strong>FC04</strong> DEVELOPMENT OF A SUBMILLIMETER MULTIPASS SPECTROMETER FOR THE STUDY OF MOLECULAR IONS</td>
<td>A. Carroll, B. Rocher, J. C. Laas, B. A. DePrince, B. Hays, S. L. Widicus Weaver, Department of Chemistry, Emory University, Atlanta, GA 30322; S. Lang, Department of Chemistry, New College of Florida, Sarasota, FL 34243.</td>
<td></td>
</tr>
<tr>
<td><strong>FC05</strong> THE DEVELOPMENT AND IMPLEMENTATION OF CHIRPED-PULSE FREQUENCY COMBS AT MILLIMETER WAVELENGTHS</td>
<td>Amanda L. Steber, Brent J. Harris, Justin L.Neill, Kevin K. Lehmann, Brooks H. Pate, Department of Chemistry, University of Virginia, McCormick Rd., P.O. Box 400319, Charlottesville, VA 22904.</td>
<td></td>
</tr>
<tr>
<td><strong>FC06</strong> CHIRPED-PULSE FOURIER TRANSFORM MM-WAVE SPECTROSCOPY FROM 260-290 GHz</td>
<td>Brent J. Harris, Amanda L. Steber, Justin L. Neill, Kevin K. Lehmann, Brooks H. Pate, Department of Chemistry, University of Virginia, Charlottesville, VA 22904.</td>
<td></td>
</tr>
</tbody>
</table>

**Intermission**
FC07 15 min 10:30

**BROADBAND MICROWAVE SPECTROSCOPY OF LARGE MOLECULES**

V. ALVIN SHUBERT, DAVID SCHMITZ, THOMAS BETZ, and MELANIE SCHNELL, *Max-Planck Advanced Study Group at the Center for Free-Electron Science, Hamburg, Germany and Max-Planck-Institut für Kernphysik, Heidelberg, Germany.*

FC08 15 min 10:47

**SENSITIVITY LIMITS OF DEEP AVERAGE BROADBAND MICROWAVE AND MM-WAVE SPECTRA**

MATT T. MUCKLE, DANIEL P. ZALESKI, AMANDA STEBER, BRENT HARRIS, AND BROOKS H. PATE, *Department of Chemistry, University of Virginia, McCormick Rd., Charlottesville, VA 22904-4319.*

FC09 10 min 11:04

**PRECISE THZ MEASUREMENTS OF HCO⁺, N₂H⁺ AND CF⁺**

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

FC10 15 min 11:16

**MOLECULAR SUPERFLUIDITY IN SMALL CLUSTERS OF (pH₂)₅-HCN STUDIED WITH ROTATIONAL SPECTROSCOPY**

STEVE P. DEMPSTER and WOLFGANG JÄGER, *Department of Chemistry, University of Alberta, Edmonton, Canada T6G 2G2.*

FC11 15 min 11:33

**PUMP/PROBE MICROWAVE-OPTICAL DOUBLE RESONANCE (PPMODR) STUDY OF TUNGSTEN CARBIDE (WC) AND PLATINUM CARBIDE (PtC)**

FANG WANG and TIMOTHY C. STEIMLE, *Department of Chemistry and Biochemistry Arizona State University Tempe, Arizona 85287-1604 U.S.A.*

FC12 15 min 11:50

**LABORATORY DETECTION AND MICROWAVE SPECTRUM of ScC₂ RADICAL (X²A₁)**

JIE MIN, DEWAYNE T. HALFEN, LUCY M. ZIURYS, *Department of Chemistry and Biochemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, AZ 85721.*
FD. MINI-SYMPOSIUM: COLD QUANTUM SYSTEMS
FRIDAY, JUNE 22, 2012 – 8:30 AM
Room: 1015 MCPHERSON LAB

Chair: DAVID ANDERSON, University of Wyoming, Laramie, Wyoming

FD01  INVITED TALK  30 min  8:30
SPECTROSCOPY AND CHEMISTRY OF COLD MOLECULES

TAKAMASA MOMOSE, Department of Chemistry, The University of British Columbia, Vancouver, CANADA.

FD02  15 min  9:05
COLD ION-MOLECULE CHEMISTRY WITH A STARK DECELERATOR BEAML INE

JAMES M. OLDHAM, MARTIN T. BELL, LEE D. HARPER, TIMOTHY P. SOFTLEY, Chemistry Research Laboratory, University of Oxford, Mansfield Road, Oxford, United Kingdom OX1 3TA.

