67th OSU INTERNATIONAL SYMPOSIUM ON MOLECULAR SPECTROSCOPY
JUNE 18-22, 2012

	MONDAY JUNE 18 8:45AM	TUESDAY JUNE 19 8:30AM	WEDNESDAY JUNE 20 8:30AM	THURSDAY JUNE 21 8:30AM	FRIDAY JUNE 22 8:30AM
AUDITORIUM INDEPENDENCE HALL	MA. PLENARY SESSION AWARDS		WA. PLENARY SESSION		
ROOM 160 MATH ANNEX*		TA. ATMOSPHERIC SPECIES		RA. ELECTRONIC	FA. ASTRONOMICAL SPECIES & PROCESSES
ROOM 170 MATH ANNEX*		TB. DYNAMICS		RB. ATMOSPHERIC SPECIES	FB. INFRARED/RAMAN
ROOM 1000 MCPHERSON LAB		TC. MICROWAVE		RC. ASTRONOMICAL SPECIES & PROCESSES	FC. MICROWAVE
ROOM 1015 MCPHERSON LAB		TD. MINI-SYMPOSIUM: PHOTODETACHMENT & PHOTOIONIZATION		RD. MINI-SYMPOSIUM: COLD QUANTUM SYSTEMS	FD. MINI-SYMPOSIUM: COLD QUANTUM SYSTEMS
ROOM 2015 MCPHERSON LAB		TE. MINI-SYMPOSIUM: SPECTROSCOPY OF INTERFACES		RE. DYNAMICS	FE. THEORY
1:30PM					
ROOM 160 MATH ANNEX*	MF. INFRARED/RAMAN	TF. INFRARED/RAMAN	WF. INFRARED/RAMAN	RF. ASTRONOMICAL SPECIES & PROCESSES	
ROOM 170 MATH ANNEX*	MG. RADICALS AND IONS	TG. ELECTRONIC	WG. ELECTRONIC	RG. ELECTRONIC	
ROOM 1000 MCPHERSON LAB	MH. MICROWAVE	TH. MICROWAVE	WH. ASTRONOMICAL SPECIES & PROCESSES	RH. MICROWAVE	
ROOM 1015 MCPHERSON LAB	MI. MINI-SYMPOSIUM: PHOTODETACHMENT & PHOTOIONIZATION	TI. RADICALS AND IONS	WI. RADICALS/IONS	RI. MINI-SYMPOSIUM: COLD QUANTUM SYSTEMS	
ROOM 2015 MCPHERSON LAB	MJ. MATRIX/CONDENSED PHASE	TJ. MINI-SYMPOSIUM: SPECTROSCOPY OF INTERFACES	WJ. MINI-SYMPOSIUM: PHOTODETACHMENT & PHOTOIONIZATION	RJ. THEORY	

*** 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[a]

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

[a]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 **5 min 11:05**
Presentation of Award by Michael L. Myrick, President, Coblentz Society

MA03 ***Coblentz Society Award Lecture*** **40 min 11:10**

IMAGING EXCITED STATE DYNAMICS WITH 2D ELECTRONIC SPECTROSCOPY

GREGORY S. ENGEL, *Department of Chemistry, The University of Chicago, Chicago USA*.

MF. INFRARED/RAMAN

MONDAY, JUNE 18, 2012 – 1:30 PM

Room: 160 MATH ANNEX

Chair: MASARU FUKUSHIMA, Hiroshima City University, Hiroshima, Japan

MF01 **10 min 1:30**

TIME RESOLVED FTIR ANALYSIS OF COMBUSTION OF AN ETHANOL/ISOPROPANOL MIXTURE IN A COMMERICIAL 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 REFERNCED SUB-DOPPLER RESOLUTION DIFFERENCE-FREQUENCY-GENERATION INFRARED SPECTROMETER

K. IWAKUNI, S. OKUBO, H. NAKAYAMA, and H. SASADA, *Department of Phisics, 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*.

MF07 **15 min 3:07**

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

MF08 **15 min 3:40**

DIRECT MEASUREMENTS OF COLLISIONALLY BROADENED (CO_2-CO_2) S-BRANCH RAMAN COHERENCE LIFETIMES OF CO_2

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 Energies, LLC, 5100 Springfield Street, Suite 301, Dayton, OH 45431*; JAMES R. GORD, *Air Force Research Laboratory, Propulsion Directorate, Wright-Patterson AFB, OH 45433*.

MF09 **10 min 3:57**

ANALYSIS OF AN ^{18}O AND D ENHANCED FT-IBBCEAS WATER SPECTRUM: NEW ASSIGNMENTS FOR $HD^{18}O$, $HD^{16}O$, $D_2{}^{18}O$ AND $D_2{}^{16}O$ 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*.

MF10 **10 min 4:09**

TOWARDS PERFECT WATER LINE INTENSITIES

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

MF11 **15 min 4:21**

HIGH-RESOLUTION INFRARED SPECTROSCOPY OF THE $(1,0,1)-(0,0,0)$ BAND OF C_3

S. THORWIRTH, J. KRIEG, I. KEPPELER, 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.*

MF12 **15 min 4:38**

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*.

MF13 **15 min 4:55**

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*.

MF14 **10 min 5:12**

VIBRATIONAL SPECTRA OF THE $MLCl_2$ 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 H_2S+: 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 H_2S+: 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 ASSYMETRIC 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,[a] MANORI PERERA,[b] 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*.

[a]Present Address: IMRA, Ann Arbor, MI 48105
[b]Present 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*.

MG06 **15 min 2:55**

SPONTANEOUS EMISSION BETWEEN ORTHO- AND PARA-LEVELS OF WATER-ION, H_2O^+

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

MG07 **15 min 3:30**

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*.

MG08 **15 min 3:47**

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*.

MG09 **15 min 4:04**

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*.

MG10 **15 min 4:21**

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*.

MG11 **15 min 4:38**

INFRARED SPECTROSCOPIC EVIDENCE FOR ISOTOPOLOGS OF THE HOHOH 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*.

MG12 **15 min 4:55**

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*.

