68th OSU INTERNATIONAL SYMPOSIUM ON MOLECULAR SPECTROSCOPY
JUNE 17-21, 2013

	MONDAY JUNE 17 8:45AM	TUESDAY JUNE 18 8:30AM	WEDNESDAY JUNE 19 8:30AM	THURSDAY JUNE 20 8:30AM	FRIDAY JUNE 21 8:30AM
AUDITORIUM INDEPENDENCE HALL	MA. PLENARY SESSION AWARDS		WA. PLENARY SESSION AWARDS		
ROOM 160 MATH ANNEX*		TA. MINI-SYMPOSIUM: SPECTROSCOPY TESTS OF FUNDAMENTAL PHYSICS		RA. MINI-SYMPOSIUM: THEORY AND SPECTROSCOPY	FA. ASTRONOMICAL SPECIES AND PROCESSES
ROOM 170 MATH ANNEX*		TB. MINI-SYMPOSIUM: SPECTROSCOPY OF PLANETARY ATMOSPHERES		RB. RADICALS AND IONS	FB. MINI-SYMPOSIUM: THEORY AND SPECTROSCOPY
ROOM 1000 MCPHERSON LAB		TC. MICROWAVE		RC. MICROWAVE	FC. MICROWAVE
ROOM 1015 MCPHERSON LAB		TD. RADICALS AND IONS		RD. ELECTRONIC	FD. ELECTRONIC
ROOM 2015 MCPHERSON LAB		TE. MATRIX/CONDENSED PHASE		RE. MINI-SYMPOSIUM: SPECTROSCOPY OF PLANETARY ATMOSPHERES	FE. DYNAMICS
1:30PM					
ROOM 160 MATH ANNEX*	MF. MINI-SYMPOSIUM: SPECTROSCOPY TESTS OF FUNDAMENTAL PHYSICS	TF. MINI-SYMPOSIUM: SPECTROSCOPY TESTS OF FUNDAMENTAL PHYSICS	WF. ASTRONOMICAL SPECIES AND PROCESSES	RF. ASTRONOMICAL SPECIES AND PROCESSES	
ROOM 170 MATH ANNEX*	MG. RADICALS AND IONS	TG. MINI-SYMPOSIUM: THEORY AND SPECTROSCOPY	WG. MINI-SYMPOSIUM: THEORY AND SPECTROSCOPY	RG. THEORY	
ROOM 1000 MCPHERSON LAB	MH. MICROWAVE	TH. MICROWAVE	WH. MICROWAVE	RH. DYNAMICS	
ROOM 1015 MCPHERSON LAB	MI. ELECTRONIC	TI. ASTRONOMICAL SPECIES AND PROCESSES	WI. INFRARED/RAMAN	RI. ATMOSPHERIC SPECIES	
ROOM 2015 MCPHERSON LAB	MJ. ATMOSPHERIC SPECIES	TJ. INFRARED/RAMAN	WJ. RADICALS AND IONS	RJ. INFRARED/RAMAN	
ROOM 1153 SMITH LAB	MK. INFRARED/RAMAN	TK. ELECTRONIC	WK. ELECTRONIC	RK. MICROWAVE	

MA. PLENARY

MONDAY, JUNE 17, 2013 – 8:45 AM

Room: AUDITORIUM, INDEPENDENCE HALL

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

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

MA01 **40 min 9:00**

LOW TEMPERATURE TRAPPING: FROM REACTIONS TO SPECTROSCOPY

S. SCHLEMMER, O. ASVANY, and S. BRÜNKEN, *I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany*.

MA02 **40 min 9:45**

DECODING THE EFFECTS OF LARGE AMPLITUDE VIBRATIONAL MOTIONS IN SPECTRA

ANNE B. McCOY, LAURA C. DZUGAN, MENG HUANG, ZHOU LIN, BERNICE OPOKU-AGYEMAN, ANDREW S. PETIT, JASON FORD, and BETHANY A. WELLEN, *Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH 43210*.

Intermission

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

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

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**

LINEAR AND NONLINEAR MOLECULAR SPECTROSCOPY WITH LASER FREQUENCY COMBS

NATHALIE PICQUÉ, *Max Planck Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching, Germany; Ludwig-Maximilians-Universität München, Fakultät für Physik, Schellingstrasse 4/III, 80799 München, Germany; Institut des Sciences Moléculaires d'Orsay, Université Paris-Sud, 91405 Orsay, France; email: nathalie.picque@mpq.mpg.de*.

MF. MINI-SYMPOSIUM: SPECTROSCOPY TESTS OF FUNDAMENTAL PHYSICS

MONDAY, JUNE 17, 2013 – 1:30 PM

Room: 160 MATH ANNEX

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

MF01 *INVITED TALK* **30 min 1:30**

SEARCH FOR A VARIATION OF FUNDAMENTAL CONSTANTS

W. UBACHS, *Department of Physics and Astronomy, VU University Amsterdam, De Boelelaan 1081, 1081 HV Amsterdam, Netherlands*.

MF02 **15 min 2:05**

AN ALCOHOL TEST FOR DRIFTING CONSTANTS

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

MF03 **15 min 2:22**

SENSITIVITY OF TRANSITIONS IN INTERNAL ROTOR MOLECULES TO A POSSIBLE VARIATION OF THE PROTON-TO-ELECTRON MASS RATIO

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

MF04 **15 min 2:39**

CH_3OH SUB-DOPPLER SPECTROSCOPY

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

MF05 **15 min 2:56**

HIGH RESOLUTION MICROWAVE SPECTROSCOPY OF CH AS A SEARCH FOR VARIATION OF FUNDAMENTAL CONSTANTS

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

MF06 **15 min 3:13**

SUB-DOPPLER AND FTMW SPECTROSCOPY OF HC_3N ISOTOPOLOGUES

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

MF07 **15 min 3:30**

THE CO A-X SYSTEM FOR CONSTRAINING COSMOLOGICAL DRIFT OF THE PROTON-ELECTRON MASS RATIO

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

MF08 **15 min 3:47**

PRECISE MEASUREMENT OF $^{40}CaH^{+}$ VIBRATIONAL TRANSITION FREQUENCY

MASATOSHI KAJITA, *Nat. Ins. Info. Comm. Tech., Koganei, Tokyo 184-8795, Japan*; MINORI ABE, *Dep. of Chemistry, Tokyo Metro. Univ., Hachioji, Tokyo 192-0397, Japan*.

MF09 **15 min 4:04**

PRECISE MEASUREMENT OF VIBRATIONAL TRANSITION FREQUENCY OF OPTICALLY TRAPPED MOLECULES

MASATOSHI KAJITA, *Nat. Ins. Info. Comm. Tech., Koganei, Tokyo 184-8795, Japan*; GEETHA GOPAKUMAR,MINORI ABE, and MASAHIKO HADA, *Dep. of Chemistry, Tokyo Metro. Univ., Hachioji, Tokyo 192-0397, Japan*.

Intermission

MF10 **15 min 4:36**

TOWARDS MORE ACCURATE MEASUREMENTS OF THE IONIZATION ENERGY OF MOLECULAR HYDROGEN

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

MF11 **15 min 4:53**

NON-ADIABATIC ENERGIES OF THE HYDROGEN MOLECULE

KRZYSZTOF PACHUCKI, *Faculty of Physics, University of Warsaw, Hoża 69, 00-681 Warsaw, Poland*; JACEK KOMASA, *Faculty of Chemistry, A. Mickiewicz University, Grunwaldzka 6, 60-780 Poznań, Poland*.

MF12 **15 min 5:10**

QED EFFECTS IN H_2

KRZYSZTOF PACHUCKI, *Faculty of Physics, University of Warsaw, Hoża 69, 00-681 Warsaw, Poland*; JACEK KOMASA, *Faculty of Chemistry, A. Mickiewicz University, Grunwaldzka 6, 60-780 Poznań, Poland*.

MF13 **15 min 5:27**

PRECISION MEASUREMENT OF THE IONIZATION ENERGY OF THE $GK\ ^1\Sigma_g^+\ (v = 1, N = 1)$ STATE OF MOLECULAR HYDROGEN.

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

MF14 **15 min 5:44**

QED TESTS AND SEARCH FOR NEW PHYSICS IN MOLECULAR HYDROGEN

E. J. SALUMBIDES, M. L. NIU, G. D. DICKENSON, K. S. E. EIKEMA, *Department of Physics and Astronomy, and LaserLaB, VU University, De Boelelaan 1081, 1081 HV Amsterdam, The Netherlands*; J. KOMASA, *Faculty of Chemistry, A. Mickiewicz University, Grunwaldzka 6, 60-780 Poznań, Poland*; K. PACHUCKI, *Faculty of Physics, University of Warsaw, Hoża 69, 00-681 Warsaw, Poland*; and W. UBACHS, *Department of Physics and Astronomy, and LaserLaB, VU University, De Boelelaan 1081, 1081 HV Amsterdam, The Netherlands*.

MG. RADICALS AND IONS

MONDAY, JUNE 17, 2013 – 1:30 PM

Room: 170 MATH ANNEX

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

MG01 **15 min** **1:30**

COMBINATION BANDS BETWEEN 2900 AND 3600 CM^{-1} OF CYCLIC O_4 CATION TRAPPED IN SOLID NEON

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

MG02 **15 min** **1:47**

FOURIER TRANSFORM FAR-INFRARED SPECTROSCOPY OF HN_2^+ ON THE AILES BEAMLINE OF SYNCHROTRON SOLEIL

O. PIRALI[a], S. GRUET[a], M. VERVLOET, *Ligne AILES, Synchrotron SOLEIL, L'Orme des Merisiers Saint-Aubin, 91192 Gif sur Yvette Cedex - France*.

[a] Also at: Institut des Sciences Moléculaires d'Orsay, UMR 8214 CNRS-Université Paris-Sud, Bât. 210, 91405 Orsay cedex, France.

MG03 **15 min** **2:04**

SUB-DOPPLER SPECTROSCOPY OF ND_3H^+ ION IN THE NH STRETCHING MODE

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

MG04 **15 min** **2:21**

INFRARED SPECTROSCOPY OF JET COOLED $ND_2H_2^+$ MOLECULAR IONS: THE SYMMETRIC AND ANTISYMMETRIC NH STRETCH MODES

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

MG05 **15 min** **2:38**

PRECISION LASER SPECTROSCOPY OF H_3^+

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

MG06 **15 min** **2:55**

SUB-DOPPLER SPECTROSCOPY OF H_3^+

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

MG07 **15 min 3:12**

HIGH PRECISION SPECTROSCOPY OF CH_5^+ USING NICE-OHVMS

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

MG08 **15 min 3:29**

INFRARED SPECTROSCOPY OF THE MASS 43 CATION: ACETYL CATION AND PROTONATED KETENE

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

MG09 **15 min 3:46**

UBIQUITOUS INTERSTELLAR MOLECULES WITH RADICALLY DIFFERENT CATION STRUCTURES: INFRARED SPECTROSCOPY OF FORMALDEHYDE AND METHANOL CATIONS

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

Intermission

MG10 **15 min 4:15**

THE CORONENE VIBRONIC STATES ABOVE THE FIRST IONIZATION POTENTIAL INVESTIGATED THROUGH TPEPICO EXPERIMENTS

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

MG11 **15 min 4:32**

MASS ANALYZED THRESHOLD IONIZATION OF LUTETIUM DIMER

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

MG12 **15 min 4:49**

C-C BOND ACTIVATION AND COUPLING OF PROPENE INDUCED BY LA ATOM

DILRUKSHI HEWAGE, *Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055*; HONG TAO, *Department of Chemistry, Southwest Forestry University, Kunming 650224, PR China*; RUCHIRA SILVA, SUDESH KUMARI, AND DONG-SHENG YANG, *Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055*.

MG13 **15 min 5:06**

HIGH-RESOLUTION PHOTOELECTRON SPECTROSCOPY OF 2-BUTYNE

UGO JACOVELLA, BÉRENGER GANS and FRÉDÉRIC MERKT, *ETH Zürich, Laboratorium für Physikalische Chemie, Wolfgang-Pauli-Strasse 10, 8093 Zürich, Switzerland*.

MG14 **15 min 5:23**

UNDERSTANDING COMPLEX SPECTRAL SIGNATURES OF EMBEDDED EXCESS PROTONS IN MOLECULAR SCAFFOLDS WITH THIRD ORDER CORRECTIONS TO THE HARMONIC POTENTIAL SURFACE

ANDREW F. DEBLASE and MARK A. JOHNSON, *Yale University, P.O. Box 208107, New Haven, CT 06520, USA*; THOMAS LECTKA, *Johns Hopkins University, 3400 North Charles Street, Baltimore, Maryland 21218, USA*; XUN WANG and KENNETH D. JORDAN, *University of Pittsburgh, 219 Parkman Avenue, Pittsburgh, PA 15260, USA*; ANNE B. McCOY, *The Ohio State University, Columbus, Ohio 43210, USA*.

MG15 **15 min 5:40**

SLOW ELECTRON VELOCITY-MAP IMAGING OF $La_2(C_6H_6)$ AND $La(C_6H_6)_2$

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

MG16 **15 min 5:57**

INFRARED SPECTROSCOPY AND STRUCTURES OF MASS-SELECTED RHODIUM CARBONYL AND RHODIUM DINITROGEN CATIONS

HEATHER L. ABBOTT, *Department of Chemistry and Biochemistry, Kennesaw State University, Kennesaw, GA 30144*; ANTONIO D. BRATHWAITE and MICHAEL A. DUNCAN, *Department of Chemistry, University of Georgia, Athens, GA 30602-2256*.

MH. MICROWAVE

MONDAY, JUNE 17, 2013 – 1:30 PM

Room: 1000 MCPHERSON LAB

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

MH01 **15 min** **1:30**

THE PROTOTYPE DIPEPTIDE GLY-GLY: A ROTATIONAL STUDY

M. VARELA, C. CABEZAS, S. MATA, J. L. ALONSO, *Grupo de Espectroscopía Molecular (GEM), Edificio Quifima, Laboratorios de Espectroscopía y Bioespectroscopía, Parque Científico, Universidad de Valladolid, 47011 Valladolid, Spain*.

MH02 **15 min** **1:47**

GAS-PHASE STRUCTURES OF LINALOOL AND COUMARIN STUDIED BY MICROWAVE SPECTROSCOPY

H. V. L. NGUYEN, W. STAHL, *Institut für Physikalische Chemie, RWTH Aachen University, Landoltweg 2, 52074 Aachen, Germany*; and J.-U. GRABOW, *Institut für Physikalische Chemie und Elektrochemie, Lehrgebiet A, Callinstrasse 3-3a, 30167 Hannover, Germany*.

MH03 **10 min** **2:04**

MW SYSTEMATIC STUDY OF ALKALOIDS: THE DISTORTED TROPANE OF SCOPOLINE

PATRICIA ECIJA, EMILIO J. COCINERO, FRANCISCO J. BASTERRETXEA, JOSÉ A. FERNANDEZ, FERNANDO CASTANO, *Departamento de Química Física, Facultad de Ciencia y Tecnología, Universidad del País Vasco (UPV/EHU), Ap.644, E-48940, Bilbao, Spain*; ALBERTO LESARRI, *Departamento de Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, E-47011 Spain*.

MH04 **15 min** **2:16**

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

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

MH05 **15 min** **2:33**

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

W. C. BAILEY, *Chemistry-Physics Department (Retired), Kean University, Union, New Jersey, USA 07083*; R. K. BOHN, *Departments of Chemistry and Physics, University of Connecticut,Storrs, Connecticut, 06269-3060, USA.*; G. S. GRUBBS II, *Department of Chemistry, Wesleyan University, Hall-Atwater Laboratories, 52 Lawn Ave, Middletown, Connecticut, 06459-0180, USA.*; Z. KISIEL, *Institute of Physics, Polish Academy of Sciences, Al. Lotnikóv 32146, 02-668 Warszawa, Poland.*; S. A. COOKE, *School of Natural and Social Sciences, Purchase College SUNY, 735 Anderson Hill Road, Purchase, NY 10577, USA*.

MH06 **15 min 2:50**

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

L. MARGULÈS, R. A. MOTIYENKO, *Laboratoire de Physique des Lasers, Atomes, et Molécules, UMR CNRS 8523, Université de Lille I, 59655 Villeneuve d'Ascq Cedex, France*; P. GRONER, *Department of Chemistry, University of Missouri-Kansas City, 5100 Rockhill Road, Kansas City, MO 64110-2499, USA*; F. De CHIRICO, A. TURK, S. A. COOKE, *School of Natural and Social Sciences, Purchase College SUNY, 735 Anderson Hill Road, Purchase, NY 10577, USA*.

MH07 **15 min 3:07**

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

NATHAN A. SEIFERT, CRISTOBAL PEREZ, DANIEL P. ZALESKI, JUSTIN L. NEILL, BROOKS H. PATE, *Department of Chemistry, University of Virginia, McCormick Rd., Charlottesville, VA 22904-4319*; ALBERTO LESARRI, MONTSERRAT VALLEJO, *Departamento de Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, E-47011 Valladolid, Spain*; EMILIO J. COCINERO, FERNANDO CASTANO, *Departamento de Química Física, Facultad de Ciencia y Tecnología, Universidad del País Vasco (UPV/EHU), Campus de Leioa, Ap. 644, E-48080 Bilbao, Spain*; ISABELLE KLEINER, *Laboratorie Interuniversitaire des Systèmes Atmosphériques (LISA), CNRS et Universités Paris Est et Paris Diderot, 61. av Général de Gaulle, 94010 Créteil, France*.

MH08 **10 min 3:24**

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

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

Intermission

MH09 **15 min 3:50**

THE COMPLETE MOLECULAR GEOMETRY OF SALICYL ALDEHYDE FROM ROTATIONAL SPECTROSCOPY

O. DOROSH, E. BIALKOWSKA-JAWORSKA, Z. KISIEL, L. PSZCZOLKOWSKI, *Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warszawa, Poland*; M. KANSKA, T. M. KRYGOWSKI, *Department of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warszawa, Poland*; H. MAEDER, *Institut für Physikalische Chemie, Christian-Albrechts-Universität zu Kiel, Olshausenstrasse 40, D-24098 Kiel, Germany*.

MH10 **10 min 4:07**

LABORATORY OBSERVATION OF THE ROTATIONAL SPECTRUM OF A POTENTIAL INTERSTELLAR SUGAR, ERYTHROSE

I. PENA, C. CABEZAS, A. M. DALY, S. MATA, J. L. ALONSO, *Grupo de Espectroscopía Molecular (GEM), Edificio Quifima, Laboratorios de Espectroscopía y Bioespectroscopía, Parque Científico, Universidad de Valladolid, 47011 Valladolid, Spain*.

MH11 **15 min 4:19**

ALDOPENTOSES IN THE GAS PHASE: ROTATIONAL SPECTRA OF D-XYLOSE, D-ARABINOSE, D-LYXOSE AND 2-DEOXY-D-RIBOSE

I. PENA, C. CABEZAS, A. M. DALY, C. BERMUDEZ, S. MATA, S. BLANCO, J. C. LOPEZ, J. L. ALONSO, *Grupo de Espectroscopía Molecular (GEM), Edificio Quifima, Laboratorios de Espectroscopía y Bioespectroscopía, Parque Científico, Universidad de Valladolid, 47011 Valladolid, Spain*.

MH12 **15 min 4:36**

A ROTATIONAL STUDY OF D-MANNOSE AND D-GALACTOSE

I. PENA, A. M. DALY, C. CABEZAS, S. MATA, J. L. ALONSO, *Grupo de Espectroscopía Molecular (GEM), Edificio Quifima, Laboratorios de Espectroscopía y Bioespectroscopía, Parque Científico, Universidad de Valladolid, 47011 Valladolid, Spain*.

MH13 **15 min 4:53**

UNVEILING THE SWEET CONFORMATIONS OF KETOHEXOSES

C. BERMUDEZ, I. PENA, C. CABEZAS, A. M. DALY, S. MATA, J. L. ALONSO, *Grupo de Espectroscopía Molecular (GEM), Edificio Quifima, Laboratorios de Espectroscopía y Bioespectroscopía, Parque Científico, Universidad de Valladolid, 47011 Valladolid, Spain*.

MH14 **15 min 5:10**

ELUCIDATING THE STRUCTURE OF SUGARS: MW SPECTROSCOPY COMBINED WITH ULTRAFAST UV LASER VAPORIZATION

EMILIO J. COCINERO, PATRICIA ECIJA, FRANCISCO J. BASTERRETXEA, JOSÉ A. FERNANDEZ, FERNANDO CASTANO, *Departamento de Química Física, Facultad de Ciencia y Tecnología, Universidad del País Vasco (UPV-EHU), Ap. 644, E-48080 Bilbao, Spain*; ALBERTO LESARRI, *Departamento de Química-Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, E-47011 Spain*; JENS-UWE GRABOW, *Institut für Physikalische Chemie, Lehrgebiet A, Universität Hannover, Callinstraße. 3A, D-30167 Hannover, Germany*; ALVARO CIMAS, *Laboratoire Analyse et Modélisation pour la Biologie et l'Environnement, Université d'Évry val d'Essonne, F-91025 Evry (France)*.

MH15 **15 min 5:27**

TOWARDS SOLVATION OF A CHIRAL ALPHA-HYDROXY ESTER: BROADBAND CHIRP AND NARROW BAND CAVITY FOUIRIER TRANSFORM MICROWAVE SPECTROSCOPY OF METHYL LACTATE-WATER CLUSTERS

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

MI. ELECTRONIC

MONDAY, JUNE 17, 2013 – 1:30 PM

Room: 1015 MCPHERSON LAB

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

MI01 **15 min** **1:30**

A DPF ANALYSIS YIELDS QUANTUM MECHANICALLY ACCURATE ANALYTIC POTENTIAL ENERGY FUNCTIONS FOR THE $A\,^1\Sigma^+$ and $X\,^1\Sigma^+$ STATES OF NaH

ROBERT J. LE ROY, SADRU WALJI, KATHERINE SENTJENS, *Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada*.