FD03  15 min  9:22
DECELERATING MOLECULES WITH MICROWAVE FIELDS

MELANIE SCHNELL, Center for Free-Electron Laser Science, Hamburg, Germany; SIMON MERZ, NICOLAS VANHAECKE, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany; WOLFGANG JÄGER, University of Alberta, Edmonton, Canada; GERARD MEIJER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany.

FD04  15 min  9:39
PROGRESS TOWARD SLOWING AND COOLING OF CaF WITH OPTICAL BICHROMATIC FORCES

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

FD05  15 min  9:56
SPECTROSCOPIC ANALYSIS OF THE A AND 3 \( ^1 \Sigma^+ \) STATES OF \(^{39}\mathrm{K}^{85}\mathrm{Rb}\)

JIN-TAE KIM, Department of Photonic Engineering, Chosun University, Gwangju, 501-759, Korea; YONGHOON LEE, Department of Chemistry, Mokpo National University, Jeonnam 534-729, Korea; BONGSOO KIM, Department of Chemistry, KAIST, Daejeon, 305-701, Korea; DAJUN WANG, Department of Physics, The Chinese University of Hong Kong, Shatin, Hong Kong; PHILLIP L. GOULD, EDWARD E. EYLER, and WILLIAM C. STWALLEY, Department of Physics, University of Connecticut, Storrs, CT 06269-3046, USA.

Intermission
DEVELOPING CONTINUOUS-WAVE RAMAN LASERS USING SOLID PARA-HYDROGEN AND BARIUM NITRATE FOR MOLECULAR SPECTROSCOPY APPLICATIONS

WILLIAM R. EVANS, Department of Physics, University of Illinois at Urbana-Champaign, Urbana, IL 61801; TAKAMASA MOMOSE, Department of Chemistry, The University of British Columbia, Vancouver, BC Canada V6T 1Z1; BENJAMIN J. McCALL, Departments of Chemistry, Astronomy and Physics, University of Illinois at Urbana-Champaign, Urbana, IL 61801.

IMPROVED ANALYTICAL POTENTIALS FOR THE $a^3\Sigma_u^+$ and $X^1\Sigma_g^+$ STATES OF Cs$_2$

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

RUBIDIUM ATOMS ON HELIUM DROPLETS: ANALYSIS OF AN EXOTIC RYDBERG COMPLEX

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

PHOTOABSORPTION OF Ag (N = 6 - 6000) CLUSTERS IN He DROPLETS: A TRANSITION FROM SINGLE- TO MULTI-CENTERED GROWTH

LUIS F. GOMEZ, EVGENY LOGINOV, RUSSELL SLITER, ANDREY F. VILEsov, Department of Chemistry, University of Southern California, Los Angeles, CA 90089-0482; AVIK HALDER, NAIHAO CHIANG, NICHOLAS GUGGEMOS, VITALY V. KRESIN, Department of Physics, University of Southern California, Los Angeles, CA 90089-0484.

MOLECULAR ION SPECTROSCOPY OF BaCl$^+$

STEVEN J. SCHOWALTER, KUANG CHEN, WADE G. REllERGERT, SCOTT T. SULLIVAN, AND ERIC R. HUDSON, Department of Physics and Astronomy, University of California, Los Angeles, California 90095, USA.
FE, THEORY
FRIDAY, JUNE 22, 2012 – 8:30 AM
Room: 2015 MCPHERSON LAB

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

FE01 10 min 8:30
OBSERVATION OF SINGLET-TRIPLET TRANSITIONS IN CAPACITIVE PHOTOCURRENT SPECTROSCOPY OF ORGANIC SOLAR CELLS

HUI LIU, JINJUN LIU, Department of Chemistry, University of Louisville, Louisville, KY 40292; HEMANT M. SHAH, AND BRUCE W. ALPHENAAAR, Department of Electrical & Computer Engineering, University of Louisville, Louisville, KY 40292.

FE02 15 min 8:42
REMARKS ON THE PHASE CHANGE OF THE ELECTRONIC WAVE FUNCTION UPON GOING ONCE AROUND A JAHN-TELLER CONICAL INTERSECTION IN VIBRATIONAL COORDINATE SPACE

JON T. HOUGEN, Sensor Sciences Division, National Institute of Standards and Technology, Gaithersburg, MD 20899-8441, USA.