MG13 **15 min 5:12**

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

N. P. ROEHR, J. SZCZEPANSKI, N. C. POLFER, *Department of Chemistry, University of Florida, Gainesville, FL 32608*.

MH. MICROWAVE

MONDAY, JUNE 18, 2012 – 1:30 PM

Room: 1000 MCPHERSON LAB

Chair: GARRY GRUBBS, Wesleyan University, Middletown, Connecticut

MH01 **15 min 1:30**

BROADBAND ROTATIONAL SPECTRUM AND MOLECULAR GEOMETRY OF OC $\cdots$AgI

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.*.

MH02 **15 min 1:47**

MICROWAVE SPECTRUM AND GEOMETRY OF $H_3P\cdots$AgI

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.*.

MH03 **15 min 2:04**

MICROWAVE SPECTROSCOPY AND INTERNAL DYNAMICS OF THE Ne-NO_2 VAN DER WAALS COMPLEX

BRIAN J. HOWARD, GEORGE ECONOMIDES and LEE DYER, *Department of Chemistry, Oxford University, South Parks Road, Oxford, OX1 3QZ, United Kingdom*.

MH04 **15 min 2:21**

FTMW SPECTROSCOPY AND DETERMINATION OF THE 3-D POTENTIAL ENERGY SURFACE FOR Ar-CS

CHISATO NIIDA, MASAKAZU NAKAJIMA, YASUKI ENDO, *Department of Basic Science, The University of Tokyo, Tokyo 153-8902, Japan*; YOSHIHIRO SUMIYOSHI, *Department of Chemistry and Chemical biology, Gunma University, Maebashi Gunma, 371-8510, Japan*; YASUHIRO OHSHIMA, *Department of Photo-Molecular Science, Institute for Molecular Science, Okazaki, 444-8585, Japan*; HIROSHI KOHGUCHI, *Department of Chemistry, Hiroshima University, Higashi-Hiroshima, 739-8511, Japan*.

MH05 **15 min 2:38**

OBSERVATION OF THE PURE ROTATIONAL SPECTRA OF THE H_2O-$trans$-HOCO COMPLEX

TAKAHIRO OYAMA, MASAKAZU NAKAJIMA, YASUKI ENDO, *Department of Basic Science, Graduate School of Arts and Sciences, The University of Tokyo, Komaba, Meguro-ku, Tokyo, 153-8902, Japan*; and YOSHIHIRO SUMIYOSHI, *Department of Chemistry and Chemical Biology, Gunma University, 4-2 Aramaki-machi, Maebashi City, Gunma, 371-8510 Japan*.

MH06 **15 min 2:55**

STRUCTURE AND INVERSION MOTIONS OF THE WEAKLY BOUND $CH_2F_2\cdots CO_2$ DIMER

REBECCA A. PEEBLES, AMELIA J. THOMAS, MICHAL M. SERAFIN and SEAN A. PEEBLES, *Department of Chemistry, Eastern Illinois University, 600 Lincoln Ave., Charleston, IL 61920*.

MH07 **10 min 3:12**

ANALYSIS OF MICROWAVE SPECTRUM, INTERNAL ROTATION AND C–H···F INTERACTIONS OF THE $CHF_3 \cdots C_2H_3F$ 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_3SiF_2-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 ***INVITED TALK*** **15 min 4:00**

MICROWAVE SPECTRA AND GEOMETRIES OF $H_2C_2 \cdots AgCl$ AND $H_2C_2 \cdots CuCl$

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 $H_2S \cdots ICF_3$ and $H_2O \cdots ICF_3$ 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_2 -$(CH_3)_2$ S

YOSHIYUKI KAWASHIMA and TAKAYUKI MORITANI, *Department of Applied Chemistry, Faculty of Engineering, Kanagawa Institute of Technology, Atsugi, Kanagawa 243-0292, JAPAN*; EIZI HIROTA, *The Graduate University for Advanced Studies, Hayama, Kanagawa 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 Espectroscopía 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

MI01 ***INVITED TALK*** **30 min 1:30**

SLOW-ELECTRON VELOCITY-MAP IMAGING OF NEGATIVE IONS: APPLICATIONS TO SPECTROSCOPY AND DYNAMICS

DANIEL NEUMARK, *Department of Chemistry, University of California at Berkeley, B64 Hildebrand Hall, Berkeley, CA 94720*.

MI02 **15 min 2:05**

STATE-RESOLVED PREDISSOCIATION DYNAMICS OF THE FORMYLOXYL RADICAL BY DISSOCIATIVE PHOTODETACHMENT OF HCO_2^- / DCO_2^-

AMELIA W. RAY, BEN B. SHEN, BERWYCK L. J. POAD and ROBERT E. CONTINETTI[a], *Department of Chemistry and Biochemistry, University of California, San Diego, La Jolla, CA 92093*.

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

MI03 **15 min 2:22**

PHOTOELECTRON-PHOTOFRAGMENT COINCIDENCE SPECTROSCOPY OF TERT-BUTOXIDE AND THE CARBANION ISOMER

BEN B. SHEN, BERWYCK L. J. POAD, AMELIA W. RAY, and ROBERT E. CONTINETTI[a], *Department of Chemistry and Biochemistry, University of California, San Diego, CA 92093*.

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

MI04 **15 min 2:39**

VIBRATIONAL AUTODETACHMENT: INTRAMOLECULAR VIBRATIONAL RELAXATION TO ELECTRONIC MOTION

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

MI05 **15 min 2:56**

PHOTOELECTRON SPECTROSCOPY OF RARE-GAS SOLVATED NUCLEOBASE ANIONS

ANGELA M. BUONAUGURIO, JING CHEN, AND KIT H. BOWEN, *Department of Chemistry, Johns Hopkins University, Baltimore, MD 21218*.

Intermission

MI06 **15 min 3:30**

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*.

MI07 **15 min 3:47**

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*.

MI08 **15 min 4:04**

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*.