MI02 **15 min** **1:47**

UNCERTAINTIES IN PROPERTIES CALCULATED FROM FITTED POTENTIAL FUNCTIONS *and* DETERMINING POTENTIAL FUNCTIONS FROM FITS TO BOUND → CONTINUUM INTENSITY DATA

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

MI03 **15 min** **2:04**

ASSIGNING COMPLEX VIBRATION-TUNNELING SPECTRA USING FRANCK-CONDON FINGERPRINTS

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

MI04 **15 min** **2:21**

OPTICAL-OPTICAL DOUBLE RESONANCE AND LIF SPECTROSCOPY OF THE JET-COOLED BORON CARBIDE (BC) FREE RADICAL

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

MI05 **10 min** **2:38**

REINVESTIGATION OF THE EMISSION SPECTRA FOLLOWING THE 266 NM PHOTOLYSIS OF IODOMETHANES

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

MI06 **15 min** **2:50**

CAVITY RINGDOWN ABSORPTION SPECTRUM OF THE $T_1(n,\pi^*) \leftarrow S_0$ TRANSITION OF 2-CYCLOHEXEN-1-ONE

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

MI07 **15 min** **3:07**

COMPUTATIONAL INVESTIGATION OF THE $T_1(n,\pi^*)$ STATE OF 2-CYCLOHEXEN-1-ONE

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

Intermission

MI08 **15 min 3:40**

PROBING COMPETITIVE NONCOVALENT INTERACTIONS: RESONANCE ENHANCED TWO-PHOTON IONIZATION (R2PI) SPECTROSCOPY OF HALOAROMATIC CLUSTERS

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

MI09 **15 min 3:57**

NONLINEAR DUAL-COMB SPECTROSCOPY WITH TWO-PHOTON EXCITATION

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

MI10 **15 min 4:14**

NEW DEVELOPMENTS OF BROADBAND CAVITY ENHANCED SPECTROSCOPIC TECHNIQUES

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

MI11 **15 min 4:31**

MEASURING THE QUENCHING OF NO FLUORESCENCE PRODUCED FROM THE EXCITATION OF PHOTOFRAGMENTED NITROBENZENE USING A PICOSECOND LASER.

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

MI12 **15 min 4:48**

SPECTROSCOPY OF LUMINESCENT CRYSTALS CONTAINING RARE EARTH ELEMENTS

MENG-LING CHEN, KWANG-HWA LII, and BOR-CHEN CHANG, *Department of Chemistry, National Central University, 300 Jhongda Road, Jhongli 32001, Taiwan*.

MI13 **15 min 5:05**

DNA-ENHANCED DYE-SENSITIZED SOLAR CELLS

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

MI14 **15 min 5:22**

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

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

MI15 **15 min 5:39**

SPECTROSCOPY OF 1,2-DIPHENYLETHANE-$(H_2O)_n$ (n=1-3) CLUSTERS

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

MI16 **15 min 5:56**

TROPOLONE COMPLEXES FORMED WITH AMPHOTERIC LIGANDS: STRUCTURE AND DYNAMICS AS VIEWED ACROSS THE VIBRONIC LANDSCAPE

DEACON J. NEMCHICK, KATHRYN CHEW, and PATRICK H. VACCARO, *Department of Chemistry, Yale University, P.O. Box 20817, New Haven, CT 06520-8107 USA*.

MJ. ATMOSPHERIC SPECIES

MONDAY, JUNE 17, 2013 – 1:30 PM

Room: 2015 MCPHERSON LAB

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

MJ01 **15 min** **1:30**

WATER BROADENING OF OXYGEN

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

MJ02 **15 min** **1:47**

LINE PARAMETERS FOR THE OXYGEN A BAND

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

MJ03 **15 min** **2:04**

AIR-BROADENING AND SHIFT PARAMETERS IN THE ν_3 BAND OF OZONE

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

MJ04 **15 min** **2:21**

AIR-BROADENED LINE SHAPES IN THE $2\nu_3$ R BRANCH OF $^{12}CH_4$ BETWEEN 6014 AND 6100 CM^{-1}

V. MALATHY DEVI, D. CHRIS BENNER, *Dept. of Physics, The College of William and Mary, Williamsburg, VA 23187*; K. SUNG, L. R. BROWN, T. J. CRAWFORD, SHANSHAN YU, *Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109*; 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*.

MJ05 **15 min** **2:38**

LINE BROADENING PARAMETERS OF METHANE AT 6000 CM^{-1}

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

MJ06 **15 min** **2:55**

EXAMINING CONTRIBUTIONS TO LINE SHAPES IN THE ν_1 + ν_3 BAND OF ACETYLENE

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

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

Intermission

MJ07 **15 min 3:30**

REFINEMENT OF THE ROBERT-BONAMY FORMALISM: TAKING INTO ACCOUNT OF CONTRIBUTIONS FROM THE LINE COUPLING

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

MJ08 **15 min 3:47**

UNDISCOVERED ERRORS OF VOIGT PROFILE BEYOND TINY W-SHAPED RESIDUALS

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

MJ09 **15 min 4:04**

WATER INTENSITIES: AB INITIO VS. EXPERIMENT

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

MJ10 **15 min 4:21**

FT-IR MEASUREMENTS OF CROSS SECTIONS OF COLD C_3H_8 IN THE 7 - 15 μm FOR TITAN

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

MJ11 **15 min 4:38**

QUANTITATIVE MEASUREMENT OF INTEGRATED BAND INTENSITIES OF ISOPRENE AND FORMALDEHYDE

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

MJ12 **15 min 4:55**

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

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

MJ13 **10 min 5:12**

COMPARISON OF EXPERIMENTAL AND THEORETICAL ABSORPTION CROSS SECTIONS OF PFBAm

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

MJ14 **15 min** **5:24**

INVESTIGATING ATMOSPHERIC OXIDATION WITH MOLECULAR DYNAMICS IMAGING AND SPECTROSCOPY

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

MJ15 **10 min** **5:41**

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

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

MJ16 **15 min** **5:53**

PHOTOCHEMISTRY OF ACETONE IN SIMULATED ATMOSPHERE

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

MK. INFRARED/RAMAN

MONDAY, JUNE 17, 2013 – 1:30 PM

Room: 1153 SMITH LAB

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

MK01 **15 min** **1:30**

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

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

MK02 **15 min** **1:47**

INFRARED SPECTROSCOPY OF $((CH_3)_3N)_n$-H^+-H_2O (n=1-3): STRUCTURES AND DISSOCIATION CHANNELS OF PROTONATED MIXED CLUSTERS AROUND A MAGIC NUMBER

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*.

MK03 **15 min** **2:04**

MAPPING CONFORMATIONAL ENERGY BARRIERS IN HYDRATED RUBIDIUM ION CLUSTERS

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

MK04 **15 min** **2:21**

IR SPECTROSCOPY OF $[Ag\cdot(CO_2)_n]^-$ CLUSTERS: IMPLICATIONS FOR REDUCTIVE ACTIVATION OF CO_2

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

MK05 **15 min** **2:38**

HIGH-RESOLUTION INFRARED SPECTROSCOPY OF Ge_2C_3

S. THORWIRTH, V. LUTTER, S. SCHLEMMER, *I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany*; T. F. GIESEN, *Universität Kassel, Fachbereich 10 - Physik, 34132 Kassel, Germany*; J. GAUSS, *Institut für Physikalische Chemie, Universität Mainz, 55099 Mainz, Germany*.

MK06 **15 min** **2:55**

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

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

MK07 **15 min 3:12**

OBSERVATION OF COMBINATION BANDS INVOLVING INTERMOLECULAR VIBRATIONS OF N_2O-N_2, N_2O-OCS AND N_2O-CO_2 COMPLEXES USING AN EXTERNAL CAVITY QUANTUM CASCADE LASER

M. REZAEI, S. SHEYBANI-DELOUI, N. MOAZZEN-AHMADI, *Department of Physics and Astronomy, University of Calgary, 2500 University Dr., N.W., Calgary, Alberta T2N 1N4, Canada*; A.R.W. McKELLAR, *National Research Council of Canada, Ottawa, Ontario, K1A 0R6, Canada*.

MK08 **15 min 3:29**

INFRARED SPECTRA OF THE NE_2-N_2O, AR_2-N_2O TRIMERS

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

Intermission

MK09 **15 min 4:00**

INFRARED SPECTRUM OF THE $(CO_2)_2$-N_2O TRIMER MEASURED IN N_2O ν_1 AND ν_3 REGIONS.

J. NOROOZ OLIAEE, N. MOAZZEN-AHMADI, *Department of Physics and Astronomy, University of Calgary, 2500 University Dr., N.W., Calgary, Alberta T2N 1N4, Canada*; A.R.W. McKELLAR, *National Research Council of Canada, Ottawa, Ontario, K1A 0R6, Canada*.

MK10 **15 min 4:17**

OBSERVATION OF A PLANAR ISOMER OF THE N_2O-$(C_2H_2)_2$ TRIMER

S. SHEYBANI-DELOUI, J. NOROOZ OLIAEE, M. REZAEI, N. MOAZZEN-AHMADI, *Department of Physics and Astronomy, University of Calgary, 2500 University Drive North West, Calgary, Alberta, Canada T2N 1N4*; A.R.W. McKELLAR, *National Research Council of Canada, Ottawa, Ontario, Canada K1A 0R6*.

MK11 **15 min 4:34**

INFRARED SPECTRUM OF THE CS_2 TETRAMER: OBSERVATION OF A STRUCTURE WITH D_{2d} SYMMETRY

M. REZAEI, J. NOROOZ OLIAEE, N. MOAZZEN-AHMADI, *Department of Physics and Astronomy, University of Calgary, 2500 University Dr., N.W., Calgary, Alberta T2N 1N4, Canada*; A.R.W. McKELLAR, *National Research Council of Canada, Ottawa, Ontario, K1A 0R6, Canada*.

MK12 **15 min 4:51**

INFRARED SPECTROSCOPIC STUDY ON FERMI RESONANCE OF THE EXCESS PROTON VIBRATION IN BINARY CLUSTERS

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 Sciences Academia Sinica, Taipei 10617, Taiwan*.

MK13 **15 min 5:08**

THEORETICAL STUDY ON FERMI RESONANCE OF THE EXCESS PROTON VIBRATION IN BINARY CLUSTERS

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

MK14 **10 min 5:25**

MUTUAL CO-ASSIGNMENT OF THE CALCULATED VIBRATIONAL FREQUENCIES IN THE GROUND AND LOWEST EXCITED ELECTRONIC STATES

YURII N. PANCHENKO, *Laboratory of Molecular Spectroscopy, Division of Physical Chemistry, Department of Chemistry, Lomonosov Moscow State University, Moscow 119991, Russian Federation..*

TA. MINI-SYMPOSIUM: SPECTROSCOPY TESTS OF FUNDAMENTAL PHYSICS

TUESDAY, JUNE 18, 2013 – 8:30 AM

Room: 160 MATH ANNEX

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

TA01 *INVITED TALK* **30 min 8:30**

TOWARDS THE FIRST MEASUREMENT OF PARITY VIOLATION IN CHIRAL MOLECULES Ð NEW ATTEMPTS AND FUTURE PROSPECTIVE

PETER SCHWERDTFEGER, *Centre for Theoretical Chemistry and Physics, The New Zealand Institute for Advanced Study, Massey University Auckland, Auckland, New Zealand*.

TA02 **15 min 9:05**

RIGOROUS RELATIVISTIC METHODS FOR ADDRESSING $\mathcal{P}$- AND $\mathcal{T}$-NONCONSERVATION IN HEAVY-ELEMENT MOLECULES

TIMO FLEIG, *Laboratoire de Chimie et Physique Quantiques, Université Paul Sabatier Toulouse 3, Toulouse, France*.

TA03 **15 min 9:22**

PARITY VIOLATION IN CHIRAL MOLECULES: CURRENT STATUS OF THEORY AND SPECTROSCOPIC EXPERIMENT

MARTIN QUACK, GEORG SEYFANG, *Physical Chemistry, ETH Zurich, CH-8093 Zurich, Switzerland*.

TA04 **15 min 9:39**

A COMBINED SYNCHROTRON-BASED HIGH RESOLUTION FTIR AND DIODE LASER JET INFRARED SPECTROSCOPY STUDY OF THE CHIRAL MOLECULE CDBrClF

S. ALBERT, K. KEPPLER ALBERT, M. QUACK, *PHYSICAL CHEMISTRY, ETH ZÜRICH, CH-8093 ZÜRICH, SWITZERLAND*; PH. LERCH, *SWISS LIGHT SOURCE, PAUL-SCHERRER-INSTITUTE, CH-5232 VILLIGEN, SWITZERLAND* ; V. BOUDON, *LABORATOIRE CARNOT DE BOURGOGNE, UNIVERSITE DE BOURGOGNE, F-21078 DIJON, FRANCE*.

TA05 **15 min 9:56**

CAVITY-ENHANCED PARITY-NONCONSERVING OPTICAL ROTATION IN Hg, Xe, AND I

L. BOUGAS, G. E. KATSORINAKIS, T. PETER RAKITZIS, *Department of Physics, University of Crete, and Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas 71110 Heraklion-Crete, Greece*.

TA06 **15 min 10:13**

CHIRAL CAVITY RING-DOWN: ABSOLUTE MEASUREMENT OF OPTICAL ROTATION IN GASES AND LIQUIDS WITH SIGNAL REVERSALS

LYKOURGOS BOUGAS, G. E. KATSOPRINAKIS, T. P. RAKITZIS, *Department of Physics, University of Crete, and Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas 71110 Heraklion-Crete, Greece*.

Intermission

TA07 **15 min 10:45**

NEW PERSPECTIVES ON THE SEARCH FOR A PARITY VIOLATION EFFECT IN CHIRAL MOLECULES

F. AUGUSTE, S. K. TOKUNAGA, A. SHELKOVNIKOV, C. DAUSSY, A. AMY-KLEIN, C. CHARDONNET and B. DARQUIÉ, *Laboratoire de Physique des Lasers, Université Paris 13, Sorbonne Paris Cité, CNRS, F-93430, Villetaneuse, France*.

TA08 **15 min 11:02**

TRAVELLING-WAVE DECELERATION OF HEAVY DIATOMIC MOLECULES

J. E. VAN DEN BERG, C. MEINEMA, S. MATHAVAN, S. HOEKSTRA, *University of Groningen, Zernikelaan 25, 9747 AA, Groningen, The Netherlands*.

TA09 **15 min 11:19**

DETECTING PARITY VIOLATION USING TRAPPED MOLECULES

J. E. VAN DEN BERG, C. MEINEMA, S. MATHAVAN, S. HOEKSTRA, *University of Groningen, Zernikelaan 25, 9747 AA, Groningen, The Netherlands*.

TA10 **15 min 11:36**

A SLOW SOURCE OF MOLECULES FOR HIGH RESOLUTION SPECTROSCOPY

MARINA QUINTERO-PÉREZ, PAUL JANSEN, THOMAS E. WALL, WIM UBACHS and HENDRICK L. BETHLEM, *LaserLaB, Department of Physics and Astronomy, VU University Amsterdam, De Boelelaan 1081, 1081 HV Amsterdam, The Netherlands*.

TA11 **15 min 11:53**

NOVEL INFRARED COHERENT SOURCES AND TECHNIQUES FOR SPECTROSCOPIC TEST OF FUNDAMENTAL PHYSICS PRINCIPLES

P. CANCIO PASTOR, I. GALLI, G. GIUSFREDI, D. MAZZOTTI, and P. DE NATALE, *Istituto Nazionale di Ottica-Consiglio Nazionale delle Ricerche (INO-CNR), and European Laboratory for Non-linear Spectroscopy (LENS) Via N. Carrara 1, 50019 Sesto Fiorentino, Italy*.

TB. MINI-SYMPOSIUM: SPECTROSCOPY OF PLANETARY ATMOSPHERES

TUESDAY, JUNE 18, 2013 – 8:30 AM

Room: 170 MATH ANNEX

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

TB01 ***INVITED TALK*** **30 min 8:30**

SATELLITE REMOTE SENSING OF THE REACTIVE LOWER ATMOSPHERE USING MEDIUM RESOLUTION INFRARED MEASUREMENTS: HIGHLIGHTS FROM IASI MISSION

P.F. COHEUR, *Atmospheric Spectroscopy / Quantum Chemistry and Photophysics, Université Libre de Bruxelles CP160/09, Brussels, Belgium.*

TB02 **15 min 9:05**

INTENSITY MODELING OF METHANOL IN THE TORSIONAL MANIFOLD

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

TB03 **15 min 9:22**

THZ SPECTROSCOPY OF DEUTERATED ETHANE

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

TB04 **15 min 9:39**

OZONE RECOVERY IN THE PRESENCE OF $O_2(a^1\Delta)$ FOR ATMOSPHERIC STUDIES

MICHAEL C. HEAVEN, *Department of Chemistry, Emory University, Atlanta, GA 30322*; VALERIY N. AZYAZOV, *P.N. Lebedev Physical Institute, Samara Branch, Samara, Russia, 443029*.

Intermission

TB05 ***INVITED TALK*** **30 min 10:15**

EXOMOL: MOLECULAR LINE LISTS FOR EXOPLANET AND OTHER ATMOSPHERES

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

TB06 **15 min 10:50**

A NEW GLOBAL FIT FOR ^{17}O ENRICHED CO_2

BEN M. ELLIOTT, CHARLES E. MILLER, *Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Drive, M/S 233-300, Pasadena, CA 91109*.

TB07 **15 min 11:07**

SEMI-EMPIRICAL DIPOLE MOMENT FUNCTION OF $X^1\Sigma^+$ CO[a]

GANG LI, IOULI E. GORDON and LAURENCE S. ROTHMAN, *Harvard-Smithsonian Center for Astrophysics, Atomic and Molecular Physics Division, Cambridge MA 02138, USA*.

[a]This effort has been supported by NASA through EOS grant NNX11AF91G and Planetary Atmospheres grant NNX10AB94G.

TB08 **15 min 11:24**

CHARACTERIZATION OF OZONE PROFILES DERIVED FROM AURA TES AND OMI RADIANCES

DEJIAN FU, JOHN R. WORDEN, SUSAN S. KULAWIK, KEVIN V. BOMAN AND VIJAY NATRAJ, *Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109*; XIONG LIU, *Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts 02138, USA*.

TB09 **15 min 11:41**

MODELING THE SPECTRUM OF THE $2\nu_2$ and ν_4 STATES OF AMMONIA TO EXPERIMENTAL ACCURACY

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

TC. MICROWAVE

TUESDAY, JUNE 18, 2013 – 8:30 AM

Room: 1000 MCPHERSON LAB

Chair: VADIM ILYUSHIN, Institute of Radio Astronomy NASU, Khazkov, Ukraine

TC01 **10 min 8:30**

ROTATIONAL SPECTRA AND ANALYSIS OF THE ARGON-MONOFLUOROPYRIDINE VAN DER WAALS COMPLEXES

MAHDI KAMAEE, MING SUN AND JENNIFER VAN WIJNGAARDEN, *Department of Chemistry, University of Manitoba, Winnipeg MB R3T 2N2 Canada*.

TC02 **15 min 8:42**

BROADBAND CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE SPECTROSCOPY AND MOLECULAR STRUCTURE OF THE ARGON-1-CHLORO-1-FLUOROETHYLENE COMPLEX

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

TC03 **15 min 8:59**

MICROWAVE SPECTRA AND MOLECULAR STRUCTURES OF 2-CHLORO-1,1-DIFLUOROETHYLENE AND ITS COMPLEX WITH ARGON

JOSEPH P. MESSINGER, GREGORY S. KNOWLTON, KATHRYN M. SUNDHEIM, HELEN O. LEUNG, AND MARK D. MARSHALL, *Department of Chemistry, Amherst College, P.O. Box 5000, Amherst, MA 01002-5000*.

TC04 **15 min 9:16**

ROTATIONAL SPECTRA OF THE TRIFLUORO ETHANOL (TFE) -WATER CLUSTERS AND THE TFE DIMERS

JAVIX THOMAS, YUNJIE XU, *Department of Chemistry, University of Alberta, Edmonton, AB, T6G 2G2, Canada*.

TC05 **15 min 9:33**

STRUCTURE FOR THE PROPIOLIC ACID - FORMIC ACID COMPLEX FROM MICROWAVE SPECTRA FOR MULTIPLE ISOTOPOLOGUES [a]

STEPHEN G. KUKOLICH, ERIK G. MITCHELL, SPENCER J. CAREY, MING SUN, and BRYAN M. SARGUS, *Department of Chemistry and Biochemistry, The University of Arizona, Tucson, Arizona 85721.*.

[a] Supported by THE NATIONAL SCIENCE FOUNDATION

TC06 **15 min 9:50**

THE EFFECT OF PROTIC ACID IDENTITY ON THE STRUCTURES OF COMPLEXES WITH VINYL CHLORIDE: FOURIER TRANSFORM MICROWAVE SPECTROSCOPY AND MOLECULAR STRUCTURE OF THE VINYL CHLORIDE-ACETYLENE COMPLEX

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

Intermission

TC07 **15 min 10:20**

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

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

TC08 **15 min 10:37**

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

NATHAN A. SEIFERT, CRISTÓBAL PÉREZ, AMANDA L. STEBER, DANIEL P. ZALESKI, JUSTIN L. NEILL, BROOKS H. PATE, *Department of Chemistry, University of Virginia, McCormick Rd., Charlottesville, VA 22904-4319*; ALBERTO LESARRI, *Departamento de Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, E-47001 Valladolid, Spain*.

TC09 **10 min 10:54**

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

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

TC10 **15 min 11:06**

ROTATIONAL SPECTRA OF ADDUCTS OF FORMALDEHYDE WITH FREONS

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

TC11 **15 min 11:23**

MICROWAVE SPECTROSCOPIC INVESTIGATIONS OF THE C–H$\cdots\pi$ CONTAINING COMPLEXES $CH_2F_2\cdots$PROPYNE AND $CH_2ClF\cdots$PROPYNE

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

TC12 **10 min 11:40**

OBSERVATION OF A C–H$\cdots$AROMATIC INTERACTION IN THE FLUOROBENZENE$\cdots$HCCH WEAKLY BOUND COMPLEX

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

TD. RADICALS AND IONS

TUESDAY, JUNE 18, 2013 – 8:30 AM

Room: 1015 MCPHERSON LAB

Chair: YUAN-PERN LEE, National Chiao Tung University, Hsinchu, Taiwan

TD01 **15 min 8:30**

THE ROLES OF ATOMIC OXYGEN AND NITRIC OXIDE IN LOW TEMPERATURE PLASMAS

SHERRIE S. BOWMAN, DAVID BURNETTE, IGOR V. ADAMOVICH, and WALTER R. LEMPERT, *M.A. Chaszeyka Non-Equilibrium Thermodynamics Laboratory, The Ohio State University, Columbus, Ohio 43210.*.