FE03 15 min 8:59
AN AB INITIO MODEL HAMILTONIAN FOR THE $e' \otimes e'$ AND $e' \otimes e''$ SINGLET STATES OF $\text{Si}_3$

D. A. MATTHEWS, J. F. STANTON, Institute for Theoretical Chemistry, The University of Texas at Austin, Austin, Texas 78712.

FE04 15 min 9:16
DIFFUSION MONTE CARLO STUDIES OF THE GROUND-STATE STRUCTURE AND ENERGETICS OF H$_5^+$ AND ITS ISOTOLOGUES

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

FE05 15 min 9:33
MODELING SPIN-ORBIT COUPLING IN THE MONOHALOCARBENES

SILVER NYAMBO AND SCOTT A. REID, Department of Chemistry, Marquette University, Milwaukee, WI 53233.

Intermission

FE06 15 min 10:10
THEORETICAL INVESTIGATION OF THE M$^+$-RG$_2$ (M = ALKALINE EARTH METAL; RG = RARE GAS) COMPLEXES

ADRIAN M. GARDNER, RICHARD J. PLOWRIGHT, JACK GRANEEK, TIMOTHY G. WRIGHT, School of Chemistry, University of Nottingham, University Park, Nottingham, NG7 2RD, UK; and W. H. BRECK-ENRIDGE, Department of Chemistry, University of Utah, 315 South 1400 East, Salt Lake City, Utah 84112, USA.
FE07  
**Post-deadline Abstract**  
15 min 10:27  
ELUCIDATION OF PROTON-ASSISTED FLUXIONALITY IN TRANSITION-METAL OXIDE CLUSTERS

RAGHUNATH O. RAMABHADRAN, NICHOLAS J. MAYHALL, EDWIN L. BECHER III, AREFIN CHOWDHURY, KRISHNAN RAGHAVACHARI(S), Department of chemistry, Indiana University, Bloomington, IN-47405.

FE08  
**Post-deadline Abstract**  
15 min 10:44  
SIGNIFICANT NON-COVALENT INTERACTIONS: CAN STILL A SINGLE MOLECULE OF H₂O BE COMPLETELY ISOLATED INSIDE THE SUB-NANO SPACE INSIDE THE FULLERENE C₆₀ CAGE? A THEORETICAL PROSPECTIVE

PRADEEP R. VARADWAI, ARPITA VARADWAI, GILLES H. PESLHERBE, Centre for Research in Molecular Modeling and Department of Chemistry Biochemistry, Concordia University, 7141 Sherbrooke Street West, Montreal, Quebec, Canada, H4B 1R6.
AUTHOR INDEX

A
ABEL, M. – RC04
ABEYSEKERA, C. – RE12
ADAM, A. G. – RA07, RA12
ADAMS, C. L. – MI04
ADANDE, G. R. – RH05
ADLER, F. – FA11
ALBERT, S. – MF12
ALEKSHEV, E. A. – FA03
ALIJAH, A. – MG01, MG02
ALLEN, H. C. – TE02, TE03, TF11, TJ01
ALLEN, S. D. – WG06
ALLPRESS, S. M. – TC10, RH13
ALMARRI, F. M. – RD04
ALONSO, J. L. – MH14
ALPHENAAR, B. W. – FE01
ALVER, O. – FB10
AMICANGELO, J. C. – MJ02
ANDERSON, D. T. – RD03, RD04, RD05
ANDERSON, J. K. – RH06
ANDREWS, D. U. – RB05
ANTONOV, I. O. – WJ02, RA05
ARISTE, A. L. – RA09
ARSENAULT, D. L. – RA07
ARUNAN, E. – TH03, RH08
AVOIRD, A. V. D. – WF04, WF05, RJ03