MI09 **15 min 4:21**

ANION PHOTOELECTRON ANGULAR DISTRIBUTIONS: ELECTRON SCATTERING RESONANCES IN PHOTODETACHMENT

RICHARD MABBS, *Washington University in St. Louis, St. Louis, Mo, 63130*.

MI10 **15 min 4:38**

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*.

MI11 **15 min 4:55**

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*.

MI12 **15 min 5:12**

ELECTRON PROPAGATOR THEORY OF AQUEOUS HALIDE PHOTOELECTRON SPECTRA

J. V. ORTIZ, *Department of Chemistry and Biochemistry*
Auburn University
Auburn, Alabama 36849-5312.

MJ. MATRIX/CONDENSED PHASE

MONDAY, JUNE 18, 2012 – 1:30 PM

Room: 2015 MCPHERSON LAB

Chair: MICHAEL HEAVEN, Emory University, Atlanta, Georgia

MJ01 **15 min 1:30**

IDENTIFICATION OF α- AND β-PROTONATED NAPHTHALENE ($C_{10}H_9{}^+$) AND THEIR NEUTRAL COUNTERPARTS 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 3:30**

HELIUM NANODROPLET ISOLATION OF IONIC LIQUID VAPOR: INRARED LASER SPECTROSCOPY OF [EMIM][Tf_2N]

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 STRELNIKOV, 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 SiC_5 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 $(PbI_2)_{(1-x)}$ $(BiI_3)_{(x)}$

IGOR VERTEGEL, EUGENE CHESNOKOV and ALEKSANDR OVCHARENKO, *Institute of Physics National Academy of Sciences of Ukraine 46, Prospect Nauki, 03680 Kiev, Ukraine*.

TA. ATMOSPHERIC SPECIES

TUESDAY, JUNE 19, 2012 – 8:30 AM

Room: 160 MATH ANNEX

Chair: LINDA BROWN, Jet Propulsion Laboratory, Pasadena, California

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), Universite 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 $X^3\Sigma_g^-$, $a^1\Delta_g$, 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 SUBSTITUTED 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*.

TA06 **10 min 9:55**

LINE MIXING EFFECTS OF O_2 A-BAND WITH PHOTOACOUSTIC SPECTROSCOPY IN SUPPORT OF REMOTE SENSING

THINH Q. BUI[a], 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*.

[a]Support from NSF Graduate Fellowship and NASA OCO Funding are gratefully acknowledged

Intermission

TA07 **10 min 10:30**

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*.

TA08 **15 min 10:42**

AIR-BROADENED LINE PARAMETERS FOR THE 2←0 BANDS OF $^{13}C^{16}O$ AND $^{12}C^{18}O$ AT 2.3 μm

V. MALATHY DEVI, D. CHRIS BENNER, *The College of William and Mary, Williamsburg, VA 23187*; M. A. H. SMITH, *Science Directorate, NASA Langley Research Center, Hampton, VA 23681*; A. W. MANTZ, *Dept. of Physics, Astronomy and Geophysics, Connecticut College, New London, CT 06320*; K. SUNG and L. R. BROWN, *Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109*.

TA09 **15 min 10:59**

SPEED DEPENDENT LINE SHAPES IN 1.61 μm AND 2.07 μm CO_2 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.*.

TA10 **15 min 11:16**

THE ν_3 AND ν_4 BANDS OF NITRIC ACID (HNO_3) AT 7.6 μm FOR ATMOSPHERIC STUDIES

A.PERRIN, J.M.FLAUD, *Laboratoire Inter Universitaire des Systemes Atmosphériques, 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), Universiy of Bologna, Viale del Risorgimento, 4 - 40136 - Bologna, Italy*.

TA11 **15 min 11:33**

FIRST HIGH RESOLUTION ANALYSIS OF THE $5\nu_3$ BAND OF NITROGEN DIOXIDE NEAR 1.3 μm

D.MONDELAIN, S.KASSI, A.CAMPARGUE, *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 Atmosphériques (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 Ã STATES OF C_3, C_3-NE, AND C_3-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 CHOLOROIODOMETHANE 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, JAEYOON SHIN, TRACY OUDENHOVEN, and F. FLEMING CRIM, *Department of Chemistry, Universtiy of Wisconsin-Madison, Madison, WI 53706*.

Intermission

TB07 **15 min 10:30**

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

ADAM D. DUNKELBERGER, RYAN D. KIEDA, JAEYOON SHIN, *Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706*; RICARDO ROSSI PACCANI, STEFANIA FUSI, *UniversitÃă di Siena, Siena, I-53100, Italy*; MASSIMO OLIVUCCI, *UniversitÃă 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*.

TB08 **15 min 10:47**

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, LIJUAN WANG, and DONGPING ZHONG, *Department of Physics, Chemistry, and Biochemistry, The Ohio State University, Columbus, OH 43210.*.

TB09 **15 min 11:04**

MOLECULAR UNDERSTANDING OF EFFICIENT DNA REPAIR MACHINERY OF PHOTOLYASE

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

TB10 **15 min 11:21**

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*.

TB11 **15 min 11:38**

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*.

TC. MICROWAVE

TUESDAY, JUNE 19, 2012 – 8:30 AM

Room: 1000 MCPHERSON LAB

Chair: PHILLIP SHERIDAN, Canisius College, Buffalo, New York

TC01 **10 min 8:30**

PURE ROTATIONAL SPECTROSCOPY OF PANHs I: 1,10-PHENANTHROLINE. IMPLICATIONS OF PANHs IN ASTROPHYSICAL 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*.

TC06 **15 min 9:40**

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*.

TC07 **15 min 9:57**

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

EMILIO J. COCINERO, PATRICIA ECIJA, 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*.

TC08 **15 min 10:14**

FOURIER TRANFORM 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 Quimica Fisica, Facultad de Ciencia y Tecnologia, Universidad del Pais Vasco, E-48080 Bilbao, Spain*; ALBERTO LESARRI, *Departamento de Quimica Fisica y Quimica Inorganica, Facultad de Ciencias, Universidad de Valladolid, E-47011 Valladolid, Spain*; ROLF MEYER, *Sonnenbergstrasse 18, CH-5621 Zufikon, Switzerland*.

