66th OSU INTERNATIONAL SYMPOSIUM ON MOLECULAR SPECTROSCOPY
JUNE 20-24, 2011

	MONDAY JUNE 20 8:45AM	TUESDAY JUNE 21 8:30AM	WEDNESDAY JUNE 22 8:30AM	THURSDAY JUNE 23 8:30AM	FRIDAY JUNE 24 8:30AM
AUDITORIUM INDEPENDENCE HALL	MA. PLENARY SESSION AWARDS		WA. PLENARY SESSION		
ROOM 160 MATH ANNEX*		TA. INFRARED/RAMAN		RA. MINI-SYMPOSIUM: FUNDAMENTAL PHYSICS	FA. MINI-SYMPOSIUM: THE THz COSMOS
ROOM 170 MATH ANNEX*		TB. DYNAMICS		RB. ATMOSPHERIC SPECIES	FB. THEORY
ROOM 1000 MCPHERSON LAB		TC. MICROWAVE		RC. MICROWAVE	FC. INFRARED/RAMAN
ROOM 1015 MCPHERSON LAB		TD. ELECTRONIC		RD. MINI-SYMPOSIUM: PERTURBATIONS	FD. MINI-SYMPOSIUM: FUNDAMENTAL PHYSICS
ROOM 2015 MCPHERSON LAB		TE. ATMOSPHERIC SPECIES		RE. DYNAMICS	FE. MATRIX/CONDENSED PHASE
1:30PM					
ROOM 160 MATH ANNEX*	MF. ELECTRONIC	TF. ASTRONOMICAL SPECIES & PROCESSES	WF. ASTRONOMICAL SPECIES & PROCESSES	RF. MINI-SYMPOSIUM: THE THz COSMOS	
ROOM 170 MATH ANNEX*	MG. INFRARED/RAMAN	TG. ELECTRONIC	WG. ELECTRONIC	RG. INFRARED/RAMAN	
ROOM 1000 MCPHERSON LAB	MH. MICROWAVE	TH. MINI-SYMPOSIUM: PERTURBATIONS	WH. MICROWAVE	RH. MICROWAVE	
ROOM 1015 MCPHERSON LAB	MI. RADICALS AND IONS	TI. INFRARED/RAMAN	WI. MINI-SYMPOSIUM: PERTURBATIONS	RI. THEORY	
ROOM 2015 MCPHERSON LAB	MJ. MATRIX/CONDENSED PHASE	TJ. THEORY	WJ. RADICALS/IONS	RJ. RADICALS AND IONS	

*** 209 W. 18th Avenue**

MA. PLENARY

MONDAY, JUNE 20, 2011 – 8:45 am

Room: AUDITORIUM, INDEPENDENCE HALL

Chair: FRANK C. DELUCIA, The Ohio State University, Columbus

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

MA01 **40 min 9:00**

SPECTROSCOPY AND DYNAMICS OF THE HOCO RADICAL

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

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

MA02 **40 min 9:45**

SPECTROSCOPIC AND THEORETICAL STUDY ON THE STRUCTURES AND DYNAMICS OF FUNCTIONAL MOLECULES - TOWARDS AN UNDERSTANDING OF THE MOLECULAR RECOGNITION FOR ENCAPSULATION COMPLEXES

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

Intermission

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

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

MA03 **40 min 11:05**

ELECTRONIC SPECTROSCOPY OF CARBON CHAINS OF ASTROPHYSICAL RELEVANCE

JOHN P. MAIER, *Department of Chemistry, University of Basel, Klingelbergstrasse 80, CH-4056 Basel, Switzerland.*

MF. ELECTRONIC

MONDAY, JUNE 20, 2011 – 1:30 pm

Room: 160 MATH ANNEX

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

MF01 **15 min** **1:30**

THEORETICAL STUDIES OF OBSERVABLE TRANSITIONS TO RECOUPLED PAIR BONDED STATES OF SULFUR HALIDE COMPOUNDS: SF/SCl ($X^2\Pi \rightarrow A^2\Sigma^-$), SF_2/SCl_2 ($X^1A_1 \rightarrow 1^1B_1$, $X^1A_1 \rightarrow 1^1A_2$), AND SFCl ($X^1A' \rightarrow A^1A''$)