B
BAGLAYAN, O. – FB09, FB10
BAHOU, M. – MJ01, RD06, RD08
BAKKER, J. M. – WJ10
BALDWIN, J. – FD07
BANDYOPADHYAY, B. – TJ04, W108
BANERJEE, J. – RG08
BARABAN, J. H. – WG01, WG02, WG03
BARKER, B. J. – WJ02
BARTELS, N. – RG07
BARTH, R. – RA03
BARTLETT, J. H. – RA05
BASTERRETXEA, F. J. – TC07
BAUDHUIN, M. A. – MI06
BAYKUSHEVA, D. – WI05
BEALE, C. – RF07
BEAMES, J. M. – TI08
BECHER III, E. L. – FE07
BECKLIN, E. E. – RF01, RF02
BEHERE, S. H. – RG04
BELL, E. – RA03
BELL, M. T. – FD02
BELL, T. – WH01
BELL, T. A. – WH13
BELLETT, D. – TB10
BELLOS, M. A. – RG08
BENNER, D. C. – TA08, TA09, RB01, FA08, FA09
BERDEN, G. – MG10
BERGIN, E. A. – WH02
BERKE, A. E. – RE10
BERMEJO, D. – RB06
BERMUDEZ, M. – RG08
BERNATH, P. F. – RA10, RF07, RG05, FB01
BESIEN, H. V. – TH06
BETZ, T. – FC07
BILLINGHURST, B. E. – TF01, RF13
BINNS, M. K. L. – RH07
BISWAL, H. S. – TD04
BISWAS, B. – WG10
BJORK, B. – FA11
BLAKE, G. A. – MF06, TC01, TC02, TC03
BLAKE, T. A. – FA08
BLOOM, S. – FB03
BOATWRIGHT, A. – RI02
BOHN, R. K. – TH07
BONNAMY, A. – TE07, WI04
BOOPALACHANDRAN, P. – MI06
BORGUET, E. – TJ02
BOTSCHWINA, P. – WI09, WI10
BOTTINELLI, S. – FA12
BOUCHEZ, A. – FA12
BOUDON, V. – RB06, RC10
BOWEN, K. H. – MI05
BOYARKIN, O. V. – TJ06
BRATHWAITE, A. D. – MG03, TJ05
BRAUER, C. S. – TH10
BRAZIER, C. – RE07
BRECKENRIDGE, W. H. – FE06
BRENNER, V. – TD04, TJ07
BROGAN, C. L. – WH11
BROQUIER, M. – TD04
BROWN, J. – RJ02
BROWN, K. R. – RD01
BROWN, L. R. – TA08, TA09, RB03, RB04, RB07, FA07, FA08
BROWN-XU, S. E. – WG12, FB11
BRUMFIELD, B. E. – FB05
BRÉCHIGNAC, P. – TE07
BUCCHINO, M. P. – RH07
BUCHANAN, E. G. – WF12, WG08
BUCHWITZ, M. – RB09
BUI, T. Q. – TA06
BUNKER, P. R. – W101
BUONAUGURIO, A. M. – MI05
BURROWS, J. – RB09
BURROWS, J. P. – TA07
BÖTTCHER, A. – MJ08