Intermission

TC09 **15 min 10:45**

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*.

TC10 **10 min 11:02**

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*.

TC11 **15 min 11:14**

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*.

TC12 **15 min 11:31**

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

I. 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*.

TC13 **15 min 11:48**

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 and 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 CYCLOOCTATERAENE

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·Ar_n and ICN·$(CO_2)_n$

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 $(CH_3)_3N\text{-}H^+\text{-}(H_2O)_n$ (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*.

TF. INFRARED/RAMAN

TUESDAY, JUNE 19, 2012 – 1:30 PM

Room: 160 MATH ANNEX

Chair: KEEYON SUN, JPL-CalTech, Pasadena, California

TF01 **15 min 1:30**

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*.

TF02 **15 min 1:47**

COMBINATION BANDS OF THE NONPOLAR OCS DIMER INVOLVING INTERMOLECULAR MODES

M. REZAEI, J. NOROOZ OLIAEE, 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*.

TF03 **15 min 2:04**

PHOTOIONIZATION INDUCED WATER MIGRATION OF 4-AMINOBENZONITRILE-$(H_2O)_1$ 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*.

TF04 **15 min 2:21**

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*.

TF05 **15 min 2:38**

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*.

TF12 **15 min 4:50**

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 $\tilde{A}\ ^2\Delta$ – $\tilde{X}\ ^2\Pi$ 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 $b^1\Sigma^+$ - $X^3\Sigma^-$ TRANSITION OF O_2 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 (Cl_2^+)

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, NiO_2

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

Intermission

TG06 **15 min 3:10**

CAVITY RINGDOWN ABSORPTION SPECTRUM OF THE $T_1(n, \pi^*) \leftarrow S_0$ TRANSITION OF ACROLEIN: ANALYSIS OF THE 0_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 **15 min 3:27**

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

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

TG08 **15 min 3:44**

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 **15 min 4:01**

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 **15 min 4:18**

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 **15 min 4:35**

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

NATHANAEL M. KIDWELL, DEEPALI 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 **15 min 4:52**

VIBRONIC SPECTROSCOPY OF PHENYLVINYLNITRILE

DEEPALI 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*.

TH. MICROWAVE

TUESDAY, JUNE 19, 2012 – 1:30 PM

Room: 1000 MCPHERSON LAB

Chair: SHANSHAN YU, Jet Propulsion Laborabory, Pasadena, California

TH01 **15 min 1:30**

PROTIC ACID HYDROGEN BONDING IN CHLOROFLUOROETHYLENES: THE HYDROGEN FLUORIDE-VINYL CHLORIDE COMPLEX

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

TH02 **15 min 1:47**

BROADBAND CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE SPECTROSCOPY AND MOLECULAR STRUCTURE OF THE ARGON-*(Z)*-1-CHLORO-2-FLUOROETHYLENE COMPLEX

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

TH03 **15 min 2:04**

ROTATIONAL SPECTRUM OF Ar...PROPARGYL ALCOHOL COMPLEX

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

TH04 **15 min 2:21**

ROTATIONALLY-RESOLVED SPECTRA OF 2-METHYLFURAN FROM THE CM-WAVE TO THE FAR INFRARED

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*.

TH05 **15 min 2:38**

THE FOURIER TRANSFORM MICROWAVE (FTMW) SPECTRA OF CYCLOHEXENE OXIDE AND ITS ARGON COMPLEX

DANIEL J. FROHMAN, STEWART E. NOVICK, and WALLACE C. PRINGLE, *Department of Chemistry, Wesleyan University, 52 Lawn Ave., Middletown, CT 06459-0180*.

TH06 **15 min 2:55**

MICROWAVE SPECTRA OF DEUTERIUM ISOTOPOLOGUES OF *cis*-HEXATRIENE

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*.

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 (NH_2CH_2CN)

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

W. STAHL, H. V. L. NGUYEN, L.W. SUTIKDJA, D. JELISAVAC, H. MOUHIB, *Institute of Physical Chemistry, RWTH Aachen University, Landoltweg 2, D-52074 Aachen, Germany*; I. KLEINER, *Laboratoire Interuniversitaire des Systèmes Atmosphériques, CNRS et Universités Paris Diderot et Paris Est, 61 av. Général de Gaulle, 94010, Créteil, France*.

TH12 **15 min 4:51**

ROTATIONAL ENERGIES IN VARIOUS TORSIONAL LEVELS OF CH_2DOH[a]

L. H. COUDERT, A. EL HILALI, *LISA, CNRS/Universités Paris Est et Paris Diderot, 61 Avenue du Général de Gaulle, 94010 Créteil, France*; L. MARGULÈS, 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*.

[a] Work 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, $(CH_3)_3CCH_2OH$

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*.

TI. RADICALS AND IONS

TUESDAY, JUNE 19, 2012 – 1:30 PM

Room: 1015 MCPHERSON LAB

Chair: JINJUN LIU, University of Louisville, Louisville, Kentucky

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[a], MOURAD ROUDJANE and TERRY A. MILLER, *Laser Spectroscopy Facility, The Ohio State University, Columbus, Ohio 43210*.

[a]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 3^1_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 ν_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 ν_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*.

Intermission

TI07 **15 min 3:30**

OXYGEN-18 STUDIES OF HOCO AND HONO FORMATION

OSCAR MARTINEZ, 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*.

TI08 **15 min 3:47**

A UV+VUV MULTIPHOTON IONIZATION SCHEME FOR OH RADICALS[a]

JOSEPH M. BEAMES, FANG LIU and MARSHA I. LESTER, *Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323*.

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

TI09 **15 min 4:04**

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*.

TI10 **15 min 4:21**

CAVITY-RINGDOWN SPECTROSCOPY OF THE VIBRONICALLY MIXED $\tilde{A}\,^2A_2 - \tilde{B}\,^2B_2$ EXCITED STATES OF THE BENZYL RADICAL AND THE $\tilde{1}\,^2A_2 \leftarrow \tilde{X}\,^2B_1$ 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*.