TD02 **15 min 8:47**

SUB-DOPPLER SPECTROSCOPY OF $trans$-HOCO RADICAL IN THE OH STRETCHING MODE

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

TD03 **15 min 9:04**

VIBRONIC ANALYSIS FOR $\widetilde{B}$ - $\widetilde{X}$ TRANSITION OF ISOPROPOXY RADICAL

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

TD04 **15 min 9:21**

ANALYSIS OF THE ROTATIONAL STRUCTURE OF $\tilde{B}^2A' \leftarrow \tilde{X}^2A'$ TRANSITION OF ISOPROPOXY RADICAL: ISOLATED STATE vs. COUPLED STATES MODEL

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*.

TD05 **15 min 9:38**

HIGH-RESOLUTION LASER-INDUCED FLUORESCENCE SPECTROSCOPY OF CYCLOHEXOXY: ROTATIONAL AND FINE STRUCTURE OF MOLECULES IN NEARLY DEGENERATE ELECTRONIC STATES

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

TD06 **15 min 9:55**

ANOMALOUS Λ-DOUBLING IN THE INFRARED SPECTRUM OF THE HYDROXYL RADICAL IN HELIUM NANODROPLETS

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

TD07 **15 min 10:12**

HELIUM NANODROPLET ISOLATION SPECTROSCOPY AND AB INITIO CALCULATIONS OF HO_3-$(O_2)_N$ CLUSTERS (N=0-4)

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

Intermission

TD08 **15 min 10:45**

FOURIER TRANSFORM INFRARED SPECTROSCOPY OF CH_3OO RADICAL IN MID-INFRARED RANGE

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

TD09 **15 min 11:02**

FARADAY ROTATION SPECTROSCOPY OF HO_2 FROM AN ATMOSPHERIC FLOW REACTOR

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

TD10 **15 min 11:19**

OBSERVATION OF THE $\widetilde{A} - \widetilde{X}$ ELECTRONIC TRANSITION OF C_6-C_{10} PEROXY RADICALS

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

TD11 **15 min 11:36**

STRUCTURE IN THE VISIBLE ABSORPTION BANDS OF JET-COOLED PHENYL PEROXY RADICALS

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

TD12 **15 min 11:53**

TERAHERTZ ROTATIONAL SPECTROSCOPY OF THE SO RADICAL

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

TE. MATRIX/CONDENSED PHASE

TUESDAY, JUNE 18, 2013 – 8:30 AM

Room: 2015 MCPHERSON LAB

Chair: MARILYN JACOX, NIST, Gaithersburg, MD

TE01 **15 min** **8:30**

INFRARED SPECTROSCOPY OF HNO AND NOH SUSPENDED IN SOLID PARAHYDROGEN

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

TE02 **15 min** **8:47**

COLD CHEMICAL REACTIONS OF H-ATOMS AND N_2O IN SOLID PARAHYDROGEN AT 2 K

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

TE03 **15 min** **9:04**

RYDBERG STATES OF Rb AND Cs ATOMS ON HELIUM NANODROPLETS: A RYDBERG-RITZ ANALYSIS

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

TE04 **15 min** **9:21**

DYNAMICS OF CH_3F-($ortho$-H_2)n CLUSTERS IN SOLID $para$-H_2 CRYSTAL STUDIED BY PUMP AND PROBE SPECTROSCOPY USING TWO CW-QUATUM CASCADE LASERS

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

TE05 **15 min** **9:38**

TERAHERTZ TIME DOMAIN SPECTROSCOPY OF SIMPLE ASTROPHYSICALLY RELEVANT ICES: THE STRUCTURE OF THE ICE

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

TE06 **15 min** **9:55**

FIRST OBSERVATION OF A VIBRATIONAL FUNDAMENTAL OF SiC_6Si TRAPPED IN SOLID Ar

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

TE07 **15 min 10:12**

NIR LASER RADIATION INDUCED CONFORMATIONAL CHANGES AND TUNNELING LIFETIMES OF HIGH-ENERGY CONFORMERS OF AMINO ACIDS IN LOW-TEMPERATURE MATRICES

GABOR BAZSO, ESZTER E. NAJBAUER, GABOR MAGYARFALVI and GYORGY TARCZAY, *Laboratory of Molecular Spectroscopy, Institute of Chemistry, Eotvos University, PO Box 32, H-1518, Budapest 112, Hungary*.

Intermission

TE08 **15 min 10:45**

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

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

TE09 **15 min 11:02**

VUV PHOTOLYSIS OF NH_3: A MATRIX ISOLATION STUDY OF THE MOLECULAR INTERACTIONS BETWEEN AMIDOGEN RADICAL AND AMMONIA MOLECULES

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

TE10 **15 min 11:19**

HOT SPOT GENERATION IN ENERGETIC MATERIALS BY APPLYING WEAK ENERGIES

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

TE11 **15 min 11:36**

THERMAL DECOMPOSITION MECHANISM OF BUTYRALDEHYDE

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

TE12 **5 min 11:53**

THE PECULIARITIES OF THE NMR SPIN-LATTICE RELAXATION IN PROTON EXCHANGED $LINBO_3$

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

TF. MINI-SYMPOSIUM: SPECTROSCOPY TESTS OF FUNDAMENTAL PHYSICS

TUESDAY, JUNE 18, 2013 – 1:30 PM

Room: 160 MATH ANNEX

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

TF01 **15 min** **1:30**

AN OVERVIEW OF PNC RELATED STUDIES INVOLVING HEAVY POLAR MOLECULES

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

TF02 **15 min** **1:47**

ThF^+ AS A CANDIDATE FOR eEDM MEASUREMENTS

MICHAEL C. HEAVEN, JOSHUA H. BARTLETT, *Department of Chemistry, Emory University, Atlanta, GA 30322*.

TF03 **15 min** **2:04**

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

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

TF04 **15 min** **2:21**

A CONCEPT OF EFFECTIVE STATE OF ATOMS-IN-COMPOUNDS TO DESCRIBE PROPERTIES DETERMINED BY THE VALENCE ELECTRON'S DENSITIES IN ATOMIC CORES

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

[a] SPbU Fundamental Science Research grant from Federal budget N 0.038.652.2013 and RFBR grant 13-02-01406 are gratefully acknowledged

TF05 **15 min** **2:38**

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

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

TF06 **15 min** **2:55**

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

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

[a] ACME COLLABORATION

TF07 **15 min 3:12**

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

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

TF08 **15 min 3:29**

PROGRESS OF THE JILA ELECTRON EDM EXPERIMENT

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

TF09 **15 min 3:46**

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

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

[a] SPbU Fundamental Science Research grant from Federal budget N 0.038.652.2013 and RFBR grant 13-02-01406 are gratefully acknowledged

TF10 **15 min 4:03**

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

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

TF11 **10 min 4:20**

PRECISE THEORETICAL STUDY OF SPECTROSCOPIC CONSTANTS IN DIATOMICS

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

[a] SPbU Fundamental Science Research grant from Federal budget N 0.038.652.2013 and RFBR grant 13-02-01406 are gratefully acknowledged

Intermission

TF12 **15 min 4:50**

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

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

TF13 **15 min 5:07**

COMB-ASSISTED QCL DOPPLER-BROADENED THERMOMETRY IN NH_3 SAMPLES

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

TF14 **15 min 5:24**

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

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

TF15 **10 min 5:41**

NARROW OPPOSITE-PARITY LEVEL CROSSINGS IN A DIATOMIC RADICAL

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

TF16 **15 min 5:53**

PHOTOELECTRON SPECTROSCOPY STUDIES OF URANIUM FLUORIDE

WEI-LI LI, TIAN JIAN, GARY V. LOPEZ, AND LAI-SHENG WANG , *Brown University, Chemistry Department, 324 Brook St, Providence, RI, 02912*.

TG. MINI-SYMPOSIUM: THEORY AND SPECTROSCOPY

TUESDAY, JUNE 18, 2013 – 1:30 PM

Room: 170 MATH ANNEX

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

TG01 ***INVITED TALK*** **30 min 1:30**

DIABATIC VERSUS ADIABATIC CALCULATION OF TORSION-VIBRATION INTERACTIONS

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

TG02 **15 min 2:05**

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

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

TG03 **15 min 2:22**

EXTENDING DIFFUSION MONTE CARLO TO INTERNAL COORDINATES

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

TG04 **15 min 2:39**

PATTERNS OF BROKEN PATTERNS

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

TG05 **15 min 2:56**

ISOMERIZATION, PERTURBATIONS, CALCULATIONS AND THE S_1 STATE OF C_2H_2

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

TG06 **15 min 3:13**

REDUCED DIMENSION ROVIBRATIONAL VARIATIONAL CALCULATIONS OF THE S_1 STATE OF C_2H_2

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

TG07 **15 min 3:30**

LEAST SQUARES FITTING OF PERTURBED VIBRATIONAL POLYADS NEAR THE ISOMERIZATION BARRIER IN THE S_1 STATE OF C_2H_2

A. J. MERER, *Department of Chemistry, University of British Columbia, Vancouver, B.C., Canada V6T 1Z1 AND Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan.*; J. H. BARABAN, P. B. CHANGALA, and R. W. FIELD, *Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139, USA*.

Intermission

TG08 **15 min 4:00**

COLLISIONAL LINE MIXING IN PARALLEL AND PERPENDICULAR BANDS OF LINEAR MOLECULES BY A NON-MARKOVIAN APPROACH

JEANNA BULDYREVA, *Institut UTINAM, UMR CNRS 6213, Université de Franche-Comté, 16 route de Gray, 25030 Besançon cedex, France*.

TG09 **15 min 4:17**

TUNNELING AND TUNNELING SWITCHING DYNAMICS IN PHENOL AND ORTHO-D-PHENOL: FTIR SPECTROSCOPY WITH SYNCHROTRON RADIATION AND THEORY

S. ALBERT, R PRENTNER, M. QUACK, *PHYSICAL CHEMISTRY, ETH ZÜRICH, CH-8093 ZÜRICH, SWITZERLAND*; PH. LERCH, *SWISS LIGHT SOURCE, PAUL-SCHERRER-INSTITUTE, CH-5232 VILLIGEN, SWITZERLAND*.

TG10 **15 min 4:34**

ANHARMONIC VIBRATIONAL MØLLER-PLESSET PERTURBATION THEORIES USING THE DYSON EQUATION

MATTHEW R. HERMES and SO HIRATA, *Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801*.

TG11 **15 min 4:51**

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

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

TG12 **15 min 5:08**

VIBRATIONAL CONSTANTS FOR TRIATOMIC MOLECULES FROM FOURTH-ORDER PERTURBATION THEORY

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

TG13 **15 min 5:25**

ROTATIONAL AND ROVIBRATIONAL CONSTANTS FOR TRIATOMIC MOLECULES FROM FOURTH-ORDER PERTURBATION THEORY

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

TG14 **15 min 5:42**

APPLICATION OF FOURTH-ORDER VIBRATIONAL PERTURBATION THEORY TO SMALL MOLECULES

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

TH. MICROWAVE

TUESDAY, JUNE 18, 2013 – 1:30 PM

Room: 1000 MCPHERSON LAB

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

TH01 **15 min** **1:30**

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

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

TH02 **15 min** **1:47**

FOURIER TRANSFORM MICROWAVE SPECTRUM OF N_2-$(CH_2)_2O$

YOSHIYUKI KAWASHIMA, *Department of Applied Chemistry, Faculty of Engineering, Kanagawa Institute of Technology, Atsugi, Kanagawa 243-0292, JAPAN*; EIZI HIROTA, *The Graduate University for Advanced Studies, Hayama, Kanagawa 240-0193, JAPAN*.

TH03 **15 min** **2:04**

THE BROADBAND ROTATIONAL SPECTRUM AND GEOMETRY OF $N_2 \cdots ICF_3$

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

TH04 **15 min** **2:21**

UNEXPECTED GENERATION AND OBSERVATION OF A T-SHAPED COMPLEX OF $H_2C_2 \cdots AgCCH$

N. R. WALKER, *School of Chemistry, Bedson Building, Newcastle University, Newcastle-upon-Tyne, NE1 7RU, U.K.*; S. L. STEPHENS, W. MIZUKAMI, D. P. TEW AND A. C. LEGON, *School of Chemistry, University of Bristol, Bristol, BS8 1TS, U.K.*.

TH05 **15 min** **2:38**

STRUCTURES OF THE CAGE, PRISM, AND BOOK HEXAMER WATER CLUSTERS FROM MULTIPLE ISOTOPIC SUBSTITUTION

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

TH06 **15 min** **2:55**

CHARACTERIZATION OF LARGE WATER CLUSTERS BY BROADBAND ROTATIONAL SPECTROSCOPY

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

TH07 **15 min 3:12**

HYDROGEN BOND NETWORK ISOMERS OF THE WATER NONAMER AND DECAMER OBSERVED BY BROADBAND ROTATIONAL SPECTROSCOPY

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

TH08 **15 min 3:29**

STRUCTURES OF THE LOWEST ENERGY NONAMER AND DECAMER WATER CLUSTERS FROM CHIRPED-PULSE ROTATIONAL SPECTROSCOPY

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

Intermission

TH09 **15 min 4:00**

MILLIMETER WAVE SPECTRA OF THE INTERNAL ROTATION EXCITED STATES OF (*o*)H_2-H_2O AND (*o*)H_2-D_2O

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

TH10 **15 min 4:17**

THE PERFORMANCE OF THE THIRD GENERATION OF CP-FTMW SPECTROMETERS ILLUSTRATED BY THE ANALYSIS OF THE WATER HEPTAMER STRUCTURE

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

TH11 **10 min 4:34**

THE CYTOSINE WATER COMPLEX

A. M. DALY, S. MATA, C. BERMUDEZ, M. BERDAKIN, I. PENA, C. CABEZAS, J. L. ALONSO, *Grupo de Espectroscopía Molecular (GEM), Edificio Quifima, Laboratorios de Espectroscopía y Bioespectroscopía, Parque Científico, Universidad de Valladolid, 47011 Valladolid, Spain*.

TH12 **10 min 4:46**

EXPERIMENTAL EVIDENCE OF LONE PAIRS - π SYSTEM INTERACTION: THE ROTATIONAL SPECTRUM OF CHLOROTRIFLUOROETHYLENE - WATER COMPLEX

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

TH13 **15 min 4:58**

MICROWAVE SPECTRA AND STRUCTURE OF H_2–CuF: OVERVIEW OF THE COMPLEXES OF HYDROGEN WITH METAL-CONTAINING DIATOMICS

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

TH14 **15 min 5:15**

EFFECTS OF A REMOTE BINDING PARTNER ON THE ELECTRIC FIELD AND ELECTRIC FIELD GRADIENT AT AN ATOM IN A WEAKLY BOUND TRIMER: MICROWAVE SPECTROSCOPY AND QUANTUM MECHANICAL COMPUTATIONS ON Kr-SO_3 AND Kr-SO_3-CO

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

TH15 **15 min 5:32**

MICROWAVE SPECTRUM AND STRUCTURE OF THE 2,6-DIFLUOROPYRIDINE-CO_2 COMPLEX

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

TH16 **15 min 5:49**

OBSERVATION OF A MODERATE STRENGTH INTERACTION OF HYDROGEN WITH A COINAGE METAL HALIDE: THE ROTATIONAL SPECTRUM AND STRUCTURE OF THE p-H_2-CuCl AND o-H_2-CuCl COMPLEXES

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

TI. ASTRONOMICAL SPECIES AND PROCESSES

TUESDAY, JUNE 18, 2013 – 1:30 PM

Room: 1015 MCPHERSON LAB

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

TI01 **15 min** **1:30**

LARGE PICTURE OF THE GALACTIC CENTER STUDIED BY H_3^+: HIGH IONIZATION RATE, PREVAILING WARM AND DIFFUSE GAS, AND NON-ROTATING EXPANDING MOLECULAR RING

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

TI02 **15 min** **1:47**

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

JULIE K. ANDERSON and LUCY M. ZIURYS, *Department of Chemistry and Biochemistry, The University of Arizona, Tucson, AZ 85719*.

TI03 **15 min** **2:04**

FORMATION OF CH^+: SHOCK CHEMISTRY IN NGC 7027

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

TI04 **15 min** **2:21**

WARM, DENSE GAS NEAR THE MASSIVE PROTOSTAR AFGL 2136 IRS 1 AS REVEALED BY ABSORPTION FROM THE ν_1, ν_2, AND ν_3 BANDS OF WATER

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

TI05 **15 min** **2:38**

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

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

TI06 **15 min** **2:55**

CSO BROADBAND MOLECULAR LINE SURVEYS I: BENCHMARKING GOBASIC ANALYSIS SOFTWARE

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

TI07 **15 min 3:12**

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

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

TI08 **15 min 3:29**

DETECTION AND FORMATION OF INTERSTELLAR c-C_3D_2

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

Intermission

TI09 **15 min 4:00**

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

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

TI10 **15 min 4:17**

THE ANALYSIS OF ACETONITRILE (CH_3CN) USING 3-D SUBMILLIMETER SPECTROSCOPY

JAMES P. MCMILLAN, SARAH M. FORTMAN, CHRISTOPHER F. NEESE, FRANK C. DE LUCIA, *Department of Physics, The Ohio State University, Columbus, OH 43210*.

TI11 **15 min 4:34**

THE COMPLETE, TEMPERATURE RESOLVED EXPERIMENTAL SPECTRUM OF METHANOL BETWEEN 560 AND 654 GHZ

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

TI12 **15 min 4:51**

SPECTROSCOPY OF ISOCYANIDES AND THEIR SEARCH IN INTERSTELLAR MEDIUM

L. MARGULÈS, R. A. MOTIYENKO, *Laboratoire PhLAM, CNRS UMR 8523, Université de Lille 1, 59655 Villeneuve d'Ascq Cedex, France*; B. TERCERO, J. CERNICHARO, *Centro de Astrobiología (CSIC-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*.

TI13 **15 min 5:08**

SUBMILLIMETERWAVE SPECTROSCOPY OF HIGHLY ASTROPHYSICAL INTEREST MOLECULE: HYDROXY-ACETONITRILE

L. MARGULÈS, R. A. MOTIYENKO, *Laboratoire PhLAM, CNRS UMR 8523, Université de Lille 1, 59655 Villeneuve d'Ascq Cedex, France*; and J.-C. GUILLEMIN, *Sciences Chimiques de Rennes, UMR 6226 CNRS-ENSCR, Avenue du Général Leclerc, CS 50837, 35708 Rennes Cedex 7, France*.

TI14 **15 min 5:25**

LABORATORY MEASUREMENTS AND ASTRONOMICAL OBSERVATIONS OF H_2NCO^+

HARSHAL GUPTA, *Morrisroe Astrocience Laboratory, California Institute of Technology, Pasadena, CA 91125*; CARL A. GOTTLIEB AND MICHAEL C. MCCARTHY, *Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138.*

TI15 **15 min 5:42**

MILLIMETER AND SUBMILLIMETER WAVE SPECTRA OF THE $HCOO^{13}CH_3$ ISOTOPOLOG OF METHYLFORMATE IN THE GROUND STATE AND IN THE FIRST EXCITED TORSIONAL STATE.

I. HAYKAL, L. MARGULÈS, T. R. HUET, R. A. MOTIYENKO, *Laboratoire PhLAM, UMR8523 CNRS-Université Lille 1, F-59655 Villeneuve d'Ascq Cedex, France*; M. CARVAJAL, *Unidad Asociada IEM-CSIC-Dpto. de Física Aplicada, Universidad de Huelva, Spain*; I. KLEINER, *LISA, CNRS et Université Paris Est et Paris Diderot, 61 av. Général de Gaulle, 94010, Créteil, France*; J. C. GUILLEMIN, *ENS de Chimie de Rennes -CNRS -35700 Rennes, France*; B. TERCERO, J. CERNICHARO, *Centro de Astrobiología (CSIC-INTA). Ctra de Ajalvir, Km 4, 28850 Torrejón de Ardoz, Madrid, Spain*.

TJ. INFRARED/RAMAN

TUESDAY, JUNE 18, 2013 – 1:30 PM

Room: 2015 MCPHERSON LAB

Chair: BRIAN BRUMFIELD, Princeton University, Princeton, NJ

TJ01 **15 min 1:30**

SUB-DOPPLER RESOLUTION SPECTROSCOPY OF THE FUNDAMENTAL BAND OF HCl WITH AN OPTICAL FREQUENCY COMB

K. IWAKUNI and M. ABE and H. SASADA, *Department of Physics, Faculty of Science and Technology, Keio University, 3-14-1, Hiyoshi, Kohoku-ku, Yokohama 223-8522, Japan*.

TJ02 **15 min 1:47**

ABSOLUTE MEASUREMENTS OF NEAR-INFRARED CO_2 TRANSITION FREQUENCIES AT THE kHz-LEVEL

DAVID A. LONG, GAR-WING TRUONG, JOSEPH T. HODGES, *Material Measurement Laboratory, National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, MD 20899, USA*; and CHARLES E. MILLER, *Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Drive, Pasadena, CA 91109, USA*.

TJ03 **15 min 2:04**

ACCURATE DETERMINATION OF ROTATIONAL ENERGY LEVELS IN THE GROUND STATE OF $^{12}CH_4$

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

TJ04 **10 min 2:21**

IR/THZ DOUBLE RESONANCE SPECTROSCOPY IN THE PRESSURE BROADENED REGIME: A PATH TOWARDS ATMOSPHERIC GAS SENSING

S. SREE HARSHA , *Aegis Technologies, 410 Jan Davis Drive, Huntsville, Alabama 35806*; DANE J. PHILLIPS, *IERUS Technologies, 2904 Westcorp Blvd, Ste 210, Huntsville, AL 35805*; FRANK C. DE LUCIA, *Department of Physics, 191 Woodruff Ave., Ohio State University, Columbus, OH 43210* ; HENRY O. EVERITT , *Army Aviation and Missile RDE Center, Redstone Arsenal, AL 35898*.