C
CAMINATI, W. – TC08, RH11
CAMPARGUE, A. – TA11
CANDEMIR, N. – RJ10
CARLOTTI, M. – TA10
CAROLLO, R. – RG08
CARR, J. M. – TF10
CARRINGTON JR., T. – WA04, RJ02
CARROLL, A. – FC04
CARROLL, P. B. – TC01, TC02, TC03
CASE, A. S. – TB02, TD06
CASTANO, F. – MH13, TB04, TB05, TC07, TC08, FA02
CATIKKAS, B. – MF14
CAZZOLI, G. – RH01, FC09
CERNICHARO, J. – WH01, FA03, FA04
CHALAYAVI, N. – TJ12
CHAN, M. – RA04, RA11
CHANDLER, D. W. – MF04
CHANG, B. – WG04
CHANGALA, P. B. – WG01, WG02
CHELIN, P. – MF09
CHEN, C. – TB01, WG04
CHEN, J. – MI05
CHEN, K. – WG11, FD10
CHEN, M. – TJ01, WI13, RE08
CHEN, Y. – WG11
CHEN, Z. – TF06
CHENG, T. C. – MG07, MG08, TJ04
CHESNOKOV, E. – MJ12
CHEUNG, A. S. – RA01
CHEUNG, A. S.- C. – RA04, RA11
CHHANTYAL-PUN, R. – TI13, RE08
<table>
<thead>
<tr>
<th>Name</th>
<th>Code</th>
</tr>
</thead>
<tbody>
<tr>
<td>CHIANG, N.</td>
<td>FD09</td>
</tr>
<tr>
<td>CHIEDA, M. A.</td>
<td>FD04</td>
</tr>
<tr>
<td>CHISHOLM, M. H.</td>
<td>WG12</td>
</tr>
<tr>
<td>CHOWDHURY, A.</td>
<td>FE07</td>
</tr>
<tr>
<td>CHRISTOPHER, C. R.</td>
<td>RG13</td>
</tr>
<tr>
<td>CICH, M. J.</td>
<td>TA01</td>
</tr>
<tr>
<td>CIRTOG, M.</td>
<td>TJ07</td>
</tr>
<tr>
<td>CLARK, B.</td>
<td>MF13</td>
</tr>
<tr>
<td>CLAYTON, R.</td>
<td>TG12</td>
</tr>
<tr>
<td>CLOUTHIER, D. J.</td>
<td>TG04, RG10</td>
</tr>
<tr>
<td>COAKLEY, J. A.</td>
<td>FA09</td>
</tr>
<tr>
<td>COCINERO, E.</td>
<td>TC08</td>
</tr>
<tr>
<td>Cookey, J. A.</td>
<td>FA09, FA07</td>
</tr>
<tr>
<td>CODY, T. J.</td>
<td>TI01, TI02, WI13</td>
</tr>
<tr>
<td>COHEN, E. A.</td>
<td>RB04</td>
</tr>
<tr>
<td>COLOMBO, A.</td>
<td>RE02</td>
</tr>
<tr>
<td>COMBS, A. B.</td>
<td>MJ09</td>
</tr>
<tr>
<td>COMPTON, R.</td>
<td>TB11</td>
</tr>
<tr>
<td>CONDE, A. P.</td>
<td>TB04, TB05</td>
</tr>
<tr>
<td>CONRAD, A. A.</td>
<td>TH06</td>
</tr>
<tr>
<td>CONROY, T.</td>
<td>RB05</td>
</tr>
<tr>
<td>CONSORTIUM, T. P.</td>
<td>WH05</td>
</tr>
<tr>
<td>CONSTABLE, S.</td>
<td>RI13</td>
</tr>
<tr>
<td>CONTINETTI, R. E.</td>
<td>MI02, MI03</td>
</tr>
<tr>
<td>Cooke, S. A.</td>
<td>TC04, TC05, TC06, TC09, TC11, RH12</td>
</tr>
<tr>
<td>COssel, K. C.</td>
<td>FA11</td>
</tr>
<tr>
<td>COUDE R, L. H.</td>
<td>TH12, FA05</td>
</tr>
<tr>
<td>COUTENS, A.</td>
<td>WH13</td>
</tr>
<tr>
<td>COX, E. G.</td>
<td>WH09</td>
</tr>
<tr>
<td>CRABTREE, K. N.</td>
<td>WJ06, WJ07, RC11</td>
</tr>
<tr>
<td>CRAIG, N. C.</td>
<td>TC13, TH06</td>
</tr>
<tr>
<td>CRAWFORD, T. D.</td>
<td>RF09, RG14</td>
</tr>
<tr>
<td>CRIM, F. F.</td>
<td>TB02, TB06, TB07, RE10, RE11</td>
</tr>
<tr>