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

MF02 **10 min** **1:47**

BLUE-DETUNED PHOTOASSOCIATION SPECTRUM IN Rb_2

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

MF03 **15 min** **1:59**

AN ACCURATE NEW POTENTIAL FUNCTION FOR GROUND-STATE Xe_2 FROM UV AND VIRIAL COEFFICIENT DATA

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

MF04 **15 min** **2:16**

LASER-INDUCED FLUORESCENCE STUDIES OF THE JET-COOLED ALUMINUM ACETYLIDE RADICAL (AlCCH/AlCCD)

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

MF05 **15 min** **2:33**

THE ELECTRONIC SPECTRUM OF H_2PO, THE PROTOTYPICAL PHOSPHORYL FREE RADICAL

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

MF06 **15 min** **2:50**

DETECTION OF THE H_2PS FREE RADICAL BY LASER SPECTROSCOPY

ROBERT A. GRIMMINGER, DENNIS J. CLOUTHIER, *Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055, USA*; RICCARDO TARRONI, *Dipartimento di Chimica Fisica ed Inorganica, Università di Bologna, 40136 Bologna, Italy*.

MF07 **15 min 3:07**

A SPECTROSCOPIC STUDY OF THE LINEAR-BENT ELECTRONIC TRANSITIONS OF JET-COOLED BCl_2 AND HBCl

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

Intermission

MF08 **15 min 3:40**

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

JINGMING LONG, HUASHENG WANG, AGUST KVARAN, *Science Institute, University of Iceland, Dunhagi 3, 107 Reykjavk, Iceland*.

MF09 **15 min 3:57**

OPTICAL STARK SPECTROSCOPY OF THE $\tilde{A}^2\Pi$- $\tilde{X}^2\Sigma^+$ BAND OF BaOH

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

MF10 **15 min 4:14**

LASER INDUCED FLUORESCENCE SPECTROSCOPY OF BORON CARBIDE

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

MF11 **15 min 4:31**

IMPROVEMENT OF SPECTROSCOPIC CONSTANTS FOR THE $A^3\Pi_{1u} \leftarrow X^1\Sigma_g^+$ SYSTEM OF Br_2

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

MF12 **15 min 4:48**

ACCURATE ANALYTIC POTENTIALS FOR THE $A\,^3\Pi_1$ and $X\,^1\Sigma^+$ STATES OF IBr FROM A COMBINED-ISOTOPOLOGUE DIRECT-POTENTIAL-FIT DATA ANALYSIS

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

MF13 **15 min 5:05**

TRANSITION STRENGTHS IN THE VISIBLE ABSORPTION SPECTRUM OF I_2: ONE MORE PASS

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

MF14 **15 min 5:22**

PHOTOELECTRON SPECTROSCOPY OF ICN^-: CHARACTERIZATION OF A CONICAL INTERSECTION IN ICN

ELISA M. MILLER, LEONID SHEPS,[a] YU-JU LU, *JILA, Department of Chemistry and Biochemistry, University of Colorado at Boulder, Boulder, CO 80309*; ANNE B. McCOY, *Department of Chemistry, The Ohio State University, Columbus, OH, 43210*; and W. CARL LINEBERGER, *JILA, Department of Chemistry and Biochemistry, University of Colorado at Boulder, Boulder, CO 80309*.

[a]Present address: Sandia National Laboratories, Livermore, CA 94551

MG. INFRARED/RAMAN

MONDAY, JUNE 20, 2011 – 1:30 pm

Room: 170 MATH ANNEX

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

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

ARE AB INITIO QUANTUM CHEMISTRY METHODS ABLE TO PREDICT VIBRATIONAL STATES UP TO THE DISSOCIATION LIMIT FOR MULTI-ELECTRON MOLECULES CLOSE TO SPECTROSCOPIC ACCURACY?