TJ05 **15 min 2:33**

DETECTION OF NO AND S-NITROSOCOMPOUNDS USING MID-IR CAVITY RING-DOWN SPECTROSCOPY

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

TJ06 **15 min 2:50**

DIFFERENTIAL OPTICAL DISPERSION SPECTROSCOPY FOR COMPARATIVE MOLECULAR QUANTIFICATION

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

Intermission

TJ07 **5 min 3:30**

STUDY OF UTILIZATION OF AUTOMOTIVE DIESEL GLOW PLUG AS AN IR SOURCE

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

TJ08 **10 min 3:37**

FTIR STUDY OF COMUSTION SPECIES IN SEVERAL REGIONS OF A CANDLE FLAME

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

TJ09 **15 min 3:49**

SPONTANEOUS RAMAN SCATTERING MEASUREMENTS OF NITROGEN VIBRATIONAL DISTRIBUTION FUNCTION IN NANOSECOND PULSED DISCHARGE

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

TJ10 **15 min 4:06**

STIMULATED INFRARED EMISSION OF C_2H_2 NEAR 3000 cm^{-1} WITH CONTINUOUS-WAVE LASERS

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

TJ11 **15 min 4:23**

CONTINUOUS WAVE STIMULATED RAMAN SPECTROSCOPY INSIDE A HOLLOW CORE PHOTONIC CRYSTAL FIBER

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

TJ12 **15 min 4:40**

DEVELOPMENT OF AN EXTERNAL CAVITY QUANTUM CASCADE LASER SPECTROMETER FOR HIGH-RESOLUTION SPECTROSCOPY OF MOLECULAR IONS

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

TJ13 **15 min 4:57**

FELION: A CRYOGENIC ION TRAP APPARATUS FOR SPECTROSCOPIC STUDIES WITH FELIX

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

TJ14 **15 min 5:14**

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

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

TJ15 **15 min 5:31**

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

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

TJ16 **15 min 5:48**

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

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

TK. ELECTRONIC

TUESDAY, JUNE 18, 2013 – 1:30 PM

Room: 1153 SMITH LAB

Chair: SCOTT REID, Marquette University, Milwaukee, WI

TK01 **15 min** **1:30**

THE CHARACTER OF THE LONG-LIVED STATE FORMED FROM S_1 OF PHENYLACETYLENE

PHILIP M. JOHNSON AND TREVOR J. SEARS[a], *Department of Chemistry, Stony Brook University, Stony Brook, New York 11794*.

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

TK02 **15 min** **1:47**

TWO-PROTON PHOTOTAUTOMERIZATION DYNAMICS OF 7-AZAINDOLE COMPLEXES

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

TK03 **15 min** **2:04**

STRUCTURE DETERMINATION AND EXCITED STATE PROTON TRANSFER REACTION OF 1-NAPHTHOL-AMMONIA CLUSTERS IN THE S_1 STATE STUDIED BY UV-IR-UV MID-IR SPECTROSCOPY

SHUNPEI YOSHIKAWA, MITSUHIKO MIYAZAKI, WEILER MARTIN, *Chemical Resources Laboratory, Tokyo Institute of Technology, 4259 Nagatsuta-cho, Midori-ku, Yokohama 226-8503 Japan*; HARUKI ISHIKAWA, *Depertment of Chemistry, School of Science, Kitasato University, Minami-ku, Sagamihara 252-0373, Japan*; MASAAKI FUJII, *Chemical Resources Laboratory, Tokyo Institute of Technology, 4259 Nagatsuta-cho, Midori-ku, Yokohama 226-8503 Japan*.

TK04 **15 min** **2:21**

LASER DESORPTION SUPERSONIC JET SPECTROSCOPY OF HYDRATED TYROSINE

HIKARI OBA, YOKO SHIMOZONO, SHUN-ICHI ISHIUCHI, MASAAKI FUJII, *Chemical Resources Lab. Tokyo Tech. 4259 Nagatsuta-cho, Midoriku, Yokohama, 226-8503, Japan*; PIERRE CARCABAL, *ISMO. Université Paris Sud XI Bâtiment 210, 91405, Orsay, Paris, France*.

TK05 **15 min** **2:38**

EXCITED-STATE DYNAMICS IN FOLIC ACID AND 6-CARBOXYPTERIN UPON UVA EXCITATION

HUIJUAN HUANG, R. AARON VOGT and CARLOS E. CRESPO-HERNÁNDEZ, *Department of Chemistry and Center for Chemical Dynamics, Case Western Reserve University, Cleveland, Ohio 44106*.

TK06 **15 min** **2:55**

RESONANCE ENHANCED MULTI-PHOTON IONIZATION (REMPI) AND DOUBLE RESONANCE (UV-UV AND IR-UV) SPECTROSCOPIC INVESTIGATION ISOCYTOSINE

SEUNG JUN LEE, AHREUM MIN, AHREUM AHN, CHEOL JOO MOON, MYONG YONG CHOI, *Department of Chemistry and Research Institute of Natural Science, Gyeongsang National University, Jinju 660-701, Korea*; SHUN-ICHI ISHIUCHI, MITSUHIKO MIYAZAKI, MASAAKI FUJII, *Tokyo Institute of Technology, Chemical Resources Laboratory, Japan*.

TK07 **15 min 3:12**

RESONANCE ENHANCED MULTI-PHOTON IONIZATION AND UV-UV HOLE-BURNING SPECTROSCOPIC STUDIES OF JET-COOLED ACETANILIDE DERIVATIVES

CEOL JOO MOON and AHREUM MIN, AHREUM AHN, SEUNG JUN LEE, MYONG YONG CHOI, *Department of Chemistry (BK21), Gyeongsang National University, 501 Jinju Daero, Jinju 600-701, South Korea*; SEONG KEUN KIM, *Department of Chemistry and Biophysics & Biophysical Chemistry (WCU) Seoul National University, Seoul 151-747, South Korea*.

TK08 **15 min 3:29**

TAILOR MADE SYNTHESIS OF T-SHAPED AND π-STACKED DIMERS IN THE GAS PHASE: CONCEPT FOR EFFICIENT DRUG DESIGN AND MATERIAL SYNTHESIS

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

Intermission

TK09 **15 min 4:00**

ROTATIONALLY RESOLVED HIGH-RESOLUTION LASER SPECTROSCOPY OF THE $S_1 \leftarrow S_0$ TRANSITION OF NAPHTHALENE AND Cl-NAPHTHALENE

SHUNJI KASAHARA, RYO YAMAMOTO, KOHEI TADA, *Molecular Photoscience Research Center, Kobe University, Kobe 657-8501, Japan*.

TK10 **15 min 4:17**

VIBRONIC SPECTROSCOPY OF 4-ISOCYANOBENZONITRILE

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

TK11 **15 min 4:34**

STEPWISE SOLVATION EFFECTS ON THE EXCITED STATES OF A WEAKLY COUPLED BICHROMOPHORE: 1,2-DIPHENOXYETHANE-$(H_2O)_N$ (N=2-4) CLUSTERS

PATRICK S. WALSH, EVAN G. BUCHANAN, JOSEPH R. GORD and TIMOTHY S. ZWIER, *Department of Chemistry, Purdue University, 560 Oval Drive, West Lafayette, IN 47907*.

TK12 **15 min 4:51**

PLANT SUNSCREENS IN NATURE: UV AND IR SPECTROSCOPY OF SINAPATE DERIVATIVES

JACOB C. DEAN, PATRICK S. WALSH, and TIMOTHY S. ZWIER, *Department of Chemistry, Purdue University, West Lafayette, IN 47907*; FLORENT ALLAIS, *AgroParisTech, Paris, France*.

TK13 **15 min 5:08**

FLUORESCENCE EXCITATION SPECTRA OF PHOTO-FRAGMENTED NITROBENZENE USING A PICOSECOND LASER: POTENTIAL EVIDENCE FOR NO PRODUCED BY TWO DISTINCT CHANNELS.

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

TK14 **15 min 5:25**

SPECTROSCOPIC CHARACTERIZATION OF A NATURAL PRODUCT: ANETHOLE

VICTORIA P. BARBER AND JOSH J. NEWBY, *Department of Chemistry and Biochemistry, Swarthmore College, Swarthmore, PA 19081*.

WA. PLENARY

WEDNESDAY, JUNE 19, 2013 – 8:30 AM

Room: AUDITORIUM, INDEPENDENCE HALL

Chair: ANNE MCCOY, The Ohio State University, Columbus, OH

WA01 **40 min 8:30**

CHARGE TRANSFER REACTIONS INDUCE BORN-OPPENHEIMER BREAKDOWN IN SURFACE CHEMISTRY: APPLICATIONS OF DOUBLE RESONANCE SPECTROSCOPY IN MOLECULE-SURFACE SCATTERING

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

WA02 **40 min 9:15**

ULTRA SENSITIVE CAVITY RING DOWN SPECTROSCOPY OF MAJOR ATMOSPHERIC SPECIES BETWEEN 1.20 AND 1.71 μm

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

Intermission

WA03 **40 min 10:20**

INFRARED STUDIES OF METAL CATION-DIHYDROGEN COMPLEXES

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

WA04 **40 min 11:05**

SPECTROSCOPIC ENGINEERING IN THE SUBMILLIMETER

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

WF. ASTRONOMICAL SPECIES AND PROCESSES

WEDNESDAY, JUNE 19, 2013 – 1:30 PM

Room: 160 MATH ANNEX

Chair: SANDRA BRUENKEN, University of Cologne, Koeln, Germany

WF01 **15 min** **1:30**

RADIATIVE LIFETIME FOR NUCLEAR SPIN CONVERSION OF WATER-ION, H_2O^+

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

WF02 **15 min** **1:47**

A MM/SUBMM WAVE SPECTROMETER TO QUANTIFY ASTROCHEMICAL REACTION RATES

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

WF03 **15 min** **2:04**

UNIFIED MICROSCOPIC-MACROSCOPIC MONTE CARLO SIMULATION OF ICE FORMATION ON INTERSTELLAR GRAINS

QIANG CHANG, *Department of Chemistry, University of Virginia, Charlottesville, Virginia, USA*; ERIC HERBST, *Department of Chemistry, Physics and Astronomy, University of Virginia, Charlottesville, Virginia, USA*.

WF04 **15 min** **2:21**

THE LOW-TEMPERATURE NUCLEAR SPIN EQUILIBRIUM OF H_3^+ IN COLLISIONS WITH H_2

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

[a]Present address: Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, 02138

WF05 **15 min** **2:38**

MOLECULAR HYDROGEN FORMATION : EFFECT OF DUST GRAIN TEMPERATURE FLUCTUATIONS

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

WF06 **15 min** **2:55**

REVISED TERM VALUES FOR THE $A - X$ ($v' = 0$-9, $v'' = 0$) BANDS IN $^{13}C^{16}O$ FROM HIGH-RESOLUTION SPECTRA ACQUIRED AT THE SOLEIL SYNCHROTRON

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

Intermission

WF07 **15 min 3:30**

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

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

WF08 **15 min 3:47**

THE '4050 Å GROUP' OF THE $\tilde{A}^1\Pi_u$ - $\tilde{X}^1\Sigma_g^+$ TRANSITION SYSTEM OF C_3

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

WF09 **15 min 4:04**

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

BRETT A. McGUIRE, *Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125*; RYAN A. LOOMIS, *Department of Chemistry, University of Virginia, Charlottesville, VA 22904*; CAMERON M. CHARNESS, JOANNA F. CORBY, *Department of Astronomy, University of Virginia, Charlottesville, VA 22904*; GEOFFREY A. BLAKE, *Division of Chemistry and Chemical Engineering and Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, CA 91125*; JAN M. HOLLIS, *NASA Goddard Space Flight Center, Greenbelt, MD 20771*; FRANK J. LOVAS, *National Institute of Standards and Technology, Gaithersburg, MD 20899*; PHILIP R. JEWELL, and ANTHONY J. REMIJAN, *National Radio Astronomy Observatory, Charlottesville, VA 22903*.

WF10 **15 min 4:21**

INDIRECT ROTATIONAL SPECTROSCOPY OF HCO^+

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

WF11 **15 min 4:38**

SLIT-JET DISCHARGE STUDIES OF POLYACETYLENIC MOLECULES: SYNTHESIS AND HIGH RESOLUTION INFRARED SPECTROSCOPY OF DIACETYLENE

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

WF12 **15 min 4:55**

SUB-DOPPLER SLIT JET DISCHARGE SPECTROSCOPY OF JET COOLED POLYACETYLENES: THE ANTI-SYMMETRIC CH STRETCH MODE OF TRIACETYLENE

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

WF13 **15 min 5:12**

A LINE LIST FOR HYDROGEN SULFIDE

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

WF14 **15 min 5:29**

ANALYSIS OF THE SUB-MILLIMETER ROTATIONAL SPECTRUM OF UREA

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

WF15 **10 min 5:46**

THE ROTATIONAL SPECTRUM OF COMPLEX ORGANIC MOLECULES: 2(N)-METHYLAMINOETHANOL

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

WG. MINI-SYMPOSIUM: THEORY AND SPECTROSCOPY

WEDNESDAY, JUNE 19, 2013 – 1:30 PM

Room: 170 MATH ANNEX

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

WG01 *INVITED TALK* **30 min 1:30**

COMBINING THEORY AND EXPERIMENT TO COMPUTE HIGHLY ACCURATE LINE LISTS FOR STABLE MOLECULES, AND PURELY AB INITIO THEORY TO COMPUTE ACCURATE ROTATIONAL AND ROVIBRATIONAL LINE LISTS FOR TRANSIENT MOLECULES

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

WG02 **15 min 2:05**

A NEW POTENTIAL ENERGY SURFACE FOR H_2–N_2O AND PIMC SIMULATION PROBING SUPERFLUIDITY AND VIBRATIONAL FREQUENCY SHIFTS IN DOPED $para$-H_2 CLUSTERS

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

WG03 **15 min 2:22**

SUPERFLUIDITY HIDDEN IN A FORGOTTEN CORNER

TAO ZENG, GREGOIRE GUILLON, and PIERRE-NICHOLAS ROY, *Department of Chemistry, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1*.

WG04 **15 min 2:39**

COMPUTATIONAL FRAMEWORK FOR STUDYING H-BONDING IN THE OH STRETCH REGION OF VIBRATIONAL SPECTRA

LAURA C. DZUGAN and ANNE B. McCOY, *Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH 43210*.

WG05 **15 min 2:56**

ESR SPECTRA OF ALKALI-METAL ATOMS ON HELIUM NANODROPLETS: A THEORETICAL MODEL FOR THE PREDICTION OF HELIUM INDUCED HYPERFINE STRUCTURE SHIFTS

ANDREAS W. HAUSER, *Institute of Experimental Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria*; MICHAEL FILATOV, *Mulliken Center for Theoretical Chemistry, Institut für Physikalische und Theoretische Chemie, Universität Bonn, Beringstrasse 4, 53115 Bonn, Germany*; WOLFGANG E. ERNST, *Institute of Experimental Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria*.

WG06 **15 min 3:13**

Xe AND Rb ATOMS ON HELIUM NANODROPLETS: IS THE VAN DER WAALS ATTRACTION STRONG ENOUGH TO FORM A MOLECULE?

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

Intermission

WG07 **15 min 3:45**

RENNER-TELLER COUPLING IN OPEN SHELL DIHYDRIDES: A COMPARISON OF THEORY WITH OPTICAL SPECTRA OF NEUTRAL AND IONIC MOLECULES

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

WG08 **15 min 4:02**

RENNER-TELLER AND SPINORBIT COUPLING IN H_2S+ AND AsH_2

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

WG09 **15 min 4:19**

COMPUTING ROVIBRATIONAL LEVELS OF POLYATOMIC MOLECULES WITH CURVILINEAR INTERNAL VIBRATIONAL COORDINATES AND AN ECKART FRAME

XIAO-GANG WANG and TUCKER CARRINGTON, JR., *Chemistry Department, Queen's University, Kingston, Canada*.

WG10 **15 min 4:36**

AN ACCURATE POTENTIAL ENERGY SURFACE FOR METHANE

XIAO-GANG WANG and TUCKER CARRINGTON, JR., *Chemistry Department, Queen's University, Kingston, Canada*.

WG11 **15 min 4:53**

THEORETICAL CALCULATIONS AND SIMULATIONS OF INTERACTION OF X-RAYS WITH HIGH-Z NANOMOITIES FOR USE IN CANCER RADIOTHERAPY

SARA N. LIM, *Biophysics Graduate Program*; ANIL K. PRADHAN, *Biophysics Graduate Program, Chemical Physics Program and Department of Astronomy, The Ohio State University*; SULTANA N. NAHAR, *Astronomy, The Ohio State University*.

WG12 **15 min 5:10**

SUPERIORITY OF LOW ENERGY 160 KV X-RAYS COMPARED TO HIGH ENERGY 6 MV X-RAYS IN HEAVY ELEMENT RADIOSENSITIZATION FOR CANCER TREATMENT

SARA N. LIM, *Biophysics Graduate Program*; ANIL K. PRADHAN, *Biophysics Graduate Program, Departments of Astronomy and Chemistry*; SULTANA N. NAHAR, *Department of Astronomy*; ROLF F. BARTH, WEILIAN YANG, ROBIN J. NAKKULA, *Pathology, The Ohio State University*; ALYCIA PALMER and CLAUDIA TURRO, *Department of Chemistry, The Ohio State University*.

WG13 **15 min 5:27**

ALKYL CH STRETCH VIBRATIONS AS A PROBE OF CONFORMATIONAL PREFERENCES

EDWIN L. SIBERT III, *Department of Chemistry and Theoretical Chemistry Institute, University of Wisconsin-Madison, WI 53706*; EVAN G. BUCHANAN AND TIMOTHY S. ZWIER, *Department of Chemistry, Purdue University, West Lafayette, IN 47907-2084*.

WG14 **15 min 5:44**

THEORETICAL STUDY OF THE VIBRATIONAL SPECTROSCOPY OF THE ETHYL RADICAL

DANIEL P. TABOR and EDWIN. L. SIBERT III, *Department of Chemistry and Theoretical Chemistry Institute, University of Wisconsin-Madison, Madison, WI 53706*.

WG15 **15 min 6:01**

SIMULATION OF HIGH RESOLUTION VIBRATIONAL AND ELECTRONIC SPECTRA WITH A MULTIFREQUENCY VIRTUAL SPECTROMETER

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

WH. MICROWAVE

WEDNESDAY, JUNE 19, 2013 – 1:30 PM

Room: 1000 MCPHERSON LAB

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

WH01 **15 min** **1:30**

THE LATEST REVISION OF THE ERHAM CODE

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

WH02 **10 min** **1:47**

GENERALIZED EQUATIONS FOR THE INERTIAL TENSOR OF A WEAKLY BOUND COMPLEX

KENNETH R. LEOPOLD, *Department of Chemistry, University of Minnesota, 207 Pleasant St., SE, Minneapolis, MN 55455*.

WH03 **15 min** **1:59**

SECOND MOMENTS (PLANAR MOMENTS) AND THEIR APPLICATION IN SPECTROSCOPY

ROBERT K. BOHN, *Dept. of Chemistry, Univ. of Connecticut, Storrs, CT 06269-3060*; JOHN A. MONTGOMERY, JR., H. HARVEY MICHELS, JASON N. BYRD, *Dept. of Physics, Univ. of Connecticut, Storrs, CT 06269-3046*.

WH04 **15 min** **2:16**

AN EMPIRICAL APPROACH TO OBTAINING ACCURATE MOLECULAR ROTATIONAL CONSTANTS FOR ISOTOPICALLY-SUBSTITUTED SPECIES FROM *AB INITIO* CALCULATIONS

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

WH05 **15 min** **2:33**

SINGULAR VALUE DECOMPOSITION-BASED MODELING OF TIME DOMAIN SIGNALS IN BROADBAND MICROWAVE SPECTROSCOPY

A. J. MINEI, *Department of Chemistry and Biochemistry, Division of Natural Sciences, College of Mount Saint Vincent, 6301 Riverdale Avenue, Riverdale, New York, 10471*; S. A. COOKE, *School of Natural and Social Sciences, Purchase College SUNY, 735 Anderson Hill Road, Purchase, NY 10577, USA*.

WH06 **15 min** **2:50**

PURE ROTATIONAL SPECTROSCOPY OF ASYMMETRIC TOPS IN THE UNDERGRADUATE CLASSROOM OR LABORATORY

A. J. MINEI, *Department of Chemistry and Biochemistry, Division of Natural Sciences, College of Mount Saint Vincent, 6301 Riverdale Avenue, Riverdale, New York, 10471*; S. A. COOKE, *School of Natural and Social Sciences, Purchase College SUNY, 735 Anderson Hill Road, Purchase, NY 10577, USA*.

WH07 **15 min 3:07**

A NEW E-BAND (60 - 90 GHz) FOURIER TRANSFORM MILLIMETER-WAVE SPECTROMETER

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

WH08 **15 min 3:24**

THE FOURIER TRANSFORM MICROWAVE/MILLIMETER SPECTRUM OF ScO ($X^2\Sigma^+$)

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

Intermission

WH09 **15 min 4:00**

SUBMILLIMETER SPECTROSCOPIC DIAGNOSTICS IN A SEMICONDUCTOR PROCESSING PLASMA

YASER H. HELAL, CHRISTOPHER F. NEESE, JENNIFER A. HOLT, FRANK C. DE LUCIA, *Department of Physics, The Ohio State University, Columbus, OH 43210*; PAUL R. EWING, *Applied Materials, Austin, TX 78724*; PHILLIP J. STOUT, MICHAEL D. ARMACOST, *Applied Materials, Sunnyvale, CA 94085*.

WH10 **15 min 4:17**

IR/THZ DOUBLE RESONANCE SPECTROSCOPY APPROACH FOR REMOTE CHEMICAL DETECTION AT ATMOSPHERIC PRESSURE

ELIZABETH A. TANNER and DANE J. PHILLIPS, *IERUS Technologies, 2904 Westcorp Blvd Ste 210, Huntsville, AL 35805*; FRANK C. DE LUCIA, *Department of Physics, 191 Woodruff Ave. Ohio State University, Columbus, OH 43210*; HENRY O. EVERITT, *Army Aviation and Missile RD&E Center, Redstone Arsenal, AL 35898*.

WH11 **15 min 4:34**

A MICRO-CANTILEVER BASED PHOTOACOUSTIC DETECTOR OF TERAHERTZ RADIATION FOR CHEMICAL SENSING

NATHAN E. GLAUVITZ, RONALD A. COUTU JR., *Department of Electrical and Computer Engineering, Air Force Institute of Technology, 2950 Hobson Way, Wright-Patterson AFB, OH 45433, USA*; MICHAEL N. KISTLER, RYAN F. HAMILTON, DOUGLAS T. PETKIE, IVAN R. MEDVEDEV, *Department of Physics, Wright State University, 3640 Colonel Glenn Highway, Dayton, OH 45435, USA*.

WH12 **15 min 4:51**

A TWO-COLOR FOURIER TRANSFORM MM-WAVE SPECTROMETER FOR GAS ANALYSIS OPERATING FROM 260-295 GHZ

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

WH13 **15 min 5:08**

GAS ANALYSIS BY FOURIER TRANSFORM MM-WAVE SPECTROSCOPY

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

WH14 **15 min 5:25**

A SEGMENTED CHIRPED-PULSE FOURIER TRANSFORM MM-WAVE SPECTROMETER (260-295 GHZ) WITH REAL-TIME SIGNAL AVERAGING CAPABILITY

BRENT J.HARRIS, AMANDA L. STEBER, and BROOKS H. PATE, *Department of Chemistry, University of Virginia, Charlottesville, VA 22904*.