<td>CRISP, D.</td>
<td>TA09</td>
</tr>
<tr>
<td>CROCKETT, N. R.</td>
<td>WH02</td>
</tr>
<tr>
<td>CROSSLEY, M. J.</td>
<td>TI12</td>
</tr>
<tr>
<td>CROZET, P.</td>
<td>RA09</td>
</tr>
<tr>
<td>DAHLSTROM, J.</td>
<td>WH07</td>
</tr>
<tr>
<td>DAILY, J. W.</td>
<td>TF08</td>
</tr>
<tr>
<td>DANGI, B.</td>
<td>WJ03</td>
</tr>
<tr>
<td>DARKHALIL, I. D.</td>
<td>TF12</td>
</tr>
<tr>
<td>DAS, A.</td>
<td>WG07</td>
</tr>
<tr>
<td>DAVIS, Z. S.</td>
<td>TF10</td>
</tr>
<tr>
<td>DAWADI, M. B.</td>
<td>WF11</td>
</tr>
<tr>
<td>DAWES, R.</td>
<td>RJ02, RJ03</td>
</tr>
<tr>
<td>DE LUCA, M.</td>
<td>WH13</td>
</tr>
<tr>
<td>DE LUCIA, F. C.</td>
<td>TF01, TH13, RC08, RE06</td>
</tr>
<tr>
<td>DE OLIVEIRA, N.</td>
<td>RC07</td>
</tr>
<tr>
<td>DE WIT, G.</td>
<td>RE09</td>
</tr>
<tr>
<td>DEAN, J.</td>
<td>FB08</td>
</tr>
<tr>
<td>DEAN, J. C.</td>
<td>TF09, WG09, WG10</td>
</tr>
<tr>
<td>DE BLASE, A. F.</td>
<td>FB03</td>
</tr>
<tr>
<td>DECHIRICO, F.</td>
<td>TC06</td>
</tr>
<tr>
<td>DEMAISON, J.</td>
<td>TC13</td>
</tr>
<tr>
<td>DEMPSTER, S. P.</td>
<td>FC10</td>
</tr>
<tr>
<td>DEO, M. N.</td>
<td>RG04</td>
</tr>
<tr>
<td>DEPRINCE, B. A.</td>
<td>RC09, FC04</td>
</tr>
<tr>
<td>DEVI, V. M.</td>
<td>TA08, TA09, RB01, FA08, FA09</td>
</tr>
<tr>
<td>DIAN, B. C.</td>
<td>WG09</td>
</tr>
<tr>
<td>DIDDAMS, S.</td>
<td>FA11</td>
</tr>
<tr>
<td>DIDRICH, K.</td>
<td>WF08</td>
</tr>
<tr>
<td>DIEZ-Y-RIEGA, H.</td>
<td>WG05</td>
</tr>
<tr>
<td>DIJK, C. W. V.</td>
<td>TH08</td>
</tr>
<tr>
<td>DOLPH, J.</td>
<td>FA09</td>
</tr>
<tr>
<td>DONTOT, L.</td>
<td>TE07</td>
</tr>
<tr>
<td>DOROFEEVA, T.</td>
<td>FB06</td>
</tr>
<tr>
<td>DOSLIC, N.</td>
<td>TD04</td>
</tr>
<tr>
<td>DOUBERLY, G. E.</td>
<td>MJ07, RI05, RI09, RI10</td>
</tr>
<tr>
<td>DOWN, M. J.</td>
<td>MF09</td>
</tr>
<tr>
<td>DRABBELS, M.</td>
<td>RI01</td>
</tr>
<tr>
<td>DROUIN, B.</td>
<td>FA03</td>
</tr>
<tr>
<td>DROUIN, B. J.</td>
<td>TA04, TA05, TH10, WH12, WH13, RB04, RC01, RF03, RF04, RF12, RF13, FA01</td>
</tr>
<tr>
<td>DRUCKER, S.</td>
<td>TG06, TG07</td>
</tr>
<tr>
<td>DU, J.</td>
<td>WG04</td>
</tr>
<tr>
<td>DUAN, C.</td>
<td>WF02</td>
</tr>
<tr>
<td>DUDDDING, T.</td>
<td>FB03</td>
</tr>
<tr>
<td>DUNBAR, R. C.</td>
<td>MG10</td>
</tr>
<tr>
<td>DUNCAN, M. A.</td>
<td>MG03, MG07, MG08, TJ04, TJ05, WJ08</td>
</tr>
<tr>
<td>DUNKELBERGER, A. D.</td>
<td>TB06, TB07</td>
</tr>
<tr>
<td>DUONG, C. H.</td>
<td>TC05</td>
</tr>
<tr>
<td>DURIG, J. R.</td>
<td>TF12</td>
</tr>
<tr>
<td>DURR, C. B.</td>
<td>WG12, FB11</td>
</tr>
<tr>
<td>DUXBURY, G.</td>