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

MG02 **10 min** **1:47**

ASSIGNMENT OF INFRARED AMMONIA SPECTRA

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

MG03 **15 min** **1:59**

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

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

MG04 **15 min** **2:16**

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

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

MG05 **15 min** **2:33**

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

L. FISSIAUX, *Laboratoire Lasers et Spectroscopies, Facultés Universitaires Notre Dame de la Paix, 61 rue de Bruxelles, B-5000 Namur, Belgium*; T. FÖLDES, *Service de Chimie Quantique et Photophysique, Université Libre de Bruxelles, CP 160/09, 50 avenue F.D. Roosevelt, B-1050 Brussels, Belgium*; F. KWABIA TCHANA, *Laboratoire Interuniversitaire des Systèmes Atmosphériques, CNRS, Universités de Paris Est Créteil et Paris 7, 61 avenue du Général De Gaulle, F-94010 Créteil cedex, France*; L. DAUMONT, *Groupe de Spectrométrie Moléculaire et Applications, UMR CNRS 6089, Université de Reims Champagne Ardenne, Campus du Moulin de la Housse, BP 1039, 51067 Reims Cedex 2, France*; M. LEPÈRE, *Laboratoire Lasers et Spectroscopies, Facultés Universitaires Notre Dame de la Paix, 61 rue de Bruxelles, B-5000 Namur, Belgium*; J. VANDER AUWERA, *Service de Chimie Quantique et Photophysique, Université Libre de Bruxelles, CP 160/09, 50 avenue F.D. Roosevelt, B-1050 Brussels, Belgium*.

MG06 **15 min 2:50**

INFRARED SPECTROSCOPY OF CARBON- AND CARBON-SILICON CLUSTERS

J. KRIEG, V. LUTTER, I. GOTTBEHÜT, T. F. GIESEN, S. SCHLEMMER, and S. THORWIRTH, *I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany*.

Intermission

MG07 **15 min 3:20**

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

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

MG08 **10 min 3:37**

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

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

MG09 **15 min 3:49**

NON-CYCLIC ISOMERS OF $(H_2O)_4$ IN HELIUM NANODROPLETS: INFRARED SPECTROSCOPY AND AB INITIO CALCULATIONS

S. D. FLYNN, A. M. MORRISON, T. LIANG, and G. E. DOUBERLY, *DEPARTMENT OF CHEMISTRY, UNIVERSITY OF GEORGIA, ATHENS, GEORGIA 30602-2556*; S. S. XANTHEAS, *CHEMICAL AND MATERIALS SCIENCES DIVISION, PACIFIC NORTHWEST NATIONAL LABORATORY, 906 BATTELLE BOULEVARD, MS K1-83, RICHLAND, WASHINGTON 99352*.

MG10 **15 min 4:06**

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

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

MG11 **15 min 4:23**

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

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

MG12 **15 min 4:40**

INTERMOLECULAR ASSOCIATION COMPLEXES OF 1,3-CYCLOHEXANEDIONE: PROBING OF KETO-ENOL TAUTOMERIC EQUILIBRIA IN COLD INERT GAS MATRIX, SOLUTION AND VAPOR PHASE BY INFRARED SPECTROSCOPY AND QUANTUM CHEMISTRY STUDY

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

MG13 **10 min 4:57**

VIBRON AND PHONON HYBRIDIZATION IN DIELECTRIC NANOSTRUCTURES

T. C. PRESTON and R. SIGNORELL, *Department of Chemistry, University of British Columbia, Vancouver, B.C., Canada*.

MH. MICROWAVE

MONDAY, JUNE 20, 2011 – 1:30 pm

Room: 1000 McPHERSON LAB

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

MH01 **15 min 1:30**

MICROWAVE SPECTRA AND STRUCTURES OF $H_4C_2\cdots AgCl$ AND $H_4C_2\cdots CuCl$

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

MH02 **15 min 1:47**

MICROWAVE SPECTRA AND STRUCTURE OF $CF_3I\cdots CO$

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

MH03 **15 min 2:04**

INTERMOLECULAR INTERACTION BETWEEN CO OR CO_2 AND ETHER OR THIOETHER OR PROPYLENE OXIDE IN A COMPLEX, INVESTIGATED BY FOURIER TRANSFORM MICROWAVE SPECTROSCOPY AND *ABINITIO* CALCULATIONS