WH15 **15 min 5:42**

COHERENT SYNCHROTRON RADIATION FOR ROTATIONAL SPECTROSCOPY: APPLICATION TO THE ROTATIONAL SPECTRUM OF PROPYNAL IN THE 200-750 GHz RANGE

J. BARROS, P. ROY, *Synchrotron SOLEIL, L'Orme des Merisiers Saint-Aubin, 91192 Gif-sur-Yvette, France*; D. APPADOO, D. Mc NAUGHTON, *Australian Synchrotron Light Source, 800 Blackburn Road Victroria 3168 and Monash University, School of Chemistry, Clayton, Victoria 3800 Australia.*; E. ROBERTSON, *La Trobe University, Department of Chemistry, Victoria, 3086, Australia*; L. MANCERON, *Laboratoire LADIR, CNRS, Université Pierre et Marie Curie, 75252 Paris Cedex, France*.

WH16 **15 min 5:59**

DEVELOPMENT OF A REDUCED-COST CHIRPED PULSE MICROWAVE SPECTROMETER

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

WI. INFRARED/RAMAN

WEDNESDAY, JUNE 19, 2013 – 1:30 PM

Room: 1015 MCPHERSON LAB

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

WI01 **15 min** **1:30**

INFRARED SPECTROSCOPIC INVESTIGATION ON HIGH ACIDITY OF DIETHYLETHER CATION

TOMOYA ENDO,YOSHIYUKI MATSUDA,ASUKA FUJII, *Depertment of Chemistry, Graduate School of Science,Tohoku University, Sendi 980-8578, Japan*; KAITO TAKAHASHI, *Institute of Atomic and Molecular Sciences, Academia Sinca,Taipei 10617, Taiwan*.

WI02 **15 min** **1:47**

STRUCTURAL, CONFORMATIONAL AND VIBRATIONAL STUDIES OF ISOCYANOCYCLOPENTANE FROM INFRARED, RAMAN SPECTRA AND AB INITIO CALCULATIONS

DATTATRAY K. SAWANT, JOSHUA J. KlAASSEN, JAMES R. DURIG, *DEPARTMENT OF CHEMISTRY, UNIVERSITY OF MISSOURI-KANSAS CITY, MO 64110 USA*.

WI03 **15 min** **2:04**

MICROWAVE AND INFRARED SPECTRA, ADJUSTED R_0 STRUCTURAL PARAMETERS, CONFORMATIONAL STABILITIES, VIBRATIONAL ASSIGNMENTS, AND AB INITIO CALCULATIONS OF CYCLOBUTYLCARBOXYLIC ACID CHLORIDE

JOSHUA J. KLAASSEN, PETER GRONER, JAMES R. DURIG, *Department of Chemistry, University of Missouri-Kansas City, Kansas City, MO 64110 USA*.

WI04 **15 min** **2:21**

LOWERING OF KETO-ENOL TAUTOMERIZATION BARRIER OF CYCLIC DIKETONES VIA CH$\cdots$O INTERACTION

T. CHAKRABORTY, B. BANDYOPADHYAY, P. BANERJEE and P. PANDEY, *Department of Physical Chemistry, Indian Association for the cultivation of science, Calcutta 700032, India. E-mail: pctc@iacs.res.in*.

WI05 **15 min** **2:38**

A SPECTROSCOPIC AND THEORETICAL STUDY OF WEAK INTRAMOLECULAR OH$\cdots\pi$ INTERACTIONS IN ALLYL CARBINOL AND METHALLYL CARBINOL

SIDSEL D. SCHROEDER, KASPER MACKEPRANG, HENRIK G. KJAERGAARD, *Department of Chemistry, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen* .

Intermission

WI06 **10 min** **3:15**

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

MAHIR TURSUN, *Department of Physics, Dumlupinar University, Kutahya, 43100, Turkey*; and GURKAN KESAN, *Institute of Physics and Biophysics, Faculty of Science, University of South Bohemia, BranisovskÃą 31, CeskÃl' BudÃl'jovice, 370 05, Czech Republic*; and CEMAL PARLAK, *Department of Physics, Dumlupinar University, Kutahya, 43100, Turkey*; MUSTAFA SENYEL, *Science Faculty, Department of Physics, Anadolu University, Eskisehir, Turkey 26470*.

WI07 **15 min 3:27**

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

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

[a]Present address: LPCA, EA 4493, Université du Littoral Côte d'Opale, 59140 Dunkerque, France
[b]Present address: CEA, IRAMIS, SPAM, Lab. Francis Perrin, 91192 Gif-sur-Yvette, France

WI08 **10 min 3:44**

TOWARD COMPUTATIONAL SPECTROSCOPY STUDIES FOR LARGE MOLECULAR SYSTEMS

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

WI09 **15 min 3:56**

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

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

WI10 **15 min 4:13**

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

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

WI11 **15 min 4:30**

CONFORMATION-SPECIFIC UV and IR SPECTROSCOPY OF CONFORMATIONALLY CONSTRAINED α/γ PEPTIDE FOLDAMERS

RYOJI KUSAKA, *Department of Chemistry, Purdue University, West Lafayette, IN 47907, and Department of Chemistry, Graduate School of Science, Hiroshima University, Higashi-Hiroshima, 739-8526, Japan*; DI ZHANG, PATRICK WALSH, JOSEPH GORD, and TIMOTHY S. ZWIER, *Department of Chemistry, Purdue University, West Lafayette, IN 47907*; BRIAN F. FISHER, and SAMUEL H. GELLMAN, *Department of Chemistry, University of Wisconsin, Madison, WI 53706*.

WI12 **15 min 4:47**

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

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

WI13 **15 min 5:04**

ACTION IRMPD SPECTROSCOPY OF B_2 FRAGMENT IONS FROM QAXIG AND NAXIG PENTAPEPTIDES

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

WI14 **15 min 5:21**

MODIFCATION OF THE PROLYL RING OF VAL-PRO-ALA AND THE IMPACT OF THIS MODIFICATION ON B2 ION STRUCTURE

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

WJ. RADICALS AND IONS

WEDNESDAY, JUNE 19, 2013 – 1:30 PM

Room: 2015 MCPHERSON LAB

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

WJ01 **15 min** **1:30**

THE INFRARED AND NEAR-INFRARED SPECTRUM OF HNO TRAPPED IN SOLID NEON

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

WJ02 **15 min** **1:47**

A NEW TYPE OF VIBRONIC INTERACTION IN THE NITRATE FREE RADICAL NO_3

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

WJ03 **15 min** **2:04**

DISPERSED FLUORESCENCE SPECTROSCOPY OF THE $\tilde{B}\ ^2E' - \tilde{X}\ ^2A_2'$ TRANSITION OF JET COOLED $^{14}NO_3$ and $^{15}NO_3$

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

WJ04 **15 min** **2:21**

ROTATIONALLY-RESOLVED HIGH-RESOLUTION LASER SPECTROSCOPY AND MAGNETIC EFFECT OF THE $B \leftarrow X$ TRANSITION OF NO_3 RADICAL

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

WJ05 **15 min** **2:38**

VIBRONIC ANALYSIS OF THE $\widetilde{A}^2E''$ STATE OF NO_3 RADICAL

TERRANCE J. CODD, MOURAD ROUDJANE, MING-WEI CHEN[a], 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

WJ06 **15 min** **2:55**

HIGH RESOLUTION CAVITY RING DOWN SPECTROSCOPY OF THE 3_0^1 and $3_0^1\ 4_0^1$ BANDS OF THE $\tilde{A}^2E''$ STATE OF NO_3 RADICAL

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

WJ07 **15 min 3:12**

THE RENNER-TELLER AND JAHN-TELLER EFFECTS IN PROTOTYPICAL MOLECULAR CATIONS SUBJECT TO A VERY LARGE SPIN-ORBIT COUPLING

BÉRENGER GANS, MONIKA GRÜTTER and FRÉDÉRIC MERKT, *Laboratorium für Physikalische Chemie, ETH Zürich, CH-8093 Zürich, Switzerland*.

WJ08 **15 min 3:29**

OBSERVATION OF THE a_1 CH STRETCHING MODES OF PHENYL RADICAL

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

WJ09 **15 min 3:46**

HIGH RESOLUTION ROVIBRATIONAL SPECTROSCOPY OF JET-COOLED PHENYL RADICAL: THE ν_{19} OUT-OF-PHASE SYMMETRIC C-H STRETCH

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

Intermission

WJ10 **15 min 4:20**

MOLECULAR CONSTANTS OF C_2 IN THE $c^3\Sigma_u^+$ STATE

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

WJ11 **15 min 4:37**

RE-ANALYSIS OF THE SPIN-ORBIT PERTURBATION FOR THE PHILLIPS SYSTEM AND THE BALLIK-RAMSAY SYSTEM OF THE SPECTRA OF C_2

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

WJ12 **15 min 4:54**

THE ETHYL RADICAL IN SUPERFLUID HELIUM NANODROPLETS: ROVIBRATIONAL SPECTROSCOPY AND AB INITIO CALCLUATIONS

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

WJ13 **15 min 5:11**

INRARED SPECTROSCOPY AND TUNNELING DYNAMICS OF THE VINYL RADICAL IN ^{4}He NANODROPLETS

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

WJ14 **15 min 5:28**

STRUCTURE AND DYNAMICS OF THE CYCLOPROPENE RADICAL CATION STUDIED BY HIGH-RESOLUTION PHOTOELECTRON SPECTROSCOPY

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

WJ15 **15 min 5:45**

STRUCTURE DETERMINATION OF NON-LINEAR HYDROCARBON CHAINS BY DEUTERIUM LABELING

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

WK. ELECTRONIC

WEDNESDAY, JUNE 19, 2013 – 1:30 PM

Room: 1153 SMITH LAB

Chair: ANTHONY MERER, Academia Sinica, Taipei, Taiwan

WK01 **15 min** **1:30**

SPECTROSCOPY OF LiCa AND RbSr MOLECULES ON HELIUM NANODROPLETS

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

WK02 **15 min** **1:47**

SPECTROSCOPY OF Li ATOMS AND Li DIMERS IN THE TRIPLET MANIFOLD ON THE SURFACE OF HELIUM NANODROPLETS

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

WK03 **10 min** **2:04**

OBSERVATION OF THE 5 $^1\Sigma_u^+$ and 5 $^1\Pi_u$ STATES OF Rb_2 BY POLARISATION LABELLING SPECTROSCOPY [a]

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

[a] Supported by the PAN-CNRS exchange programme, 2011-12

WK04 **5 min** **2:16**

DOUBLE RESONANCE EXCITATION OF THE RUBIDIUM DIMER : THE 2 $^1\Pi_g$ STATE

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

WK05 **15 min** **2:23**

EXCITATION OF ULTRACOLD MOLECULES TO “TRILOBITE-LIKE" LONG-RANGE MOLECULAR RYDBERG STATES

M. A. BELLOS, R. CAROLLO, J. BANERJEE, E. E. EYLER, P. L. GOULD, W. C. STWALLEY, *Department of Physics, University of Connecticut, Storrs, CT 06269-3046*.

WK06 **15 min** **2:40**

HIGH RESOLUTION PHOTOELECTRON SPECTROSCOPY OF Au_2^- and Au_4^- BY PHOTOELECTRON IMAGING

IKER LEON, ZHENG YANG, and LAI-SHENG WANG, *DEPARTMENT OF CHEMISTRY, BROWN UNIVERSITY, PROVIDENCE, RI 02912, USA*.

WK07 **15 min 2:57**

INTRACAVITY LASER ABSORPTION SPECTROSCOPY OF PLATINUM NITRIDE IN THE NEAR INFRARED

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

WK08 **10 min 3:14**

REANALYSIS OF THE NEAR INFRARED ELECTRONIC TRANSITIONS OF NiCl

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

WK09 **10 min 3:26**

INTRACAVITY LASER ABSORPTION SPECTROSCOPY OF ZIRCONIUM FLUORIDE IN THE NEAR INFRARED

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

Intermission

WK10 **15 min 4:00**

ROTATIONAL AND HYPERFINE STRUCTURE IN THE [17.6]2.5−X2.5 AND [23.3]2.5−X2.5 TRANSITIONS OF IRIDIUM MONOXIDE

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

WK11 **15 min 4:17**

ELECTRONIC TRANSITIONS OF YTTRIUM MONOXIDE

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

WK12 **10 min 4:34**

ELECTRONIC TRANSITIONS OF PALLADIUM AND VANADIUM DIMER

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

WK13 **15 min 4:46**

ELECTRONIC TRANSITIONS OF RUTHENIUM MONOXIDE

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

WK14 **10 min** **5:03**

PRECISION SPECTROSCOPY OF TELLURIUM

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

WK15 **15 min** **5:15**

IONIZATION MEASUREMENT AND SPECTROSCOPY OF ThS AND ThS^{+}

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

WK16 **15 min** **5:32**

A STUDY OF NbCr AND $NbCr^{-}$ BY ANION PHOTOELECTRON SPECTROSCOPY

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

RA. MINI-SYMPOSIUM: THEORY AND SPECTROSCOPY

THURSDAY, JUNE 20, 2013 – 8:30 AM

Room: 160 MATH ANNEX

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

RA01 ***INVITED TALK*** **30 min 8:30**

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

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

RA02 **15 min 9:05**

TUNNELING SPLITTINGS IN VIBRONIC STRUCTURE OF CH_3F^+ ($\tilde{X}^2E$): STUDIED BY HIGH RESOLUTION PHOTOELECTRON SPECTRA AND $AB\ INITIO$ THEORETICAL METHOD

YUXIANG MO, SHUMING GAO, ZUYANG DAI, and HUA LI, *Department of Physics and State Key Laboratory of Low-Dimensional Quantum Physics, Tsinghua University, Beijing 100084, China*.

RA03 **15 min 9:22**

ANALYSIS OF THE ROTATIONALLY-RESOLVED SPECTRA OF THE VIBRONICALLY-ACTIVE MOLECULES

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

RA04 **15 min 9:39**

A THEORETICAL PREDICTION OF ELECTRONIC TRANSITIONS IN C_3

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

RA05 **15 min 9:56**

THE RENNER EFFECT IN THE $\widetilde{X}\ ^2A''$ AND $\widetilde{A}\ ^2A'$ ELECTONIC STATES OF HSO/HOS

ROMAN I. OVSYANNIKOV, *Institute of Applied Physics, Russian Academy of Science, Ulyanov Street 46, Nizhny Novgorod, Russia 603950, and Physical and Theoretical Chemistry, Faculty of Mathematics and Natural Sciences, University of Wuppertal, D-42097 Wuppertal, Germany*; PER JENSEN, *Physical and Theoretical Chemistry, Faculty of Mathematics and Natural Sciences, University of Wuppertal, D-42097 Wuppertal, Germany*; TSUNEO HIRANO, *Department of Chemistry, Faculty of Science, Ochanomizu University, 2-1-1 Otsuka, Bunkyo-ku, Tokyo 112-8610, Japan*.

Intermission

RA06 **15 min 10:30**

PHOTODISSOCIATION SPECTROSCOPY OF BARE AND HYDRATED PERMANGANATE IONS

JORGEN HOUMOLLER, KRISTIAN STOCHKEL, STEEN BRONDSTED NIELSEN, *Department of Physics and Astronomy, Aarhus University, Ny Munkegade 120, 8000 Aarhus C, Denmark*; SYDNEY H. KAUFMAN, J. MATHIAS WEBER, *JILA, and Department of Chemistry and Biochemistry, University of Colorado, Boulder, Colorado 80309, USA*.

RA07 **15 min 10:47**

MANIFESTATION OF NONADIABATIC EFFECTS IN THE IR SPECTRUM OF PARA-BENZOQUINONE RADICAL CATION

KRZYSZTOF PIECH, THOMAS BALLY, *Department of Chemistry, University of Fribourg, CH-1700 Fribourg, Switzerland*; TAKATOSHI ICHINO and JOHN F. STANTON, *Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, TX 78712*.

RA08 **15 min 11:04**

NUMERICALLY EXACT DYNAMICS OF FUNCTIONAL QUANTUM SYSTEMS - APPLICATIONS TO GaAs QUANTUM DOT QUBITS AND 2-DIMENSIONAL SPECTRA OF VERY LARGE PHOTOSYNTHEITC COMPLEXES

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

RA09 **15 min 11:21**

OBSERVATION AND ANALYSIS OF BOUND → FREE TRANSITION OF ScI_3 PHOTOEXCITED IN THE ULTRAVIOLET

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

RA10 **15 min 11:38**

EXCITED STATES OF THE DIATOMIC MOLECULE CrHe

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

RA11 **15 min 11:55**

POLARIZATION EFFECTS AND IONIC BONDING IN A POLAR DIATOMIC: THE CaF^+ $X^1\Sigma^+$ STATE

STEPHEN L. COY, JOSHUA H. BARABAN, ROBERT W. FIELD, *MIT Dept. of Chemistry, Cambridge, MA 02139*; BRYAN M. WONG, *Materials Chemistry Dept., Sandia National Lab., Livermore, CA 94551*.

RB. RADICALS AND IONS

THURSDAY, JUNE 20, 2013 – 8:30 AM

Room: 170 MATH ANNEX

Chair: HEATHER ABBOTT-LYON, Kennesaw State University, Kennesaw, GA

RB01 **15 min** **8:30**

VIBRATIONAL SPECTROSCOPY OF SYMPATHETICALLY COOLED CaH^+ MOLECULAR IONS

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

RB02 **15 min** **8:47**

INTRACLUSTER REACTIONS IN Ni-CO_2 CLUSTERS

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

RB03 **15 min** **9:04**

INFRARED PHOTODISSOCIATION SPECTROSCOPY OF METAL OXIDE CARBONYL CATIONS.

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

RB04 **15 min** **9:21**

ACCURATE POTENTIAL ENERGY CURVES FOR THE GROUND ELECTRONIC STATES OF NeH^+ AND ArH^+

JOHN A. COXON, *Department of Chemistry, Dalhousie University, Halifax, Nova Scotia, Canada B3H 4J3*; PHOTOS G. HAJIGEORGIOU, *Department of Life and Health Sciences, University of Nicosia, Nicosia 1700, Cyprus*.

RB05 **15 min** **9:38**

EXPANSION DISCHARGE SOURCE FOR ION BEAM LASER SPECTROSCOPY OF COLD MOLECULAR IONS

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

Intermission

RB06 **15 min** **10:15**

INFRARED PHOTODISSOCATION SPECTROSCOPY OF METAL BENZENE CATION COMPLEXES

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

RB07 **15 min** **10:32**

SPECTROSCOPY OF BENZYL-TYPE RADICALS GENERATED BY ELECTRIC DISCHARGE : JET-COOLED DICHLOROBENZYL RADICALS

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

RB08 **15 min 10:49**

ROVIBRATIONAL SPECTROSCOPY OF THE OH-O_3 AND C_2H_4-O_3 COMPLEXES IN ^{4}He NANODROPLETS

EMMANUEL I. OBI, and GARY E. DOUBERLY, *Department of Chemistry, University of Georgia, Athens, Georgia 30602, USA*.

RB09 **15 min 11:06**

SPECTROSCOPY OF THE CH_3-HCL COMPLEX IN HELIUM NANODROPLETS

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

RB10 **15 min 11:23**

BIMOLECULAR PYROLYSIS REACTIONS STUDIED BY CHIRPED-PULSE MILLIMETER-WAVE SPECTROSCOPY

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

RB11 **5 min 11:40**

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

AHMED MAHJOUB and MAJDI HOCHLAF, *Universite Paris-Est, Laboratoire Modelisation et Simulation Multi Echelle, MSME UMR 8208 CNR, 77454 Marne la vallee (France)*; LIONEL POISSON, *Laboratoire Francis Perrin CNR- URA 2453, CEA âĂŞIRAMIS, 91192, Gif sur Yvette (France)*; GUSTAVO A. GARCIA and LAURENT NAHON, *Synchrotron SOLEIL, LOrme des Merisiers, Saint Aubin BP 48, 91193 (France)*.

RB12 **15 min 11:47**

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

RAGHUNATH O. RAMABHADRAN, JENNIFFER E. MANN, SARAH. E. WALLER, DAVID W. ROTHGEB, CAROLINE C. JARROLD, KRISHNAN RAGHAVACHARI, *DEPARTMENT OF CHEMISTRY, INDIANA UNIVERSITY, BLOOMINGTON, IN-47405*.

RC. MICROWAVE

THURSDAY, JUNE 20, 2013 – 8:30 AM

Room: 1000MCPHERSON LAB

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

RC01 **15 min 8:30**

THE ROTATIONAL SPECTRUM OF RUTHENIUM MONOCARBIDE USING PPMODR[a]

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

[a]Funded by DoE-BES

RC02 **15 min 8:47**

PURE ROTATIONAL SPECTRA OF THE REACTION PRODUCTS OF LASER ABLATED THORIUM METAL AND OXYGEN MOLECULES ENTRAINED WITHIN SUPERSONIC EXPANSIONS OF NOBLE GASES

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

RC03 **15 min 9:04**

DETECTION OF THE ROTATIONAL SPECTRUM OF SULFOXYLIC ACID (HOSOH)

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

[a]Present address: École Normale Supérieure de Cachan, 94235 Cachan Cedex, France

RC04 **15 min 9:21**

GLOBAL ANALYSIS OF BROADBAND ROTATION AND VIBRATION-ROTATION SPECTRA OF SULFUR DICYANIDE

ZBIGNIEW KISIEL, *Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warszawa, Poland*; MANFRED WINNEWISSSER, BRENDA P. WINNEWISSER, FRANK C. DE LUCIA, *Department of Physics, The Ohio State University, Columbus, OH 43210, USA*; DENNIS W. TOKARYK, *Department of Physics and Centre for Laser, Atomic, and Molecular Sciences, University of New Brunswick, P.O.Box. 4400, New Brunswick E3B 5A3, Canada*; BRANT E. BILLINGHURST, *Canadian Light Source Inc., University of Saskatchewan, 101 Perimeter Road, Saskatoon, Saskatchewan S7N 0X4, Canada*.