<td>MG01, MG02, TA03</td>
</tr>
<tr>
<td>DYER, L.</td>
<td>MH03</td>
</tr>
<tr>
<td>ECOGNIDES, G.</td>
<td>MH03</td>
</tr>
<tr>
<td>EDWARDS, J. L.</td>
<td>WH09</td>
</tr>
<tr>
<td>EHARA, M.</td>
<td>TD07</td>
</tr>
<tr>
<td>EIDELBERG, M.</td>
<td>RC07</td>
</tr>
<tr>
<td>EILERS, H.</td>
<td>WG05</td>
</tr>
<tr>
<td>EIJCA, P.</td>
<td>TC08</td>
</tr>
<tr>
<td>ELKINS, M.</td>
<td>TE10</td>
</tr>
<tr>
<td>ELLIS, A. M.</td>
<td>RI02</td>
</tr>
<tr>
<td>ELLISON, G. B.</td>
<td>TF08</td>
</tr>
<tr>
<td>ELMUTI, L. F.</td>
<td>MH07, MH08</td>
</tr>
<tr>
<td>ELSAYED, M.</td>
<td>WI02</td>
</tr>
<tr>
<td>ENDO, Y.</td>
<td>MH04, MH05</td>
</tr>
<tr>
<td>ENDRES, C. P.</td>
<td>RC01, RC02, RF11, FA12</td>
</tr>
<tr>
<td>ENGEL, G. S.</td>
<td>MA03</td>
</tr>
<tr>
<td>ERNST, W. E.</td>
<td>WJ05, WJ06, FD08</td>
</tr>
<tr>
<td>ESSELMAN, B. J.</td>
<td>MJ04</td>
</tr>
<tr>
<td>EVANGELISTI, L.</td>
<td>TC08, RH11</td>
</tr>
<tr>
<td>EVANS, C. J.</td>
<td>TC10, RH13</td>
</tr>
<tr>
<td>EVANS, W. R.</td>
<td>FD06</td>
</tr>
<tr>
<td>EVERITT, H. O.</td>
<td>RB08, RE06</td>
</tr>
<tr>
<td>EYLER, E. E.</td>
<td>RG08, FD04, FD05</td>
</tr>
<tr>
<td>F</td>
<td></td>
</tr>
<tr>
<td>FALGarONE, E.</td>
<td>WH13</td>
</tr>
<tr>
<td>FAILO, C.</td>
<td>TE07</td>
</tr>
<tr>
<td>FARRELLY, D.</td>
<td>WF06</td>
</tr>
<tr>
<td>FAUER, A.</td>
<td>WJ04, WJ05, RC03</td>
</tr>
<tr>
<td>FAVERO, L. B.</td>
<td>TC08</td>
</tr>
<tr>
<td>FAWZY, W. M.</td>
<td>WJ02, WJ03</td>
</tr>
<tr>
<td>FEAUTRIER, N.</td>
<td>RC03</td>
</tr>
<tr>
<td>FEDERMAN, S. R.</td>
<td>RC07</td>
</tr>
<tr>
<td>FEHNEL, R. R.</td>
<td>RI03, RI04</td>
</tr>
<tr>
<td>FENG, C.</td>
<td>RI02</td>
</tr>
<tr>
<td>FENG, G.</td>
<td>TC08, RH11</td>
</tr>
<tr>
<td>FERMANN, M.</td>
<td>MF07</td>
</tr>
<tr>
<td>FERNANDEZ, J. A.</td>
<td>TC08, FA02</td>
</tr>
<tr>
<td>FERNÁNDEZ, B.</td>
<td>WF06</td>
</tr>
<tr>
<td>FERNÁNDEZ, J. A.</td>
<td>TC07</td>
</tr>
<tr>
<td>FERNÁNDEZ-FERNÁNDEZ, M.</td>
<td>TB04</td>
</tr>
<tr>
<td>FIELD, R.</td>
<td>RE02</td>
</tr>
<tr>
<td>FIELD, R. W.</td>
<td>TG04, WG01, WG02, WG03, RE12, RG07</td>
</tr>
<tr>
<td>FILLION, J. H.</td>
<td>RC07</td>
</tr>
<tr>
<td>FINNERAN, I. A.</td>
<td>TC01, TC02, TC03, TH04</td>
</tr>
<tr>
<td>FISHER, A. P.</td>
<td>RB08</td>
</tr>
<tr>
<td>FITZGERALD, S.</td>
<td>MJ11</td>
</tr>
<tr>
<td>FLAUD, J. M.</td>
<td>TA10</td>
</tr>
<tr>
<td>FLEISHER, A. J.</td>
<td>FA11</td>
</tr>
<tr>
<td>FLETCHER, L. N.</td>
<td>FA08</td>
</tr>
<tr>
<td>FLYNN, S. D.</td>
<td>MJ07, RI05</td>
</tr>
</tbody>
</table>