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

MH04 **10 min 2:21**

DOES WATER PREFER TO DONATE A PROTON TO AN F OR TO a Cl ATOM? - A ROTATIONAL STUDY OF $CH_3CHClF...H_2O$

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

MH05 **15 min 2:33**

DETERMINATION OF THE STRUCTURE OF THE ARGON CYCLOPENTANONE AND NEON VAN DER WAALS COMPLEXES

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

MH06 **15 min 2:50**

IMPROVED DIPOLE MOMENTS FOR ACRYLONITRILE AND PROPIONITRILE

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

MH07 **15 min 3:07**

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

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

MH08 **15 min 3:24**

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

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

Intermission

MH09 **15 min 4:00**

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

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

MH10 **15 min 4:17**

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

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

MH11 **15 min 4:34**

THE ROTATIONAL SPECTRUM OF BIOMOLECULAR RELATED COMPOUNDS.[a]

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

[a]Work supported by NSF(CHE-0911117)

MH12 **15 min 4:51**

FLUORINE SUBSTITUTION IN NEUROTRANSMITTERS: MICROWAVE SPECTROSCOPY AND MODELLING OF THE CONFORMATIONAL SPACE AND NON BONDING INTERACTIONS

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

MH13 **15 min 5:08**

NEUROTRANSMITTERS IN THE GAS PHASE: LA-MB-FTMW STUDIES

C. CABEZAS, 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)*.

MH14 **15 min 5:25**

LA-MB-FTMW STUDIES OF SUGARS

M. LOZOYA, C. CABEZAS, 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)*.

MI. RADICALS AND IONS

MONDAY, JUNE 20, 2011 – 1:30 pm

Room: 1015 McPHERSON LAB

Chair: DMITRY MELNIK, The Ohio State University, Columbus, OH

MI01 **10 min** **1:30**

ISOTOPIC EFFECTS IN CHEMICAL REACTIONS OF SINGLE IONS

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

MI02 **15 min** **1:42**

MODELING THE INFLUENCE OF NUCLEAR SPIN IN THE REACTION OF H_3^+ WITH H_2

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

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

MI03 **15 min** **1:59**

SPECTROSCOPIC MEASUREMENTS OF THE REACTION $H_3^+ + H_2 \rightarrow H_2 + H_3^+$

KYLE N. CRABTREE, CARRIE A. KAUFFMAN, BRIAN A. TOM,[a] EFTALDA BEÇKA, BRETT A. McGUIRE,[b] BENJAMIN J. McCALL, *Department of Chemistry, University of Illinois, Urbana, IL 61801, USA*.

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

MI04 **15 min** **2:16**

INFRARED PHOTODISSOCIATION SPECTROSCOPY OF FIRST ROW TRANSITION METAL-CARBONYL CATIONS

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

MI05 **15 min** **2:33**

INFRARED PHOTODISSOCIATION SPECTROSCOPY OF METAL ION WATER COMPLEXES

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

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

VIBRATIONALY DRIVEN ELECTRON TRANSFER IN $CH_3NO_2^- \cdot CH_3I$ CLUSTERS

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

MI07 **15 min 3:07**

PHOTOELECTRON IMAGING OF NITROETHANE, NITROPROPANE AND NITROBUTANE

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

Intermission

MI08 **15 min 3:40**

ROTATIONAL SPECTRA OF N_2OH^+ AND CH_2CHCNH^+ MOLECULAR IONS

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

MI09 **15 min 3:57**

NOISE IMMUNE CAVITY ENHANCED OPTICAL HETERODYNE VELOCITY MODULATION SPECTROSCOPY

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

MI10 **15 min 4:14**

LINESHAPE AND SENSITIVITY OF SPECTROSCOPIC SIGNALS OF N_2^+ IN A POSITIVE COLUMN COLLECTED USING NOISE IMMUNE CAVITY ENHANCED OPTICAL HETERODYNE VELOCITY MODULATION SPECTROSCOPY