TI11 **15 min 4:38**

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*.

TI12 **15 min 4:55**

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

G. D. O'CONNOR, T. P. TROY, D. A. ROBERTS, N. CHALYAVI, B. FÜCKEL, M. J. CROSSLEY, K. NAUTA, T.W. 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*.

TI13 **15 min 5:12**

LASER INDUCED FLUORESCENCE STUDY OF $\widetilde{B}$ - $\widetilde{A}$ TRANSITION OF ISOPROPOXY RADICAL

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

[a]Present address: Department of Chemistry, University of Louisville, 2320 South Brook Street, Louisville, Kentucky 40292

TI14 **15 min 5:29**

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 SPECTROSCOPY

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

TJ06 **15 min 3:30**

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, Higashi-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, Higashi-Hiroshima 739-8526, Japan*; TAKEHARU HAINO, *Department of Chemistry, Faculty of Science, Hiroshima University, Higashi-Hiroshima 739-8526, Japan*; TAKAYUKI EBATA, *Department of Chemistry, Faculty of Science, Hiroshima University, Higashi-Hiroshima 739-8526, Japan*; and THOMAS R. RIZZO, *Laboratoire de Chimie Physique Moléculaire, École Polytechnique Fédérale de Lausanne, Lausanne CH-1015, Switzerland*.

TJ07 **15 min 3:47**

GAS PHASE HYDRATION OF MODEL PEPTIDE CHAINS: FAR/MID INFRARED SIGNATURE OF WATER INTER-MOLECULAR 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*.

TJ08 **15 min 4:04**

IR SPECTROSCOPY OF $Au^{-}\cdot(CO_2)_n$ CLUSTERS: STRONG CLUSTER SIZE DEPENDENCE OF METAL-LIGAND INTERACTION

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

TJ09 **15 min 4:21**

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 WOOTTEN, *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*.

WF. INFRARED/RAMAN

WEDNESDAY, JUNE 20, 2012 – 1:30 PM

Room: 160 MATH ANNEX

Chair: ISABELLE KLEINER, CNRS, University Paris 7, Paris Est, Creteil, France

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 H_2-H_2O 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 FAURE, *CNRS, Institut de Planétologie et d'Astrophysique de Grenobleï£¡(IPAG), France*; AD VAN DER AVOIRD, *Radboud University, 6525 AJ Nijmegen, The Netherlands*.

WF05 **15 min 2:38**

OVERTONE VIBRATIONAL SPECTROSCOPY AND DYNAMICS IN H_2-H_2O 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-UniversitÂt'e de Bourgogne, Dijon, France*; ALEXANDRE FAURE, *CNRS, Institut de PlanÂt'etologie et dâĂŹAstrophysique 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_2D_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_2O DIMER AND INFRARED SPECTRA OF $(C_2D_4)_2$ AND $(C_2D_4)_3$ 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

K. DIDRICHE, T. FOLDES, M. HERMAN, *Service de Chimie quantique et Photophysique CP160/09, Faculté des Sciences, Université Libre de Bruxelles (U.L.B.), Av. Roosevelt, 50, B-1050, Bruxelles, Belgium.*

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*.

WG. ELECTRONIC

WEDNESDAY, JUNE 20, 2012 – 1:30 PM

Room: 170 MATH ANNEX

Chair: J. MATHIAS WEBER, University of Colorado, Boulder, Colorado

WG01 **15 min 1:30**

UNGERADE POLYADS IN THE $45800 - 46500$ CM^{-1} REGION OF THE S_1 STATE OF C_2H_2

J. H. BARABAN, P. B. CHANGALA, R. G. SHAVER, R. W. FIELD, *Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139, USA*; A. J. MERER, *Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan*.

WG02 **15 min 1:47**

IDENTIFICATION OF NEW *CIS* VIBRATIONAL LEVELS IN THE S_1 STATE OF C_2H_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_2H_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*.

WG07 **15 min 3:12**

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

WG08 **15 min 3:45**

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*.

WG09 **15 min 4:02**

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*.

WG10 **15 min 4:19**

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*.

WG11 **15 min 4:36**

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*.

WG12 **15 min 4:53**

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*.

WG13 **15 min 5:10**

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*.

WH. ASTRONOMICAL SPECIES AND PROCESSES

WEDNESDAY, JUNE 20, 2012 – 1:30 PM

Room: 1000 MCPHERSON LAB

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

WH01 **15 min 1:30**

A CONFUSION LIMITED SPECTRAL SURVEY OF ORION

J. CERNICHARO, B. TERCERO, N. MARCELINO, T. BELL, *CAB. Dpt Astrophysics. Crta Torrejón Km 4. 28850 Torrejón de Ardoz. Madrid. Spain*; A. PALAU, *ICE, Campus UAB, Torre C5, 08193 Bellaterra. Spain*.

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^+, H_2O^+, AND H_3^+ 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 H_2O^+ 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 H_3^+

TAKESHI 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, MüÃijnchen Germany 81679*.

Intermission

WH07 **15 min 3:30**

CH^+ SPECTRUM AND DIFFUSE INTERSTELLAR BANDS TOWARD HERSCHEL 36 EXCITED BY DUST EMISSION

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 Chemistry 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 OBSERVATORY

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, *National 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*[a], *Pasadena, CA 91109*.

[a] 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*[a]*, 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] 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 $\tilde{X}\ ^1\Sigma_g^+$ AND $\tilde{a}\ ^3\Sigma_u^+$

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

WAFAA 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 WAFAA 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, Univeristy of Illinois, Urbana, IL 61801*.

WI07 **15 min 3:12**

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

WI08 **15 min 3:45**

INFRARED PHOTODISSOCATION SPECTROSCOPY OF ALUMINUM BENZENE CATION COMPLEXES

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

WI09 **15 min 4:02**

STRUCTURES AND SPECTROSCOPIC PROPERTIES CALCULATED FOR $C_6H_7^+$ 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*.

WI10 **15 min 4:19**

ROVIBRATIONAL STATES OF $ClHCl^-$ 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*.

WI11 **15 min 4:36**

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*.