RC05 **15 min 9:38**

CONTINUATION OF THE PURSUIT OF THE FAR-INFRARED SPECTRUM OF NCNCS, AT THE CANADIAN LIGHT SOURCE

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

RC06 **15 min 9:55**

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

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

Intermission

RC07 **15 min 10:30**

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

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

RC08 **15 min 10:47**

MILLIMETER AND SUB-MILLIMETER SPECTROSCOPY OF CRCCH ($X^6\Sigma^+$)

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

RC09 **15 min 11:04**

CHARACTERIZATION OF SILICON SULFIDES BY CHIRPED-PULSE ROTATIONAL SPECTROSCOPY

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

RC10 **15 min 11:21**

DETECTION OF TWO HIGHLY-STABLE SILICON NITRIDES BY CHIRPED-PULSE ROTATIONAL SPECTROSCOPY: HSiNSi and SiH_3NSi

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

RC11 **15 min 11:38**

FOURIER-TRANSFORM MICROWAVE SPECTROSCOPY OF HCCNSi AND NCNSi

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

RC12 **15 min 11:55**

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

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

RD. ELECTRONIC

THURSDAY, JUNE 20, 2013 – 8:30 AM

Room: 1015 MCPHERSON LAB

Chair: ALLAN S. C. CHEUNG, University of Hong Kong, Hong Kong

RD01 **15 min 8:30**

METHODS FOR MANIPULATING CaF USING OPTICAL POLYCHROMATIC FORCES

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

RD02 **15 min 8:47**

NEW LINE LISTS INCLUDING INTENSITIES FOR THE C_2 SWAN SYSTEM ($d^3\Pi_g$-$a^3\Pi_u$), C_2 SINGLET SYSTEMS AND ROVIBRATIONAL TRANSITIONS WITHIN THE NH $X^3\Sigma^-$ GROUND STATE.

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

RD03 **15 min 9:04**

MEASUREMENT OF ABSOLUTE HYDROXYL RADICAL CONCENTRATION IN LEAN FUEL-AIR MIXTURES EXCITED BY NANOSECOND PULSED DISCHARGE[a].

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

[a]Funded by AFRL MURI for plasma assisted combustion research grant

RD04 **15 min 9:21**

LASER INDUCED FLUORESCENCE SPECTROSCOPY OF JET COOLED SiCN : ROTATIONAL ANALYSIS OF THE HOT BANDS

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

RD05 **15 min 9:38**

THE ELECTRIC DIPOLE MOMENT OF IRIDIUM MONOSILICIDE, IrSi

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

RD06 **15 min 9:55**

TRIPLE-SINGLET MIXING in Si_3: the $1^3A_1''$ - $\tilde{a}^3A_2'$ TRANSITION[a]

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

[a]Funded by the NSF

RD07 **15 min 10:12**

MULTIPLEXED MODR WITH APPLICATIONS TO THE ELECTRONIC SPECTRUM OF SO_2

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

Intermission

RD08 **15 min 10:45**

SPECTROSCOPY OF THE NO-Ar COMPLEX IN THE VICINITY OF THE $3p \leftarrow X^2\Pi$ TRANSITIONS IN NITRIC OXIDE

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

RD09 **15 min 11:02**

AN INTRODUCTION TO HIGH RESOLUTION COHERENT MULTIDIMENSIONAL SPECTROSCOPY

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

RD10 **15 min 11:19**

STRATEGIES FOR INTERPRETING HIGH RESOLUTION COHERENT MULTIDIMENSIONAL SPECTRA

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

RD11 **15 min 11:36**

HIGH RESOLUTION COHERENT 3D SPECTROSCOPY OF BROMINE

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

RD12 **10 min 11:53**

HIGH RESOLUTION COHERENT THREE-DIMENSIONAL SPECTROSCOPY OF IODINE

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

RE. MINI-SYMPOSIUM: SPECTROSCOPY OF PLANETARY ATMOSPHERES

THURSDAY, JUNE 20, 2013 – 8:30 AM

Room: 2015 MCPHERSON LAB

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

RE01 ***INVITED TALK*** **30 min 8:30**

THE ROLE OF SPECTROSCOPY IN RESEARCH ON THE NEUTRAL ATMOSPHERES OF THE OUTER SOLAR SYSTEM

GLENN S. ORTON, *JET PROPULSION LABORATORY, CALIFORNIA INSTITUTE OF TECHNOLOGY, PASADENA, CA 91109*.

RE02 **15 min 9:05**

THE REVISED METHANE DATABASE IN HITRAN 2012

LINDA R. BROWN, *Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr., Pasadena, CA 91109*.

RE03 **15 min 9:22**

HITRAN2012 AND REMOTE SENSING OF PLANETARY ATMOSPHERES

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

RE04 **15 min 9:39**

COSMIC-RAY IONIZATION AND HAZES ON HOT JUPITERS

PAUL B RIMMER, CHRISTIANE HELLING, *SUPA, School of Physics and Astronomy, University of St Andrews, KY16 9SS*; CATHERINE WALSH, *Leiden Observatory, P.O. Box 9513, NL-2300 RA Leiden, The Netherlands*.

RE05 **15 min 9:56**

SPECTROSCOPY FOR HOT SUPER-EARTH EXOPLANETS

P.F. BERNATH and M. DULICK, *Department of Chemistry & Biochemistry, Old Dominion University, 4541 Hampton Boulevard, Norfolk, VA, 23529-0126, USA*.

Intermission

RE06 **10 min 10:30**

SPECTROSCOPIC STUDY OF CYANOACETYLENE CATION: SLOW PHOTO-ELECTRON SPECTROSCOPY AND AB-INITIO INVESTIGATIONS

AHMED MAHJOUB, MARTIN SCHWELL, YVES BENILAN, NICOLAS FRAY and MARIE-CLAIRE GAZEAU, *LISA UMR CNRS 7583, Univ. Paris Est Creteil & Univ. Paris Diderot, Institut Pierre Simon Laplace,61 Ave du General de Gaulle, 94010, Creteil, France*; GUSTAVO A. GARCIA and FRANCOIS GAIE-LEVERL, *Synchrotron SOLEIL, LâĂŹOrme des Merisiers, St.Aubin, B.P. 48, 91192, Gif-sur-Yvette Cedex, France*; NORBERT CHAMPION and SYDNEY LEACH, *LERMA UMR CNRS 8112, Observatoire de Paris-Meudon, 5 place Jules-Jansen, 92195, Meudon, France*.

RE07 **15 min 10:42**

THE $\nu_{12} + \nu_6 - \nu_6$ AND $\nu_{11} - \nu_{12}$ BANDS OF $^{12}CH_3^{13}CH_3$: A FREQUENCY ANALYSIS INCLUDING DATA FROM THE FOUR LOWEST VIBRATIONAL STATES

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

RE08 **15 min 10:59**

IDENTIFICATION OF PROTONATED PYRENE (1-$C_{16}H_{11+}$) AND ITS NEUTRAL COUNTERPART 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*.

RE09 **15 min 11:16**

VIBRONIC SPECTROSCOPY OF A STRUCTURAL ISOMER OF QUINOLINE: (Z)-PHENYLVINYLNITRILE

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

RE10 **15 min 11:33**

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

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

RF. ASTRONOMICAL SPECIES AND PROCESSES

THURSDAY, JUNE 20, 2013 – 1:30 PM

Room: 160 MATH ANNEX

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

RF01 **15 min** **1:30**

DISTRIBUTION OF SO_2 AND SO IN THE ENVELOPE OF VY-CANIS MAJORIS: INSIGHT INTO CIRCUMSTELLAR SULFUR CHEMISTRY

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

RF02 **15 min** **1:47**

RADIO INTERFEROMETRIC DETECTION OF TiO AND TiO_2 IN VY CANIS MAJORIS: "SEEDS" OF INORGANIC DUST FORMATION

S. BRÜNKEN, H.S.P. MÜLLER, *I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany* ; T. KAMIŃSKI, K.M. MENTEN, *Max-Planck Institut für Radioastronomie, 53121 Bonn, Germany*; C.A. GOTTLIEB, N.A. PATEL, K.H. YOUNG, M.C. McCARTHY, *Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 02138, USA*; J.M. WINTERS, *Institut de Radioastronomie Millimétrique, 38406 Saint-Martin d'Héres, France*; L. DECIN, *Instituut voor Sterrenkunde, Katholieke Universiteit Leuven, 3001 Leuven, Belgium, and Sterrenkundig Instituut Anton Pannekoek, University of Amsterdam, 1098 Amsterdam, The Netherlands*.

RF03 **15 min** **2:04**

TRANSITION-METAL OXIDES IN WARM CIRCUMSTELLAR ENVIRONMENTS

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

RF04 **15 min** **2:21**

OBSERVATIONS AND ANALYSIS OF EXTENDED TAIL TOWARD RED IN THE DIFFUSE INTERSTELLAR BANDS OF HERSCHEL 36

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

RF05 **15 min** **2:38**

MULTI-RESOLUTION STUDIES OF COMPLEX MOLECULES IN HIGH MASS STAR FORMING REGIONS

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

RF06 **15 min** **2:55**

IONIZATION OF H_2 BY X-RAYS IN THE CENTRAL MOLECULAR ZONE OF THE GALACTIC CENTER

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

RF07 **15 min 3:12**

CARMA OBSERVATIONS OF PAH RICH SOURCES: NGC 2023, L134N AND GGD 27

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

RF08 **15 min 3:29**

A SEARCH FOR HCO^+ AND HCN EMISSION IN PLANETARY NEBULAE

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

Intermission

RF09 **15 min 4:00**

IDENTIFICATION AND ASSIGNMENT OF THE FIRST EXCITED TORSIONAL STATE OF CH_2DOH WITHIN THE o_2, e_2, AND o_3 TORSIONAL LEVELS

JOHN C. PEARSON, SHANSHAN YU, *Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr., Pasadena, CA 91109, USA*; L. H. COUDERT, *LISA, CNRS/Universités Paris Est et Paris Diderot, 61 Avenue du Général de Gaulle, 94010 Créteil, France*; L. 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*.

RF10 **15 min 4:17**

ANALYSIS OF THE ROTATION-TORSION SPECTRUM OF CH_2DOH WITHIN THE e_0, e_1, AND o_1 TORSIONAL LEVELS

L. H. COUDERT, *LISA, CNRS/Universités Paris Est et Paris Diderot, 61 Avenue du Général de Gaulle, 94010 Créteil, France*; JOHN C. PEARSON, SHANSHAN YU, *Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr., Pasadena, CA 91109, USA*; L. 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*.

RF11 **15 min 4:34**

A GLOBAL FIT OF THE $X^2\Pi$, $A^2\Sigma^+$, $B^2\Sigma^+$ AND $C^2\Sigma^+$ STATES OF SIX OH ISOTOPOLOGUES

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

RF12 **15 min 4:51**

MICROWAVE SPECTROSCOPY OF *TRANS*-ETHYL METHYL ETHER IN THE GROUND STATE

KAORI KOBAYASHI, YUSUKE SAKAI, SHOZO TSUNEKAWA, *Department of Physics, University of Toyama, 3190 Gofuku, Toyama, 930-8555 Japan*; TAIHEI MIYAMOTO, MASAHARU FUJITAKE and NOBUKIMI OHASHI, *Kanazawa University, Japan*.

RF13 **15 min 5:08**

JET-COOLED EXCITATION SPECTRA OF LARGE BENZANNULATED BENZYL RADICALS: 9-ANTHRACENYLMETHYL ($C_{15}H_{11}$) and 1-PYRENYLMETHYL ($C_{17}H_{11}$)

GERARD D. O'CONNOR, GEORGE B. BACSKAY, GABRIELLE V.G. WOODHOUSE, TYLER P. TROY, KLAAS NAUTA, SCOTT H. KABLE and TIMOTHY W. SCHMIDT, *School of Chemistry, The University of Sydney, NSW 2006, Australia*.

RF14 **15 min 5:25**

ROTATIONAL STRUCTURE OF THE IR/FIR BANDS OF SMALL PAHS

O. PIRALI[a], S. GRUET[a], M. VERVLOET, *Ligne AILES, Synchrotron SOLEIL, L'Orme des Merisiers Saint-Aubin, 91192 Gif sur Yvette Cedex - France*; M. GOUBET, T. R. HUET, *Laboratoire de Physique des Lasers, Atomes et Molécules, UMR 8523 CNRS - Université Lille 1, Bâtiment P5, F-59655 Villeneuve d'Ascq Cedex, France*; R. GEORGES, *Université de Rennes 1, Institut de Physique de Rennes, CNRS, UMR 6251, F-35042 Rennes Cedex, France*; P. SOULARD, P. ASSELIN, *UPMC Université Paris 06, UMR 7075 CNRS, Laboratoire de Dynamique, Interactions et Réactivité (LADIR), F-75005, Paris, France*.

[a]Also at: Institut des Sciences Moléculaires d'Orsay, UMR 8214 CNRS-Université Paris-Sud, Bât. 210, 91405 Orsay cedex, France.

RF15 **15 min 5:42**

SYNCHROTRON-BASED HIGHEST RESOLUTION FTIR SPECTROSCOPY OF AZULENE, NAPHTHALENE ($C_{10}H_8$), INDOLE (C_8H_6N) AND BIPHENYL ($C_{12}H_{10}$)

S. ALBERT, M. QUACK, *PHYSICAL CHEMISTRY, ETH ZÜRICH, CH-8093 ZÜRICH, SWITZERLAND*; PH. LERCH, *SWISS LIGHT SOURCE, PAUL-SCHERRER-INSTITUTE, CH-5232 VILLIGEN, SWITZERLAND*.

RF16 **15 min 5:59**

PHOTOGENERATION OF, AND EFFICIENT COLLISIONAL ENERGY TRANSFER FROM, VIBRATIONALLY EXCITED HYDROGEN ISOCYANIDE (HNC)

MICHAEL J. WILHELM[a], *Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104*; and HAI-LUNG DAI, *Department of Chemistry, Temple University, Philadelphia, PA 19122*.

[a]Present Address: Department of Chemistry, Temple University, Philadelphia, PA 19122

RG. THEORY

THURSDAY, JUNE 20, 2013 – 1:30 PM

Room: 170 MATH ANNEX

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

RG01 **15 min** **1:30**

SYMMETRY, DEGENERACY, AND STATISTICAL WEIGHTS OF H_3^+

KYLE N. CRABTREE, *Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, 02138*; BENJAMIN J. McCALL, *Departments of Chemistry, Astronomy, and Physics, University of Illinois, Urbana, IL, 61801*.

RG02 **15 min** **1:47**

INVESTIGATION OF LARGE-AMPLITUDE MOTIONS OF H_5^+ AND THE DYNAMICS OF THE PROTON TRANSFER BETWEEN H_3^+ and H_2

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

RG03 **10 min** **2:04**

EINSTEIN A COEFFICIENTS FOR VIBRATION-ROTATIONAL TRANSITIONS OF NO

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

RG04 **15 min** **2:16**

OZONE PHOTOLYSIS: STRONG ISOTOPOLOGUE/ISOTOPOMER SELECTIVITY IN THE STRATOSPHERE

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

RG05 **15 min** **2:33**

LINE SHAPE PARAMETERS FOR CO_2 TRANSITIONS: ACCURATE PREDICTIONS FROM COMPLEX ROBERT-BONAMY CALCULATIONS

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

RG06 **15 min** **2:50**

AB INITIO CLASSICAL DYNAMICS SIMULATIONS OF CO_2 LINE-MIXING EFFECTS IN INFRARED BANDS

JULIEN LAMOUROUX[a], JEAN-MICHEL HARTMANN, HA TRAN, *Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA, CNRS UMR 7583),Université Paris-Est Créteil, Université Paris Diderot, Institut Pierre-Simon Laplace, 94010 Créteil Cedex, France*; MARCEL SNELS, *ISAC-CNR, Via del Fosso del Cavaliere, 100 00133 Rome, Italy*; STEFANIA STEFANI and GIUSEPPE PICCIONI, *IAPS-IASF, Via del Fosso del Cavaliere, 100 00133 Rome, Italy*.

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

RG07 **15 min 3:07**

TOWARDS EXPERIMENTAL ACCURACY FROM THE FIRST PRINCIPLES

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

RG08 **15 min 3:24**

HOW MANY VIBRATIONAL LEVELS DOES THE GROUND ELECTRONIC STATE OF THE SODIUM DIMER SUPPORT?

PHOTOS G. HAJIGEORGIOU, *Department of Life and Health Sciences, University of Nicosia, Nicosia 1700, Cyprus*.

Intermission

RG09 **15 min 4:00**

RESONANCE AND REVIVALS IN QUANTUM ROTORS: COMPARING HALF-INTEGER SPIN AND INTEGER SPIN

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

RG10 **15 min 4:17**

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

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

RG11 **15 min 4:34**

EXACT QUANTUM DYNAMICS CALCULATIONS USING PHASE SPACE WAVELETS

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

RG12 **15 min 4:51**

ACHIEVING THE COMPLETE-BASIS LIMIT IN LARGE MOLECULAR CLUSTERS: COMPUTATIONALLY EFFICIENT PROCEDURES TO ELIMINATE BASIS-SET SUPERPOSITION ERROR

RYAN M. RICHARD, JOHN M. HERBERT, *Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH 43210*.

RG13 **15 min 5:08**

VIBRATIONAL ANYLASIS ON $I(H_2O)^-$ and $I(D_2O)^-$ SPECTRA

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

RG14 **10 min 5:25**

AB-INITIO STUDY OF THE GROUP 2 HYDRIDE ANIONS

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

RG15 **15 min 5:37**

ACCURATE INTERMOLECULAR INTERACTIONS AT DRAMATICALLY REDUCED COST AND A MANY-BODY ENERGY DECOMPOSITION SCHEME FOR XPol+SAPT

KA UN LAO and JOHN M. HERBERT, *Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH 43210.*

RH. DYNAMICS

THURSDAY, JUNE 20, 2013 – 1:30 PM

Room: 1000 MCPHERSON LAB

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

RH01 **15 min** **1:30**

TORSION-INVERSION TUNNELING PATTERNS IN THE CH-STRETCH VIBRATIONALLY EXCITED STATES OF THE G_{12} MOLECULES

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

RH02 **15 min** **1:47**

COUPLING OF THE C-H STRETCH TO LARGE-AMPLITUDE TORSION AND INVERSION MOTIONS: COMPARISON OF $CH_3CH_2^{\cdot}$, $CH_3OH_2^+$ AND CH_3NH_2

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

RH03 **15 min** **2:04**

HYDROGEN ABSTRACTION FROM METHANE BY BROMINE AND CHLORINE RADICALS: A DYNAMICS COMPARISON

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

RH04 **15 min** **2:21**

A NEW APPROACH TOWARD TRANSITION STATE SPECTROSCOPY

KIRILL PROZUMENT, RACHEL G. SHAVER, MONIKA A. CIUBA, *Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139*; JOHN S. MUENTER, *Department of Chemistry, University of Rochester, Rochester, NY 14627*; G. BARRATT PARK, *Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139*; JOHN F. STANTON, *Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, TX 78712*; HUA GUO, *Department of Chemistry, University of New Mexico, Albuquerque, NM 87131*; BRYAN M. WONG, *Materials Chemistry Department, Sandia National Laboratories, Livermore, CA 94550*; DAVID S. PERRY, *Department of Chemistry, The University of Akron, Akron, OH 44325*; ROBERT W. FIELD, *Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139*.

RH05 **15 min** **2:38**

PHOTODISSOCIATION DYNAMICS OF VINYL CYANIDE STUDIED BY CHIRPED-PULSE MILLIMETER-WAVE SPECTROSCOPY OF HCN AND HNC PRODUCTS

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

RH06 **15 min 2:55**

ENERGY TRANSFER AND LASING OF THE LOWER Ar($3p^5 4p$) STATES IN Ar and He

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

RH07 **15 min 3:12**

GRAVITATON WAVES AND GRAVITON-PHOTON INTERACTIONS

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

Intermission

RH08 **15 min 3:45**

PROBING CHEMICAL DYNAMICS WITH HIGH RESOLUTION SPECTROSCOPY: CHIRPED-PULSE FOURIER-TRANSFORM MICROWAVE SPECTROSCOPY COUPLED WITH A HYPERTHERMAL SOURCE

NATHANAEL M. KIDWELL, VANESA VAQUERO VARA , DEEPALI N. MEHTA-HURT, JOSEPH A. KORN, BRIAN C. DIAN, and TIMOTHY S. ZWIER, *Department of Chemistry, Purdue University, West Lafayette, IN 47907-2084*.

RH09 **15 min 4:02**

J-SPECIFIC DYNAMICS IN AN OPTICAL CENTRIFUGE USING TRANSIENT IR SPECTROSCOPY

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

RH10 **15 min 4:19**

OBSERVATION OF NEW DYNAMICS IN THE STATE-RESOLVED COLLISIONAL RELAXATION OF HIGHLY EXCITED MOLECULES

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

RH11 **10 min 4:36**

TIME RESOLVED INFRARED EMISSION FROM VIBRATIONAL EXCITED ACETYLENE FOLLOWING SUPER ENERGY TRANSFER COLLISIONS WITH HOT HYDROGEN

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

RH12 **15 min 4:48**

TIME-RESOLVED IR-IR DOUBLE RESONANCE FOR THE ν_4 and $2\nu_4 - \nu_4$ VIBRATION-ROTATION TRANSITIONS OF CH_3F

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

RH13 **15 min 5:05**

VIBRATIONAL ENERGY RELAXATION OF CHOLOROIODOMETHANE IN COLD ARGON

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

RH14 **15 min 5:22**

DETERMINATION OF DIFFERENTIAL CROSS SECTIONS OF THE STATE-TO-STATE INELASTIC COLLISIONS IN BULBS. A THREE-DIMENSIONAL SLICED FLUORESCENCE IMAGING STUDY

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

RH15 **15 min 5:39**

ION IMAGING STUDIES OF CH_2I_2 PHOTODISSOCIATION AT 248 NM

JULIA H. LEHMAN, HONGWEI LI and MARSHA I. LESTER, *Department of Chemsitry, University of Pennsylvania, Philadelphia, PA 19104-6323*.

RI. ATMOSPHERIC SPECIES

THURSDAY, JUNE 20, 2013 – 1:30 PM

Room: 1015 MCPHERSON LAB

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

RI01 **15 min 1:30**

HITRAN2012: DOWN TO EARTH

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

RI02 **15 min 1:47**

CAVITY-ENHANCED, FREQUENCY-AGILE RAPID SCANNING (FARS) SPECTROSCOPY: MEASUREMENT PRINCIPLES

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

RI03 **15 min 2:04**

CAVITY-ENHANCED, FREQUENCY-AGILE RAPID SCANNING (FARS) SPECTROSCOPY: EXPERIMENTAL REALIZATIONS AND MEASUREMENT RESULTS

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

RI04 **15 min 2:21**

PERFORMANCE OF A CRYOGENIC 21 METER-PATH COPPER HERRIOTT CELL VACUUM COUPLED TO A BRUKER 125HR SYSTEM

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

RI05 **15 min 2:38**

FREQUENCY-COMB REFERENCED, SUB-DOPPLER SPECTROSCOPY OF HOT BANDS OF ACETYLENE IN THE REGION OF THE $\nu_1 + \nu_3$ COMBINATION BAND

CHRISTOPHER P. MCRAVEN, *Chemistry Department, Brookhaven National Laboratory, Upton, New York 11973*; MATTHEW J. CICH, SALVATORE M. CAIOLA, *Department of Chemistry, Stony Brook University, Stony Brook, New York 11794*; TREVOR J. SEARS[a], *Chemistry Department, Brookhaven National Laboratory, Upton, New York 11973*; GREGORY E. HALL, *Chemistry Department, Brookhaven National Laboratory, Upton, New York 11973*.