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

MI11 **15 min 4:31**

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

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

MI12 **15 min 4:48**

PHOTODISSOCIATION SPECTROSCOPY OF Ca^+-H_2O IN THE TEMPERATURE-VARIABLE ION TRAP

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

[a]Present address: Osaka Prefecture University, Japan

MI13 **15 min 5:05**

HIGH-RESOLUTION IR ACTION SPECTRUM OF $C_2H_2^+$

SABRINA GÄRTNER, JÜRGEN KRIEG, OSKAR ASVANY and STEPHAN SCHLEMMER, *I. Physikalisches Institut, Universität zu Köln*.

MJ. MATRIX/CONDENSED PHASE

MONDAY, JUNE 20, 2011 – 1:30 pm

Room: 2015 McPHERSON LAB

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

MJ01 **15 min 1:30**

FLUORESCENCE OF MATRIX-ISOLATED BIACETYL

ERIN E. GATRONE, NATHAN G. KUCHMAS and C. A. BAUMANN, *Department of Chemistry, The University of Scranton, Scranton, PA 18510-4626*.

MJ02 **15 min 1:47**

EXPERIMENTAL THERMOCHEMISTRY OF GAS PHASE CYTOSINE TAUTOMERS

A. M. MORRISON and G. E. DOUBERLY, *DEPARTMENT OF CHEMISTRY, UNIVERSITY OF GEORGIA, ATHENS, GEORGIA 30602-2556*.

MJ03 **10 min 2:04**

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

GÁBOR BAZSÓ, GYÖRGY TARCZAY, *Laboratory of Molecular Spectroscopy, Institute of Chemistry, Eötvös Loránd University, Pf. 32, Budapest, H-1518, Hungary*; GÉZA FOGARASI, PÉTER G. SZALAY, *Laboratory of Theoretical Chemistry, Institute of Chemistry, Eötvös Loránd University, Pf. 32, Budapest, H-1518, Hungary*.

MJ04 **15 min 2:16**

PULSED JET DISCHARGE MATRIX ISOLATION AND COMPUTATIONAL STUDY OF HALOGEN ATOM COMPLEXES: $Br–BrCH_2X$ (X=H,Cl,Br)

AIMABLE KALUME, LISA GEORGE AND SCOTT A. REID, *Department of Chemistry, Marquette University, Milwaukee, WI 53233*.

MJ05 **15 min 2:33**

PHOTOINDUCED ELECTRON TRANSFER IN THE $C_2H_4–Br_2$ COMPLEX

AIMABLE KALUME, LISA GEORGE AND SCOTT A. REID, *Department of Chemistry, Marquette University, Milwaukee, WI 53233*.

MJ06 **15 min 2:50**

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

JAY C. AMICANGELO, *School of Science, Penn State Erie, Erie, PA 16563*; MOHAMMED BAHOU, BARBARA GOLEC, AND YUAN-PERN LEE, *Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu 30010, Taiwan and Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan*.

Intermission

MJ07 **15 min 3:30**

FTIR ISOTOPIC AND DFT STUDIES OF SiC_5 TRAPPED IN SOLID Ar

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

MJ08 **15 min 3:47**

FTIR AND DFT STUDIES OF THE MgC_3^- ANION IN SOLID Ar

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

MJ09 **15 min 4:04**

DIMINISHED CAGE EFFECT IN p-H_2: IR IDENTIFICATION OF INTERMEDIATES IN ADDITION REACTIONS OF CL ATOM WITH UNSATURATED HYDROCARBONS

YUAN-PERN LEE, *Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu 30010, Taiwan and Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan*; MOHAMMED BAHOU, BARBARA GOLEC, *Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu 30010, Taiwan*.