WI12 **15 min 4:53**

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*.

WI13 **15 min 5:10**

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

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

[a]Present Address: Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL, 61801

WI14 **15 min 5:27**

SPECTROSCOPIC AND KINETIC MEASUREMENTS OF ORGANIC PEROXY RADICALS BY DUAL-WAEVELENGTH 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

WJ01 ***INVITED TALK*** **30 min 1:30**

HIGH-RESOLUTION PHOTOELECTRON AND PHOTOIONIZATION SPECTROSCOPY

F. MERKT, *Laboratorium für Physikalische Chemie, ETH Zurich, CH 8093 Zurich, Switzerland*.

WJ02 **15 min 2:05**

THE GAS-PHASE SPECTROSCOPY STUDY OF ThN and ThN^+

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

WJ03 **15 min 2:22**

MASS-ANALYZED THRESHOLD IONIZATION OF M_2O_2 (M = Ce and Pr)

LU WU, BENI DANGI, MOURAD ROUNJANE, and DONG-SHENG YANG, *Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055*.

WJ04 **15 min 2:39**

PREFERRED METAL BINDING SITE OF ANILINE

SUDESH KUMARI, BRAD SOHNLEIN AND DONG-SHENG YANG, *Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055*.

Intermission

WJ05 **15 min 3:10**

PHOTOIONIZATION OF ALKALI-DOPED HELIUM NANODROPLETS

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*.

WJ06 **15 min 3:27**

PHOTOIONIZATION SPECTROSCOPY OF ISOLATED Cr ATOMS IN ULTRACOLD HELIUM NANODROPLETS

ANDREAS KAUTSCH, MATTHIAS HASEWEND, MARTIN RATSCHEK, MARKUS KOCH, and WOLFGANG E. ERNST, *Institute of Experimental Physics, TU Graz, Petersgasse 16, 8010 Graz, Austria*.

WJ07 **15 min 3:44**

PHOTOIONIZATION OF HIGHLY CHARGED ARGON IONS AND THEIR DIAGNOSTIC LINES

SULTANA N. NAHAR, *Department of Astronomy, The Ohio State University, Columbus, OH 43210*.

WJ08 **15 min 4:01**

HIGH-RESOLUTION PFI-ZEKE PHOTOELECTRON SPECTROSCOPY OF Cl_2: THE GROUND ($X^+\ ^2\Pi_g$) AND FIRST EXCITED ($A^+\ ^2\Pi_u$) ELECTRONIC STATES OF Cl_2^+

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

WJ09 **15 min 4:18**

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*.

WJ10 **15 min 4:35**

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*.

RA. ELECTRONIC

THURSDAY, JUNE 21, 2012 – 8:30 AM

Room: 160 MATH ANNEX

Chair: JOEL TELLINGHUISEN, Vanderbilt University, Nashville, Tennessee

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 $[17.8]0^+ - X^1\Sigma^+$ 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 Ω-TYPE DOUBLING IN THE Ω=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-Pyrenées (CNRS) 14 Av Edouard Belin, 31400 Toulouse, France*; ARTURO LÓPEZ ARISTE, *THEMIS Telescope, CNRS UPS 853, C/Via 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*.

RA12 **15 min 11:50**

MEASUREMENT OF HYPERFINE STRUCTURE AND PERMANENT ELECTRIC DIPOLE MOMENTS IN THE ELECTRONIC SPECTRUM OF IRIDIUM 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*; KEEYOON 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, Akademician Zuev square, Tomsk 634021, Russia*.

RB03 **15 min 9:04**

EVALUATION OF THE EXPERIMENTAL AND THEORETICAL INTENSITIES OF WATER-VAPOR LINES IN THE 2 μm 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 ν_6 REGION AND THE $2\nu_6$ 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

D.U. ANDREWS, B.R. HEAZLEWOOD, A.T. MACCARONE, T. CONROY, R.J. PAYNE, M.J.T. JORDAN and S.H. KABLE , *School of Chemistry, University of Sydney, Sydney, NSW, 2006, Australia*.

RB06 **15 min 9:55**

HIGH RESOLUTION STIMULATED RAMAN SPECTROSCOPY OF CARBON TETRAFLUORIDE CF_4

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

RB07 **15 min 10:30**

PRELIMINARY MODELING OF CH_3D 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, Vl. 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*.

RB08 **15 min 10:47**

SUBMILLIMETER SPECTRUM OF METHYL CHLORIDE: ANALYSIS OF THE ν_3=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*.

RB09 **15 min 11:04**

IMPROVED LINE PARAMETERS FOR CH4 AROUND 1.6 MICRONS

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

RB10 **15 min 11:21**

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*.

RC. ASTRONOMICAL SPECIES AND PROCESSES

THURSDAY, JUNE 21, 2012 – 8:30 AM

Room: 1000 MCPHERSON LAB

Chair: HARSHAL GUPTA, Jet Propulsion Laboratory, Pasadena, California

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 1/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

RC06 **15 min 10:10**

TIME-SLICE VELOCITY-MAP ION IMAGING STUDIES OF THE PHOTODISSOCIATION OF ASTROPHYSIC 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*.

RC07 **15 min 10:27**

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 Califormia, 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*.

RC08 **15 min 10:44**

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*.

RC09 **15 min 11:01**

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

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

RC10 **15 min 11:18**

HIGH RESOLUTION SPECTROSCOPY OF HEXAMETHYLENETETRAMINE (HMT) $C_6N_4H_{12}$

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. PIRALI[a], *Ligne AILES – Synchrotron SOLEIL, L'Orme des Merisiers, F-91192 Gif-sur-Yvette, France*.

[a] Also at: Institut des Sciences Moléculaires d'Orsay, UMR8214 CNRS-Université Paris-Sud, Bat.210, 91405 Orsay cedex, France.

RC11 **15 min 11:35**

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*.

RC12 **15 min 11:52**

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 **30 min 8:30**

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 **15 min 9:05**

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 **15 min 9:22**

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 **15 min 9:39**

PHOTOCHEMICAL STUDIES OF CH_3OH 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 **15 min 9:56**

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 **15 min 10:30**

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*.