[a] also: *Department of Chemistry, Stony Brook University, Stony Brook, New York 11794*

RI06 **15 min 2:55**

DIAGNOSTIC CHEMICAL ANALYSIS OF EXHALED HUMAN BREATH USING A NOVEL SUB-MILLIMETER/TERAHERTZ SPECTROSCOPIC APPROACH

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

RI07 **15 min 3:12**

TERAHERTZ CHEMICAL ANALYSIS OF EXHALED HUMAN BREATH - BROAD ESSAY OF CHEMICALS

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

Intermission

RI08 **15 min 3:45**

SF_6: THE FORBIDDEN BAND UNVEILED

V. BOUDON, *Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR 6303 CNRS–Université de Bourgogne, 9 Av. A. Savary, BP 47870, F-21078 Dijon Cedex, France*; L. MANCERON, *Laboratoire de Dynamique, Interactions et Réactivité, CNRS UMR 7075, 4 Place Jussieu, F-75252 Paris Cedex, France*; F. KWABIA-TCHANA, *Laboratoire Interuniversitaire des Systèmes Atmosphériques, UMR CNRS 7583, Université Paris-Est Créteil et Université Paris-Diderot, 61 Avenue du Général de Gaulle, 94010 Créteil Cedex, France*; P. ROY, *Ligne AILES – Synchrotron SOLEIL, L'Orme des Merisiers, F-91192 Gif-sur-Yvette, France*.

RI09 **15 min 4:02**

FREQUENCY ANALYSIS OF THE 10 μm REGION OF THE ETHYLENE SPECTRUM USING THE D_{2h} TOP DATA SYSTEM.

M.-T. BOURGEOIS, M. ROTGER, *Groupe de Spectrométrie Moléculaire et Atmosphérique, CNRS UMR 7331, Université de Reims Champagne-Ardenne, Moulin de la Housse, B.P. 1039, Cases 16-17, F-51687 Reims Cedex, France*; M. TUDORIE, J. VANDER AUWERA, *Service de Chimie Quantique et Photophysique, C.P. 160/09, Université Libre de Bruxelles, 50, avenue F. D. Roosevelt, B-1050 Brussels, Belgium*; V. BOUDON, *Laboratoire Interdisciplinaire Carnot de Bourgogne, CNRS UMR 6303, Université de Bourgogne, 9, Avenue Alain Savary, BP 47870, F-21078 Dijon Cedex, France*.

RI10 **15 min 4:19**

INFRARED ABSORPTION SPECTRUM OF THE SIMPLEST CRIEGEE INTERMEDIATE CH_2OO

YU-TE SU, YU-HSUAN HUANG, HENRYK WITEK, *Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu 30010, Taiwan*; YUAN-PERN LEE, *Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu 30010, Taiwan and Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan*.

RI11 **15 min 4:36**

OBSERVATION OF THE $^3A' - {}^1A'$ ELECTRONIC TRANSITION OF THE METHYLENE PEROXY CRIEGEE INTERMEDIATE

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

RI12 **15 min 4:53**

UV SPECTRUM AND PHOTOCHEMISTRY OF THE SIMPLEST CRIEGEE INTERMEDIATE CH_2OO

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

RI13 **15 min 5:10**

SPECTROSCOPIC CHARACTERIZATION OF AN ALKYL-SUBSTITUTED CRIEGEE INTERMEDIATE CH_3CHOO AND ITS OH RADICAL PRODUCTS

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

RI14 **15 min 5:27**

RATE CONSTANTS AND DEUTERIUM KINETIC ISOTOPE EFFECTS FOR METHOXY RADICAL REACTING WITH NO_2 AND O_2

J. CHAI, H. HU, T. S. DIBBLE, *Department of Chemistry, College of Environmental Science and Forestry, State University of New York, Syracuse, New York 13210*; G. S. TYNDALL, J. J. ORLANDO, *Atmospheric Chemistry Division, National Center for Atmospheric Research, Boulder, Colorado 80305*.

RI15 **15 min 5:44**

ABSOLUTE VUV PHOTOIONIZATION SPECTRA FOR HCHO, HO_2, AND H_2O_2 FROM 10.5-12.0 eV

LEAH G. DODSON[a], LINHAN SHEN, NATHAN C. EDDINGSAAS[b], KANA TAKEMATSU, *California Institute of Technology, Division of Chemistry and Chemical Engineering, Pasadena, CA*; JOHN D. SAVEE, OLIVER WELZ, CRAIG A. TAATJES, DAVID L. OSBORN, *Sandia National Lab, Livermore, CA*; STANLEY P. SANDER, *Jet Propulsion Laboratory, Pasadena, CA*; MITCHIO OKUMURA, *California Institute of Technology, Division of Chemistry and Chemical Engineering, Pasadena, CA*.

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

RI16 **15 min 6:01**

LABORATORY INVESTIGATION OF THE AIRGLOW BANDS

BRIAN DROUIN, SHANSHAN YU, TIMOTHY J. CRAWFORD, CHARLES E. MILLER, *Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr., Pasadena, CA 91109*; JENG-HWA YEE, *Applied Physics Laboratory, The Johns Hopkins University, 111000, Johns Hopkins Rd, Laurel, MD 20723-6099*.

RJ. INFRARED/RAMAN

THURSDAY, JUNE 20, 2013 – 1:30 PM

Room: 2015 MCPHERSON LAB

Chair: LAURA MCCUNN, Marshall University, Huntington, WV

RJ01 **15 min** **1:30**

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

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

RJ02 **15 min** **1:47**

INFRARED SPECTROSCOPY OF PHENOL-TRIETHYLSILANE DIHYDROGEN-BONDED CLUSTER

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

RJ03 **10 min** **2:04**

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

F. KWABIA TCHANA, F. WILLAERT, X. LANDSHEERE, J.M. FLAUD, *Laboratoire Interuniversitaire des Systémes Atmosphériques (LISA), UMR CNRS 7583, Université Paris-Est Créteil (UPEC) et Université Paris-Diderot (UPD), 61 Avenue du Général de Gaulle, 94010 Créteil Cedex, France*; L. LAGO, M. CHAPUIS, P. ROY,, *Synchrotron SOLEIL, L'Orme des Merisiers Saint-Aubin, 91192 Gif-sur-Yvette, France*; L. MANCERON, *Laboratoire LADIR, UMR7075 CNRS, Université Pierre et Marie Curie, 75252 Paris Cedex, France*.

RJ04 **10 min** **2:16**

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

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

RJ05 **15 min** **2:28**

SYNCHROTRON-BASED STUDY OF THE FAR IR SPECTRUM OF SILACYCLOBUTANE: THE ν_{29} AND ν_{30} BANDS

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

RJ06 **15 min** **2:45**

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

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

RJ07 **15 min 3:02**

SYNCHROTRON BASED FOURIER TRANSFORM FAR-INFRARED SPECTROSCOPY OF CH3NO2

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

Intermission

RJ08 **15 min 3:40**

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

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

RJ09 **15 min 3:57**

CHARACTERIZATION OF STRUCTURAL MOTIFS FOR CO_2 ACCOMMODATION BY IONIC SPECIES RELEVANT TO PHOTOELECTROCATALYSIS USING CRYOGENIC VIBRATIONAL PREDISSOCIATION SPECTROSCOPY

JOSEPH A. FOURNIER, CHRISTOPHER J. JOHNSON, CONRAD T. WOLKE, ARRON B. WOLK, CHRISTOPHER M. LEAVITT, KRISTEN J. BREEN, and MARK A. JOHNSON, *DEPARTMENT OF CHEMISTRY, YALE UNIVERSITY, NEW HAVEN, CT 06520*.

RJ10 **15 min 4:14**

IRMPD SPECTROSCOPY OF GAS-PHASE PEPTIDE IONS: HISTSTIDYL-GLYCINE COMPLEXES OF METAL IONS.

ROBERT C. DUNBAR, *Chemistry Department, Case Western Reserve Univ., Cleveland, OH 44106*; GIEL BERDEN, *Radboud University Nijmegen, Netherlands*; JOS OOMENS, *Radboud University Nijmegen, and University of Amsterdam, Netherlands*; JUSTIN KAI-CHI LAU, *York University, Toronto, Canada*; UDO H. VERKERK, *York University, Toronto, Canada*; ALAN C. HOPKINSON, *York University, Toronto, Canada*; K. W. MICHAEL SIU, *York University, Toronto, Canada*.

RJ11 **15 min 4:31**

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

FUMIYA MORISHIMA, YOSHIYA INOKUCHI and TAKAYUKI EBATA, *Graduate School of Science, Hiroshima University 1-3-1, Kagamiyama, Higashi-Hiroshima 739-8526, JAPAN*.

RJ12 **15 min 4:48**

DEUTERATION EFFECT ON THE NH/ND STRETCH BAND OF THE JET-COOLED 7-AZAINDOLE AND ITS TAUTOMERIC DIMERS: RELATION TO THE GROUND-STATE DOUBLE PROTON-TRANSFER REACTION

HARUKI ISHIKAWA, *Department of Chemistry, School of Science, Kitasato University, Minami-ku, Sagamihara 252-0373, Japan*; TAKUMI NAKANO, TSUKIKO TAKASHIMA, HIROKI YABUGUCHI, and KIYOKAZU FUKE, *Department of Chemistry, Graduate School of Scinec, Kobe University, Nada-ku, Kobe 657-8501, Japan*.

RJ13 **10 min 5:05**

SOLVENT EFFECTS ON IR MODES OF (R)-3-METHYLCYCLOPENTANONE CONFORMERS: A COMPUTATIONAL INVESTIGATION

WATHEQ AL-BASHEER, *Physics Department, King Fahd University of Petroleum and Minerals, Dhahran 31261 Saudi Arabia*.

RJ14 **15 min 5:17**

CHIRAL RECOGNITION IN NEUTRAL AND IONIC MOLECULAR COMPLEXES

ANANYA SEN, AUDE BOUCHET, VALERIA LEPERE, KATIA LE BARBU-DEBUS, and ANNE ZEHNACKER-RENTIEN, *CNRS, Institut des Sciences Moléculaires d'Orsay (ISMO), UMR 8214, Orsay F-91405, and Univ. Paris-Sud, Orsay F-91405, France*.

RK. MICROWAVE

THURSDAY, JUNE 20, 2013 – 1:30 PM

Room: 1153 SMITH LAB

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

RK01 **10 min 1:30**

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

VADIM V. ILYUSHIN[a], IVAN SMIRNOV, EUGENE A. ALEKSEEV, *Institute of Radio Astronomy of NASU, Chervonopraporna 4, 61002 Kharkov, Ukraine*; LAURENT MARGULÈS[b], ROMAN A. MOTIYENKO, *Laboratoire de Physique des Lasers, Atomes et Molècules, UMR 8523 CNRS-Universitè Lille 1, Bâtiment P5, F-59655 Villeneuve d'Ascq Cedex, France*; BRIAN DROUIN, *Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Drive, Pasadena, CA 91109-8099, USA*.

[a]Part of this work was done within the Ukrainian-French CNRS-PICS 6051 project.
[b]This work was supported by the CNES and the Action sur Projets de l'INSU, PCMI.

RK02 **15 min 1:42**

A SEMIEXPERIMENTAL EQUILIBRIUM STRUCTURE OF *cis*-HEXATRIENE FROM MICROWAVE SPECTROSCOPY

NORMAN C. CRAIG, YIHUI CHEN, HANNAH A. FUSON, HENGFENG TIAN, and HERMAN VAN BESIEN, *Department of Chemistry and Biochemistry, Oberlin College, Oberlin, Ohio 44074*; H. D. RUDOLPH, *Department of Chemistry, University of Ulm, D-89069 Ulm, Germany*; JEAN DEMAISON, *Laboratoire de Physique des Lasers, Atomes et Molécules, Université de Lille I, 59655 Villeneuve d'Ascq Cedex, France*.

RK03 **15 min 1:59**

ANALYSIS OF THE ROTATIONAL STRUCTURE IN THE HIGH-RESOLUTION INFRARED SPECTRA OF cis, cis- AND $trans, trans$-1,4-DIFLUOROBUTADIENE-1-d_1 AND $trans, trans$-1,4-DIFLUOROBUTADIENE-1,4-d_2

NORMAN C. CRAIG, YIHUI CHEN, YUHUA LU, CHRISTOPHER F. NEESE, and DEACON J. NEMCHICK, *Department of Chemistry and Biochemistry, Oberlin College, Oberlin, OH 44074*; THOMAS A. BLAKE, *Pacific Northwest National Laboratory, Richland, WA 99352*.

RK04 **10 min 2:16**

THE DELICATE BALANCE OF HYDROGEN BOND FORCES IN D-THREONINOL

DI ZHANG, VANESA VAQUERO VARA, BRIAN C. DIAN and TIMOTHY S. ZWIER, *Department of Chemistry, Purdue University, West Lafayette, IN 47907*; DAVID W. PRATT, *Department of Chemistry, University of Vermont, Burlington VT 05405*.

RK05 **10 min 2:28**

WAVEGUIDE CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF 2-ETHOXYETHANOL

MARIA A. PHILLIPS and STEVEN T. SHIPMAN, *Division of Natural Sciences, New College of Florida, Sarasota, FL 34243*.

RK06 **10 min 2:40**

WAVEGUIDE CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF 1-PROPANETHIOL

BRITTANY P. GORDON and STEVEN T. SHIPMAN, *Division of Natural Sciences, New College of Florida, Sarasota, FL 34243*.

RK07 **15 min 2:52**

SPECTROSCOPIC FEATURES OF 2,6-DIFLUOROPHENOL

VANESA VAQUERO VARA , JACOB C. DEAN, DAVID S. WILCOX, BRIAN C. DIAN and TIMOTHY S. ZWIER, *Department of Chemistry, Purdue University, West Lafayette, IN 47907.*.

RK08 **15 min 3:09**

MILLIMETER WAVE TUNNELING-ROTATIONAL SPECTRUM OF PHENOL

L. KOLESNIKOVÁ, A. M. DALY, J. L. ALONSO, *Grupo de Espectroscopía Molecular (GEM), Edificio Quifima, Laboratorios de Espectroscopía y Bioespectroscopía, Parque Científico, Universidad de Valladolid, 47011 Valladolid, Spain*; B. TERCERO, J. CERNICHARO, *Departamento de Astrofísica, Centro de Astrobiología CAB, CSIC-INTA, Ctra. de Torrejón a Ajalvir km 4, 28850 Madrid, Spain*.

Intermission

RK09 **15 min 3:40**

ROTATIONAL SPECTROSCOPY UNVEILS ELEVEN CONFORMERS OF ADRENALINE

C. CABEZAS, V. CORTIJO, S. MATA, J. C. LÓPEZ, J. L. ALONSO, *Grupo de Espectroscopía Molecular (GEM), Edificio Quifima, Laboratorios de Espectroscopía y Bioespectroscopía, Parque Científico, Universidad de Valladolid, 47011 Valladolid, Spain*.

RK10 **10 min 3:57**

PROBING THE TAUTOMERISM OF HISTIDINE

C. BERMÚDEZ, C. CABEZAS, S. MATA, J. L. ALONSO, *Grupo de Espectroscopía Molecular (GEM), Edificio Quifima, Laboratorios de Espectroscopía y Bioespectroscopía, Parque Científico, Universidad de Valladolid, 47011 Valladolid, Spain*.

RK11 **15 min 4:09**

DEUTERIUM QUADRUPOLE COUPLING IN PROPIOLIC ACID AND FLUOROBENZENES MEASURED WITH FTMW SPECTROMETER USING MULTIPLE FIDS [a]

MING SUN, BRYAN M. SARGUS, SPENCER J. CAREY and STEPHEN G. KUKOLICH, *Department of Chemistry and Biochemistry, The University of Arizona, Tucson, Arizona 85721.*.

[a] Supported by THE NATIONAL SCIENCE FOUNDATION

RK12 **15 min 4:26**

MICROWAVE SPECTRA OF FLUORINATED PROPIONIC ACIDS AND THEIR HYDRATES

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

RK13 **10 min 4:43**

MW SPECTROSCOPY COUPLED WITH ULTRAFAST UV LASER VAPORIZATION: SUCCINIC ACID IN THE GAS PHASE

ESTIBALIZ MENDEZ, PATRICIA ECIJA, EMILIO J. COCINERO, FERNANDO CASTANO, FRANCISCO J. BASTERRETXEA, *Departamento de Química Física, Facultad de Ciencia y Tecnología, Universidad del País Vasco (UPV/EHU), Ap.644, E-48940, Bilbao, Spain*; PETER D. GODFREY, DON MCNAUGHTON, *School of Chemistry, Box 23 Victoria 3800 Monash University, Australia*; MICHAELA K. JAHN, K.P. RAJAPPAN NAIR, JENS-UWE GRABOW, *Institut für Physikalische Chemie und Elektrochemie, Gottfried-Wilhelm-Leibniz-Universität, 30167 Hannover, Germany*.

RK14 **15 min 4:55**

CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF 3-VINYLBENZALDEHYDE

MIRANDA SMITH and GORDON G. BROWN, *Department of Science and Mathematics, Coker College, 300 E College Ave., Hartsville, SC 29550.*.

RK15 **10 min 5:12**

CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF *META*-CHLOROBENZALDEHYDE

SEAN T. ARNOLD, JESSICA A. GARRETT, and GORDON G. BROWN, *Department of Science and Mathematics, Coker College, 300 E College Ave., Hartsville, SC 29550.*.

RK16 **15 min 5:24**

ROTATIONAL SPECTRUM OF HEXAFLUOROISOPROPANOL AND COMAPRISION TO HEXAFLUOROISOBUTENE

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

FA. ASTRONOMICAL SPECIES AND PROCESSES

FRIDAY, JUNE 21, 2013 – 8:30 AM

Room: 160 MATH ANNEX

Chair: KYLE CRABTREE, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA

FA01 **15 min** **8:30**

THE PUBLICLY AVAILABLE PREBIOTIC INTERSTELLAR MOLECULAR SURVEY (PRIMOS): EXPANDING SPECTROSCOPIC CHARACTERIZATIONS, EXTENDING TO NEW SOURCES, AND ADDING TO THE KNOWN MOLECULAR INVENTORY

BRETT A. McGUIRE, P. BRANDON CARROLL, *Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125*; JOANNA F. CORBY, *Department of Astronomy, University of Virginia, Charlottesville, VA 22904*; RYAN A. LOOMIS, *Department of Chemistry, University of Virginia, Charlottesville, VA 22904*; GEOFFREY A. BLAKE, *Division of Chemistry and Chemical Engineering and Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, CA 91125*; JAN M. HOLLIS, *NASA Goddard Space Flight Center, Greenbelt, MD 20771*; FRANK J. LOVAS, *National Institute of Standards and Technology, Gaithersburg, MD 20899*; PHILIP R. JEWELL, and ANTHONY J. REMIJAN, *National Radio Astronomy Observatory, Charlottesville, VA 22903*.

FA02 **15 min** **8:47**

THE IONIZATION TOWARD THE HIGH-MASS STAR-FORMING REGION NGC 6334 I

J. MORALES, *University of Puerto Rico, Rio Piedras Campus, Physics Department, San Juan, Puerto Rico 00931*; C. CECCARELI, *Institut de Planétologie et d'Astrophysique de Grenoble (IPAG) UMR 5274, Grenoble, F-38041, France*; L. OLMI, *Osservatorio Astrofisico di Arcetri - INAF, Largo E. Fermi 5, I-50125, Firenze, Italy*; D. LIS, *California Institute of Technology, Pasadena, CA 91125, USA*; R. PLUME, *Department of Physics and Astronomy, University of Calgary, Calgary, AB T2N 1N4, Canada*; P. SCHILKE, *I. Physikalisches Institut der Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany*.

FA03 **15 min** **9:04**

ROTATIONAL SPECTRA OF ISOTOPIC CH_3CN IN THEIR $v_8 = 1$ EXCITED VIBRATIONAL STATES

HOLGER S. P. MÜLLER, *I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany*; B. J. DROUIN, J. C. PEARSON, *Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109, USA*; A. BELLOCHE, K. M. MENTEN, *Max-Planck Institut für Radioastronomie, 53121 Bonn, Germany*.

FA04 **15 min** **9:21**

THE FIRST EXTENSIVE MOLECULAR STUDY OF AN OXYGEN-RICH PLANETARY NEBULA: OBSERVATIONS OF SiO, SO_2, AND SO

JESSICA L. EDWARDS, LUCY M. ZIURYS, *Department of Chemistry and Biochemistry, Department of Astronomy, Steward Observatory, The University of Arizona, Tucson, AZ 85721*.

FA05 **15 min** **9:38**

MAPPING THE MOLECULAR OUTFLOWS OF THE HIGH EXCITATION RED SPIDER NEBULA (NGC 6537)

JESSICA L. EDWARDS, LUCY M. ZIURYS, *Department of Chemistry and Biochemistry, Department of Astronomy, Steward Observatory, The University of Arizona, Tucson, AZ 85721*.

FA06 **15 min 9:55**

STRUCTURE OF THE DENSE MOLECULAR GAS IN THE HELIX NEBULA: LARGE SCALE MAPPING OF HCO^+

N. R. ZEIGLER, L. M. ZIURYS, *Department of Chemistry, University of Arizona, PO Box 210041, 1306 East University Blvd, Tucson, AZ, 85721, USA*; L. N. ZACK, *Department of Chemistry, University of Basel, Klingelbergstrasse 80, CH-4056 Basel, Switzerland*.