RD07 **15 min 10:47**

THEORETICAL SPIN-ORBIT SPECTROSCOPY OF Cl DOPANTS IN SOLID PARAHYDROGEN

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

RD08 **15 min 11:04**

INFRARED SPECTROSCOPY OF 1-CHOLOROMETHYLALLYL AND 1-METHYLALLYL 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*.

RD09 **15 min 11:21**

IR-IR DOUBLE RESONANCE EXPERIMENT OF CH_3F-($ortho$-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*.

RD10 **15 min 11:38**

LINESHAPE ANALYSIS OF CH_3F-(*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 CO_2 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, N_2, Ar, He, CO_2, 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

RE07 **15 min 10:20**

ULTRAVIOLET PHOTODISSOCIATION 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 [a], *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*.

[a]Corresponding author.

RE08 **15 min 10:37**

OBSERVATION OF VIBRATIONALLY HOT CH_2CHO IN THE 351NM PHOTODISSOCIATION OF XCH_2CH_2ONO (X=F,Cl,Br,OH)

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

[a]Present address: School of Chemical Science, University of Illinois at Urbana Champaign,106 Noyes Lab, 505 S. Mathews, Urbana, IL 61801

RE09 **15 min 10:54**

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*.

RE10 **15 min 11:11**

HYDROGEN ABSTRACTION FROM CH_3D 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*.

RE11 **15 min 11:28**

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*.

RE12 **15 min 11:45**

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

CHAMARA ABEYSEKERA, JAMES M. OLDHAM, ARTHUR G. SUITS, *Department of Chemsitry, 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 ISOTOPOLOGUES

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

RF07 **15 min 3:30**

USING HOT EMISSION SPECTRA IN GENERATING LINE LISTS OF MOLECULES (NH_3, CH_4) 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. BERNATH, *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*.

RF08 **15 min 3:47**

BROADBAND SCREENING FOR INTERSTELLAR SPECIES: ADDITIONAL LABORATORY MEASUREMENTS AND INTERSTELLAR DETECTION OF ETHANIMINE (CH_3CHNH) 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*.

RF09 **10 min 4:04**

UNRAVELING THE COMPLEX NEAR-UV SPECTRUM OF Si_2C

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*.

RF10 **15 min 4:16**

LABORATORY DETECTIONS OF CYANOTHIOFORMALDEHYDE (HCSCN) AND MERCAPTOACETONITRILE ($HSCH_2CN$) 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.*.

RF11 **10 min 4:33**

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*.

RF12 **15 min 4:45**

ASSIGNMENTS, PERTURBATIONS, PATHOLOGIES AND A ROTATIONAL ANALYSIS OF THE SPECTRUM OF CH_2DOH

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

RF13 **15 min 5:02**

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*.

RF14 **15 min 5:19**

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*.

RG. ELECTRONIC

THURSDAY, JUNE 21, 2012 – 1:30 PM

Room: 170 MATH ANNEX

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

RG01 **10 min 1:30**

DIRECT POTENTIAL FITTING FOR THE $A\,^3\Pi_{1u}$ and $X\,^1\Sigma_g^+$ STATES OF Br_2

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

RG02 **15 min 1:42**

ANALYSIS OF THE VISIBLE ABSORPTION SPECTRUM OF I_2 IN INERT SOLVENTS USING A PHYSICAL MODEL

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

RG03 **5 min 1:59**

WAVELENGTH ANOMALIES IN UV-Vis SPECTROPHOTOMETRY

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

RG04 **15 min 2:06**

DEPERTURBATION STUDIES OF AlO : INTERACTIONS IN THE $A^2\Pi \sim X^2\Sigma^+$ STATES

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*.

RG05 **15 min 2:23**

FOURIER TRANSFORM EMISSION SPECTROSCOPY OF THE $A^2\Pi$–$X^2\Sigma^+$ (RED) SYSTEM OF $^{13}C^{14}N$.

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*.

RG06 **15 min 2:40**

HYPERFINE-RESOLVED SATURATION SPECTROSCOPY OF METASTABLE N_2 IN THE (1-0) BAND OF THE $\tilde{B}^3\Pi_g - \tilde{A}^3\Sigma_u^+$ ELECTRONIC TRANSITION

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*.

RG07 **15 min 2:57**

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*.

RG08 **15 min 3:14**

OBSERVATION OF BLUE-DETUNED PHOTOASSOCIATION TO THE 2 (0_g^+) STATE OF $^{85}Rb_2$ VIA REMPI

M. A. BELLOS, R. CAROLLO, D. RAHMLOW, J. BANERJEE, M. BERMUDEZ, E. E. EYLER, P. L. GOULD, and W. C. STWALLEY, *Department of Physics, University of Connecticut, Storrs, CT 06269*.

Intermission

RG09 **15 min 3:45**

IS THE EQUILIBRIUM STRUCTURE OF BeOH LINEAR OR BENT?

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

RG10 **15 min 4:02**

AN EXPERIMENTAL AND QUANTUM CHEMICAL STUDY OF THE ELECTRONIC SPECTRUM OF THE HBCl 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*.

RG11 **15 min 4:19**

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*.

RG12 **15 min 4:36**

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*.

RG13 **15 min 4:53**

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*.

RG14 **15 min 5:10**

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*.

RH. MICROWAVE

THURSDAY, JUNE 20, 2012 – 1:30 PM

Room: 1000 MCPHERSON LAB

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

RH01 **15 min 1:30**

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*.

RH02 **15 min 1:47**

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*.

RH03 **15 min 2:04**

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*.

RH04 **15 min 2:21**

FTMW SPECTROSCOPY OF SILYL MERCAPTAN, H_3SiSH

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*.

RH05 **15 min 2:38**

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*.

RH06 **15 min 2:55**

THE CCN ($\tilde{X}^2\Pi_{1/2}$) 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*.

RH07 **15 min 3:12**

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

RH08 **15 min 3:45**

MICROWAVE SPECTRUM OF HEXAFLUOROISOPROPANOL

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

RH09 **15 min 4:02**

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*.

RH10 **15 min 4:19**

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

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

RH11 **15 min 4:36**

HALOGEN BOND AND INTERNAL MOTIONS: THE LOW-BARRIER CASE OF CF_3Cl-DIMETHYLETHER

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

RH12 **15 min 4:53**

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*.

RH13 **15 min 5:10**

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*** **30 min 1:30**

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 SHEPPERSON, 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 NO_2 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 NO_2 $\nu_1 + \nu_3$ AND THE CH_4 ν_3 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-C_2H_2 EMBEDDED IN HELIUM NANODROPLETS

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

Intermission

RI06 ***INVITED TALK*** **30 min 3:30**

DOPANT ROTATION IN MOLECULAR SUPERFLUID CLUSTERS

PIERRE-NICHOLAS 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-$(O_2)_n$ 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_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 M5S 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 ***INVITED TALK*** **30 min 1:30**

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 S_1 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 H_2D^+

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*.

FA. ASTRONOMICAL SPECIES AND PROCESSES

FRIDAY, JUNE 22, 2012 – 8:30 AM

Room: 160 MATH ANNEX

Chair: JOHN C. PEARSON, Jet Propulsion Laboratory, Pasadena, California

FA01 **15 min 8:30**

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 1/CNRS, Institut de Planétologie et d'Astrophysique de Grenoble (IPAG) UMR 5274, Grenoble, F-38041, France*.

FA02 **15 min 8:47**

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*.

FA03 **15 min 9:04**

TERAHERTZ SPECROSCOPY 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, Chervonopraporna 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 Torrejòn de Ardoz, Madrid, Spain*.

FA04 **15 min 9:21**

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, Chervonopraporna 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*.

FA05 **15 min 9:38**

SPECTROSCOPY OF A MAJOR COMPLEX ORGANIC MOLECULE: MONO-DEUTERATED DIMETHYL ETHER

C. RICHARD, L. MARGULÈS, 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

FA06 **15 min 10:10**

TOWARDS AN ACCURATE INFRARED LINELIST FOR SO_2

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*.

FA07 **15 min 10:27**

THEORETICAL NH_3 SPECTRA IN 5800-7000 CM^{-1} REGION AND CO_2 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*; KEEYOON 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*.

FA08 **15 min 10:44**

LINE PARAMETERS OF THE PH_3 PENTAD IN THE $4-5\mu$m 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-Universites Paris-ESt 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*.

FA09 **15 min 11:01**

LINE BY LINE SPECTRAL PARAMETERS IN THE $4\nu_3$ 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 $^{13}CH_3CH_3$ INCLUDING DATA FROM THE LOWEST FOUR VIBATIONAL 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, Fin-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, Department of Physics, 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 KOERBER, CHRISTIAN P. ENDRES, STEPHAN SCHLEMMER, *I. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany*.

FB. INFRARED/RAMAN

FRIDAY, JUNE 22, 2012 – 8:30 AM

Room: 170 MATH ANNEX

Chair: SVEN THORWIRTH, University of Cologne, Koeln, Germany

FB01 **15 min 8:30**

HIGH RESOLUTION EMISSION SPECTROSCOPY OF THE VIBRATION-ROTATION BANDS OF HBO AND HBS.

G. LI[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*.

[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. Catherines, 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_{60} AND PYRENE

JACOB T. STEWART, BRIAN E. BRUMFIELD,[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*.

[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

NATHANAEL M. KIDWELL, DEEPALI 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. KESAN, *Faculty of Science, University of South Bohemia, Czech Republic*; C. PARLAK, *Department of Physics, Dumlupýnar University, Kutahya, 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, Dumlupýnar University, Kutahya, 43100, Turkey*; C. PARLAK, *Department of Physics, Dumlupýnar University, Kutahya, 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 ORGANOMETALLIC 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

Chair: SUSANNA WIDICUS WEAVER, Emory University, Atlanta, Georgia

FC01 **15 min 8:30**

A NEW U-BAND (40 - 60 GHz) FOURIER TRANSFORM MICROWAVE SPECTROMETER

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

FC02 **15 min 8:47**

FOURIER TRANSFORM MICROWAVE SPECTRUM OF THE AlC_2 ($\tilde{X}^2A_1$) RADICAL

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

FC03 **15 min 9:04**

THE FOURIER TRANSFORM MICROWAVE SPECTRUM OF YOH AND YOD ($\tilde{X}^1\Sigma^+$)

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

FC04 **15 min 9:21**

DEVELOPMENT OF A SUBMILLIMETER MULTIPASS SPECTROMETER FOR THE STUDY OF MOLECULAR IONS

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*.

FC05 **15 min 9:38**

THE DEVELOPMENT AND IMPLEMENTATION OF CHIRPED-PULSE FREQUENCY COMBS AT MILLIMETER WAVELENGTHS

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*.

FC06 **10 min 9:55**

CHIRPED-PULSE FOURIER TRANSFORM MM-WAVE SPECTROSCOPY FROM 260-290 GHz

BRENT J.HARRIS, AMANDA L. STEBER, JUSTIN L. NEILL, KEVIN K. LEHMANN, BROOKS H. PATE, *Department of Chemistry, University of Virginia, Charlottesville, VA 22904*.

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^+, N_2H^+ 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 $(pH_2)_N$-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 ScC_2 RADICAL (X^2A_1)

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 BEAMLINE

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}K^{85}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

FD06 **15 min 10:30**

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*.

FD07 **15 min 10:47**

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*.

FD08 **15 min 11:04**

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*.

FD09 **10 min 11:21**

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*.

FD10 ***Post-deadline Abstract*** **15 min 11:33**

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. ALPHENAAR, *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 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. BRECKENRIDGE, *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 H_2O BE COMPLETELY ISOLATED INSIDE THE SUB-NANO SPACE INSIDE THE FULLERENE C_{60} CAGE? A THEORETICAL PROPSPECTIVE

PRADEEP R. VARADWAJ, ARPITA VARADWAJ, 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*.

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