Intermission

FA07 **15 min 10:30**

THE CM-, MM- AND SUBMM-WAVE SPECTRUM OF ALLYL ISOCYANIDE AND RADIOASTRONOMICAL OBSERVATIONS IN ORION KL AND THE PRIMOS LINE SURVEY

I. HAYKAL, R. A. MOTIYENKO, L. MARGULÈS, and T. R. HUET, *Laboratoire PhLAM, UMR8523 CNRS-Université Lille 1, F-59655 Villeneuve d'Ascq Cedex, France*; P. ECIJA, E J. COCINERO, F BASTERRETXEA, J. A. FERNÁNDEZ, F. CASTANO, *Departamento de Química Física, Facultad de Ciencia y Tenología, Universidad del País Vasco, Barrio Sarriena s/n, 48940 Leioa (Spain)*; B. TERCERO, J. CERNICHARO, *Centro de Astrobiología (CSIC-INTA). Ctra de Ajalvir, Km 4, 28850 Torrejón de Ardoz, Madrid, Spain*; A. LESARRI, *Departamento de Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, 47011 Valladolid (Spain)*; J. C. GUILLEMIN, *Sciences Chimiques de Rennes -Ecole Nationale Supérieure de Chimie de Rennes -CNRS -35700 Rennes, France*.

FA08 **15 min 10:47**

TORSION-ROTATION-VIBRATION EFFECTS IN THE ν_{20}, $2\nu_{21}$, $2\nu_{13}$ AND $\nu_{21} + \nu_{13}$ STATES OF CH_3CH_2CN

ADAM M. DALY, JOHN C. PEARSON, SHANSHAN YU, BRIAN J. DROUIN, *Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr., Pasadena, CA 91109*; C. BERMÚDEZ, J. L. ALONSO, *Grupo de Espectroscopia Molecular (GEM), Edificio Quifima, Laboratorios de Espectroscopia y Bioespectroscopia, Parque Cientfíco, Universidad de Valladolid, 47011 Valladolid, Spain*.

FA09 **15 min 11:04**

MILLIMETER- WAVE SPECTRUM OF CARBONYL DIAZIDE IN PURSUIT OF DIAZIRINONE

BRENT K. AMBERGER, BRIAN J. ESSELMAN, R. CLAUDE WOODS and ROBERT J. McMAHON, *The University of Wisconsin - Madison Department of Chemistry, 1101 University Avenue, Madison, WI 53705*.

FA10 **15 min 11:21**

MILLIMETER- WAVE SPECTRUM OF PYRIDAZINE

BRENT K. AMBERGER, BRIAN J. ESSELMAN, JOSH D. SHUTTER, R. CLAUDE WOODS and ROBERT J. McMAHON, *The University of Wisconsin - Madison Department of Chemistry, 1101 University Avenue, Madison, WI 53705*.

FA11 **15 min 11:38**

MILLIMETER-WAVE SPECTROSCOPY OF AMINOMALONONITRILE

ROMAN A. MOTIYENKO, LAURENT MARGULÈS, *Laboratoire PhLAM, UMR 8523 CNRS - Université Lille 1, 59655 Villeneuve d'Ascq Cedex, France*; JEAN-CLAUDE GUILLEMIN, *Institut des Sciences Chimiques de Rennes, UMR 6226 CNRS - ENSCR, 35708 Rennes Cedex 7, France*.

FA12 ***Post-deadline Abstract*** **15 min 11:55**

A LABORATORY SEARCH FOR THE CARRIER OF U-LINES ATTRIBUTED TO l-C_3H^+ IN THE HORSEHEAD NEBULA PDR

MICHAEL C. McCARTHY, KYLE N. CRABTREE, and OSCAR MARTINEZ, JR., *Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 02138*.

FB. MINI-SYMPOSIUM: THEORY AND SPECTROSCOPY

FRIDAY, JUNE 21, 2013 – 8:30 AM

Room: 170 MATH ANNEX

Chair: STEPHEN COY, Massachusetts Institute of Technology, Cambridge, MA

FB01 *INVITED TALK* **30 min 8:30**

ROTATIONAL SPECTROSCOPY MEETS THEORY

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

FB02 **15 min 9:05**

ROTATIONAL SPECTROSCOPY AND QUANTUM CHEMICAL CALCULATIONS OF A FRUIT ESTER: THE MICROWAVE SPECTRUM OF n-BUTYL ACETATE

T. ATTIG, L.W. SUTIKDJA, R. KANNENGIEßER, W. STAHL, *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*.

FB03 **15 min 9:22**

EXTENSION OF THE MEASUREMENT, ASSIGNMENT, AND FIT IN THE GROUND STATE OF THE TWO-TOP MOLECULE METHYL ACETATE

H. V. L. NGUYEN, I. KLEINER, *Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA), UMR 7583 (CNRS/Univ. Paris Est et Paris Diderot), Université de Paris Est, 61 avenue du Général de Gaulle, F-94010 Créteil cedex, France*; S. SHIPMAN, *Division of Natural Sciences, New College of Florida, 5800 Bay Shore Road, Sarasota, FL 34243-2109, USA*; and K. KOBAYASHI, *Department of Physics, Faculty of Science, Toyama University, 3190 Gofuku Toyama, Toyama, 930-8555, Japan*.

FB04 **15 min 9:39**

A FITTING PROGRAM FOR MOLECULES WITH TWO EQUIVALENT TOPS AND C_{2V} POINT-GROUP SYMMETRY AT EQUILIBRIUM: APPLICATION TO EXISTING MICROWAVE, MILLIMETER, AND SUB-MILLIMETER WAVE MEASUREMENTS OF ACETONE

VADIM V. ILYUSHIN, *Institute of Radio Astronomy of NASU, Chervonoproporna 4, 61002 Kharkov, Ukraine. NIST Guest Worker June - August 2009.*; JON T. HOUGEN, *Sensor Science Division, National Institute of Standards and Technology, Gaithersburg, MD 20899-8441, USA*.

FB05 **15 min 9:56**

GAS PHASE ROVIBRATIONAL SPECTROSCOPY OF DMSO, PART.I: WHEN A SYNCHROTRON SOURCE REVEALS AN UNUSUAL ROTATIONAL BEHAVIOUR

ARNAUD CUISSET, DMITRII A. SADOVSKII , *Laboratoire de Physico-Chimie de l'Atmosphère, 189A Ave. Maurice Schumann, 59140 Dunkerque, France*; OLIVIER PIRALI, *Ligne AILES, synchrotron SOLEIL, L'Orme des Merisiers, Saint Aubin, BP 48, 91192 Gif-sur-Yvette, France.*.

FB06 **15 min 10:13**

GAS PHASE ROVIBRATIONAL SPECTROSCOPY OF DMSO, PART II: TOWARDS THE TERAHERTZ OBSERVATION OF 4-FOLD CLUSTERS

ARNAUD CUISSET, MARIE-ALINE MARTIN-DRUMEL, FRANCIS HINDLE, GAEL MOURET, DMITRII A. SADOVSKII , *Laboratoire de Physico-Chimie de l'Atmosphère, 189A Ave. Maurice Schumann, 59140 Dunkerque, France*.

Intermission

FB07 **15 min 10:45**

WHAT IS THE NATURE OF THE DOUBLETS IN THE E-METHANOL LAMB-DIP SPECTRA?

S. P. BELOV, A.V. BURENIN, G. Yu. GOLUBIATNIKOV and A.V. LAPINOV, *Institute of Applied Physics of RAS, 46 Ul'yanova str., GSP-120, Nizhny Novgorod 603950, Russia*.

FB08 **15 min 11:02**

ANALYSIS OF THE MICROWAVE SPECTRUM OF THE THREE-TOP MOLECULE TRIMETHOXYLMETHANE

L. H. COUDERT, *LISA, CNRS/Universités Paris Est et Paris Diderot, 61 Avenue du Général de Gaulle, 94010 Créteil, France*; G. FENG, AND W. CAMINATI, *Dipartimento di Chimica "G. Ciamician," Università di Bologna, Via F. Selmi, 40126 Bologna, Italy*.

FB09 **15 min 11:19**

HIGH RESOLUTION THZ AND FIR SPECTROSCOPY OF $SOCl_2$

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

FB10 **15 min 11:36**

STRUCTURE OF THE BENZENE DIMER—GOVERNED BY DYNAMICS

MELANIE SCHNELL, *Center for Free-Electron Laser Science, 22761 Hamburg, Germany; Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany*; UNDINE ERLEKAM, GERT VON HELDEN, GERARD MEIJER, *Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany*; PHILIP R. BUNKER, *National Research Council of Canada, Ottawa, Ontario K1A 0R6, Canada*; JENS-UWE GRABOW, *Institut für Physikalische Chemie und Elektrochemie, Gottfried-Wilhelm-Leibniz-Universtät, 30167 Hannover, Germany*; AD VAN DER AVOIRD, *Institute for Molecules and Materials, Radboud University, 6525 AJ Nijmegen, The Netherlands*.

FB11 **15 min 11:53**

HOW TO CALCULATE SPIN-SPIN COUPLING AND SPIN-ROTATION COUPLING STRENGTHS AND THEIR UNCERTAINTIES FROM SPECTROSCOPIC DATA: APPLICATION TO THE $c(1^3\Sigma_g^+)$ STATE OF DIATOMIC LITHIUM

NIKESH S. DATTANI, *Department of Chemistry, Oxford University, Oxford, OX1 3QZ, UK*; XUAN LI, *Chemical Science Division, Lawrence Berkeley National Laboratory, Berkeley, 94720-8176, USA*.

FC. MICROWAVE

FRIDAY, JUNE 21, 2013 – 8:30 AM

Room: 1000 MCPHERSON LAB

Chair: STEPHEN COOKE, Purchase College SUNY, Purchase, NY

FC01 **15 min 8:30**

FLUORINE SUBSTITUTION AND COMPLEXATION EFFECTS ON FLEXIBILITY AND TUNNELING PATHWAYS: THE ROTATIONAL SPECTRUM 2-FLUOROBENZYLAMINE AND BENZYLAMINE-WATER

S. MELANDRI, A. MARIS, C. CALABRESE, L EVANGELISTI AND W. CAMINATI, *Dipartimento di Chimica Ciamician, Università di Bologna, via Selmi 2,40126 Bologna, Italy*.

FC02 **15 min 8:47**

FTMW OBSERVATION AND ANALYSIS OF THE p-H_2–AgCl AND o-H_2–AgCl COMPLEX

G. S. GRUBBS II, DANIEL A. OBENCHAIN, HERBERT M. PICKETT and STEWART E. NOVICK, *Department of Chemistry, Wesleyan University, 52 Lawn Avenue, Middletown, CT, 06459-0180, USA (email to GSG2: ggrubbs@wesleyan.edu)*.

FC03 **15 min 9:04**

HYDROGEN INTERACTION WITH METAL HALIDES: THE NUCLEAR QUADRUPOLE COUPLING CONSTANT OF GOLD IN THE p-H_2-AuCl COMPLEX AND TRENDS IN THE OTHER HYDROGEN-COINAGE METAL HALIDE INTERACTIONS

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

FC04 **15 min 9:21**

THE SUBMILLIMETER SPECTRUM OF NdO

JENNIFER A. HOLT, CHRISTOPHER F. NEESE, FRANK C. DE LUCIA, *Microwave Laborotory, The Ohio State University, Columbus, Ohio 43210.*

Intermission

FC05 **15 min 10:00**

THE ROTATIONAL SPECTRUM OF H_2S: THE $H_2{}^{33}S$ ISOTOPOLOGUE AND THE SUB-DOPPLER RESOLUTION IN THE THz REGIME

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

FC06 **15 min 10:17**

EXAMINING PREBIOTIC CHEMISTRY USING O(^{1}D) INSERTION REACTIONS

BRIAN M. HAYS, JACOB C. LAAS, SUSANNA L. WIDICUS WEAVER, *Emory University, Department of Chemistry, Atlanta, GA 30322*.

FC07 **15 min 10:34**

LABORATORY DETECTION OF $IZnCH_3$ (X^1A_1) : FURTHER EVIDENCE FOR ZINC INSERTION

MATTHEW P. BUCCHINO, *Department of Chemistry and Biochemistry, University of Arizona, Tucson, Arizona 85721*; JUSTIN P. YOUNG, *Department of Chemistry, Canisius College, Buffalo, New York 14208*; PHIL M. SHERIDAN, *Department of Chemistry, Canisius College, Buffalo, New York 14208*; and LUCY M. ZIURYS, *Department of Chemistry and Biochemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, Arizona 85721*.

FC08 **15 min 10:51**

FURTHER STUDIES OF POTASSIUM-BEARING MOLECULES : THE MILLIMETER-WAVE SPECTRUM OF KSH (X^1A')

MATTHEW P. BUCCHINO, *Department of Chemistry and Biochemistry, University of Arizona, Tucson, Arizona 85721*; JUSTIN P. YOUNG, PHIL M. SHERIDAN and DAVID EWING, *Department of Chemistry, Canisius College, Buffalo, New York 14208*; LUCY M. ZIURYS, *Department of Chemistry and Biochemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, Arizona 85721*.

FC09 **15 min 11:08**

ENERGY TRANSFER COLLISIONAL PROCESS INVOLVING HETEROMOLECULAR COLLISIONS BETWEEN METHYL FLUORIDE AND N_2, Ar, He, CO_2, AND AIR

DANE J. PHILLIPS, *IERUS Technologies, 2904 Westcorp Blvd Ste 210, Huntsville, AL 35805*; HENRY O. EVERITT, *Army Aviation and Missile RD&E Center, Redstone Arsenal, AL 35898*.

FC10 ***Post-deadline Abstract*** **15 min 11:25**

ROTATIONAL SPECTRUM OF PROPARGYL ALCOHOL DIMER

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

FD. ELECTRONIC

FRIDAY, JUNE 21, 2013 – 8:30 AM

Room: 1015 MCPHERSON LAB

Chair: MOURAD ROUDJANE, The Ohio State University, Columbus, OH

FD01 **15 min 8:30**

A THEORETICAL STUDY OF CN SPECTROSCOPY FROM THE IR TO THE VUV

DAVID W. SCHWENKE, *NASA Ames Research Center, Moffett Field, CA 94035*.

FD02 **15 min 8:47**

LINE STRENGTHS IN THE FORM OF EINSTEIN A COEFFICIENTS AND OSCILLATOR STRENGTHS OF THE $A^2\Pi$-$X^2\Sigma^+$ (RED) AND $B^2\Sigma^+$-$X^2\Sigma^+$ (VIOLET) SYSTEMS OF CN

R. S. RAM and J. S. A. BROOKE, *Department of Chemistry, University of York, York, YO10 5DD, UK*; G. LI, *Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 02138, USA*; D. W. SCHWENKE, *NASA Ames Research Center, Moffett Field, CA 94035-1000, USA*; P. F. BERNATH, *Department of Chemistry and Biochemistry, Old Dominion University, Norfolk, VA 23529, USA*.

FD03 **15 min 9:04**

ARGON-INDUCED PRESSURE BROADENING, SHIFTING AND NARROWING IN THE CN $\tilde{A}^2\Pi - \tilde{X}^2\Sigma^+$ (1-0) BAND

D. FORTHOMME, C. P. MCRAVEN, T. J. SEARS[a], G. E. HALL, *Chemistry Department, Brookhaven National Laboratory, Bldg. 555A, P.O. Box 5000, Upton, NY 11973, USA*.

[a]also : *Department of Chemistry, Stony Brook University, Stony Brook, New York 11794, USA*

FD04 **10 min 9:21**

LIFETIMES OF THE $\tilde{A}$ STATES OF C_3

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.*.

FD05 **10 min 9:33**

LIFETIMES OF THE $\tilde{A}$ STATES OF THE C_3-NE AND C_3-AR COMPLEXES

YI-JEN WANG, CHIAO-WEI CHEN, 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.*.

Intermission

FD06 **15 min 10:00**

QUASILINEAR EVIDENCE FOR THE EQUILIBRIUM STRUCTURE OF BeOH

KYLE MASCARITOLO, JERMEY M. MERRIT, MICHAEL C. HEAVEN, *Emory University, Department of Chemistry, Atlanta, GA 30322*.

FD07 **15 min 10:17**

A MODEL OF ELECTRONICALLY-EXCITED STATES OF N_2 AND ITS EXTREME-ULTRAVIOLET SPECTRUM.

A.N. HEAYS, *Leiden Observatory, Leiden University, P.O. Box 9513, 2300 RA Leiden, The Netherlands*; B.R. LEWIS and S.T. GIBSON, *Research School of Physics and Engineering, The Australian National University, Canberra, ACT 0200, Australia*.

FD08 **10 min 10:34**

TWO-DIMENSIONAL SUBPICOSECOND TIME-RESOLVED FLUORESCENCE ANISOTROPY: OPTICAL KERR-GATING WITH A DYNAMIC POLARIZATION EXCITATION.

TAKASHIGE FUJIWARA, *Department of Chemistry and Biochemistry, The Ohio State University, Columbus OH 43210*; NATALIE C. ROMANO, DAVID A. MODARELLI, and EDWARD C. LIM, *Department of Chemistry and The Center for Laser and Optical Spectroscopy, The University of Akron, Akron OH 44325-3601*.

FD09 **15 min 10:46**

THE ORIGIN OF ANOMALOUS ELECTRONIC CIRCULAR DICHROISM SPECTRA OF $[RuPt_2(tppz)_2Cl_2]^{4+}$ IN ACETONITRILE

H.-G. YU[a], *Department of Chemistry, Brookhaven National Laboratory, Upton, NY 11973-5000, USA*.

[a]This work was performed at the Brookhaven National Laboratory under Contract No. DE-AC02-98CH10886 with the U.S. Department of Energy and supported by its Division of Chemical Sciences, Office of Basic Energy Sciences, and also used the resource at NERSC.

FD10 **15 min 11:03**

AB INITIO STUDY OF ION-PAIR STATES OF THE IODINE MOLECULE

VADIM A. ALEKSEEV, *Institute of Physics, St.Petersburg State University, Uljanovskaja St.1, Peterhof, 198504 St.Petersburg, Russia*.

FD11 ***Post-deadline Abstract*** **15 min 11:20**

MEASURING THE ELECTRON ELECTRIC DIPOLE MOMENT USING YTTERBIUM FLUORIDE MOLECULES

I.J. SMALLMAN, J.A. DEVLIN, D.M. KARA, J.J. HUDSON, B.E. SAUER, M.R. TARBUTT, E.A. HINDS, *Centre for Cold Matter, Imperial College London, The Blackett Laboratory, London, SW72BW*.

FE. DYNAMICS

FRIDAY, JUNE 21, 2013 – 8:30 AM

Room: 2015 MCPHERSON LAB

Chair: TERRY GUSTAFSON, The Ohio State University, Columbus, OH

FE01 **15 min 8:30**

CRYOGENIC ION VIBRATIONAL SPECTROSCOPY OF PT(II)-METHANE CH ACTIVATION INTERMEDIATES

BRETT MARSH, ETIENNE GARAND, *Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706*.

FE02 **15 min 8:47**

EXPERIMENTAL CHARACTERIZATION OF IDEALIZED METAL-CENTERED REACTIONS

DARRIN BELLERT, ADAM MANSELL, and ZACHARY THEIS, *Department of Chemistry, Baylor University, Waco, TX 76798*.

FE03 **15 min 9:04**

UTILIZING METAL TO LIGAND CHARGE TRANSFER STATES OF MM QUADRUPLY BONDED COMPLEXES FOR PHOTOVOLTAIC APPLICATIONS

SHARLENE A. LEWIS, SAMANTHA E. BROWN-XU, MALCOLM H. CHISHOLM, *The Ohio State University, Department of Chemistry and Biochemistry, Columbus, Ohio 43210*; ARTHUR J. EPSTEIN, *The Ohio State University, Department of Chemistry and Biochemistry and Department of Physics, Columbus, Ohio 43210*.

FE04 **15 min 9:21**

VIBRATIONALLY DRIVEN HYDROGEN ABSTRACTION REACTION BY BROMINE RADICAL IN SOLUTION

JAE YOON SHIN, MICHAEL A. SHALOWSKI, and F. FLEMING CRIM, *Department of Chemistry, University of Wisconsin-Madison, WI 53706*.

FE05 **15 min 9:38**

STRUCTURAL MOTIONS AND CHARGE DELOCALIZATION IN ELECTRONICALLY EXCITED N,N'-DIMETHYLPIPERAZINE

XINXIN CHENG , *Department of Chemistry, Brown University, Providence, RI 02912*; SANGHAMITRA DEB , *Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104*; and PETER M. WEBER , *Department of Chemistry, Brown University, Providence, RI 02912*.

Intermission

FE06 **15 min 10:10**

THEORETICAL STUDIES OF PHOTODISSOCIATION DYNAMICS OF $BrCN^-$

BERNICE OPOKU-AGYEMAN and ANNE B. McCOY, *Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH 43210*.

FE07 **15 min 10:27**

USING TRYPTOPHAN AS A PROBE FOR STUDYING PROTEIN HYDRATION DYNAMICS

YANGZHONG QIN, CHIH-WEI CHANG, LIJUAN WANG AND DONGPING ZHONG, *DEPARTMENT OF PHYSICS, THE OHIO STATE UNIVERSITY, COLUMBUS, OH, 43210*.

FE08 **15 min 10:44**

FEMTOSECOND CONICAL INTERSECTION DYNAMICS OF TRYPTOPHAN IN PROTEINS AND VALIDATION OF SLOWDOWN OF HYDRATION LAYER DYNAMICS

J. YANG, *Department of Physics, The Ohio State University, Columbus, OH 43210*; L. ZHANG, *Department of Chemistry, Columbia University, New York, NY 10027*; L. WANG, and D. ZHONG, *Department of Physics, Department of Chemistry and Biochemistry, and Programs of Biophysics, Chemical Physics, and Biochemistry, The Ohio State University, Columbus, OH 43210*.

FE09 **15 min 11:01**

PHOTOISOMERIZATION DYANAMICS OF THE SUNSCREEN MOLECULE AVOBENZONE

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

FE10 **15 min 11:18**

STUDY OF PROTON TRANSFER IN *E. COLI* PHOTOLYASE

MENG ZHANG, ZHEYUN LIU, JIANG LI, LIJUAN WANG and DONGPING ZHONG, *191 W. Woodruff Ave., Columbus, Ohio 43210.*.

FE11 ***Post-deadline Abstract*** **15 min 11:35**

DETECTION AND INTERPRETATION OF COLLISIONAL TRANSFER AND ROTATIONAL ANISOTROPY FINGERPRINTS IN RESONANT FOUR-WAVE MIXING SPECTRA.

A. KOUZOV, *Department of Physics, Saint-Petersburg State University, Peterhof, Saint-Petersburg 198504, Russia*; P. RADI, P. MAKSYUTENKO, *Department General Energy, Paul Scherrer Institute, CH-5232 Villigen, Switzerland*; and D. KOZLOV, *A.M. Prokhorov General Physics Institute, Russian Academy of Sciences, Vavilov str. 38, 119991 Moscow, Russia*.

AUTHOR INDEX

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