MJ10 **15 min 4:21**

MOLECULAR HYDROGEN INTERACTIONS WITHIN METAL-ORGANIC FRAMEWORKS

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

MJ11 **15 min 4:38**

ELECTRON SPIN RESONANCE INVESTIGATION OF FORMATION MECHANISMS OF MATRIX ISOLATED H_4^+

M. CORRENTI, J. BANISAUKAS, L. B. KNIGHT, JR., *Department of Chemistry, Furman University, Greenville, SC*.

TA. INFRARED/RAMAN

TUESDAY, JUNE 21, 2011 – 8:30 am

Room: 160 MATH ANNEX

Chair: NASSER MOAZZEN-AHMADI, University of Calgary, Calgary, Canada

TA01 **10 min 8:30**

TIME RESOLVED FTIR ANALYSIS OF COMBUSTION OF ETHANOL AND GASOLINE COMBUSTION IN AN INTERNAL COMBUSTION ENGINE

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

TA02 **10 min 8:42**

TIME RESOLVED FTIR ANALYSIS OF TAILPIPE EXHAUST FOR SEVERAL AUTOMOBILES

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

TA03 **15 min 8:54**

HIGH-RESOLUTION MID-INFRARED SPECTROSCOPY OF DEUTERATED WATER CLUSTERS USING A QUANTUM CASCADE LASER-BASED CAVITY RINGDOWN SPECTROMETER

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

TA04 **15 min 9:11**

MID-IR CAVITY RING-DOWN SPECTROMETER FOR BIOLOGICAL TRACE NITRIC OXIDE DETECTION

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

TA05 **15 min 9:28**

OFF-AXIS CAVITY RING DOWN SPECTROSCOPY BASED ON A CONTINUOUS-WAVE OPTICAL PARAMETRIC OSCILLATOR

JARI PELTOLA, MIKAEL SILTANEN and LAURI HALONEN, *Laboratory of Physical Chemistry, Department of Chemistry, P.O. BOX 55 (A.I. Virtasen aukio 1), FI-00014 University of Helsinki, Finland*; MARKKU VAINIO, *Laboratory of Physical Chemistry, Department of Chemistry, P.O. BOX 55 (A.I. Virtasen aukio 1), FI-00014 University of Helsinki, Finland and Centre for Metrology and Accreditation, P.O. Box 9, FIN-02151 Espoo, Finland*.

TA06 **15 min 9:45**

OH DETECTION USING OFF-AXIS INTEGRATED CAVITY OUTPUT SPECTROSCOPY (OA-ICOS)

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

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

[b]thanks the IRENI program for the postdoctoral support.

Intermission

TA07 **15 min 10:15**

CAVITY RINGDOWN LASER ASORPTION SPECTROSCOPY(CRLAS) of ISOTOPICALLY LABELED ACETYLENE BETWEEN 12,500 - 13,600 cm^{-1}

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

TA08 **15 min 10:32**

AUTOMATIC TUNING OF AN ACULIGHT OPTICAL PARAMETRIC OSCILLATOR

A. M. MORRISON, T. LIANG, and G. E. DOUBERLY, *DEPARTMENT OF CHEMISTRY, UNIVERSITY OF GEORGIA, ATHENS, GEORGIA 30602-2556*.

TA09 **15 min 10:49**

PRECISION MEASUREMENT OF CARBON DIOXIDE HOTBAND TRANSITION AT 4.3 MICRON USING A HOT CELL

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

TA10 **15 min 11:06**

HIGH PRECISION MID-IR SPECTROSCOPY OF $^{14}N_2{}^{16}O$ NEAR 4.5 μm

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

TA11 **15 min 11:23**

MIR-IR SATURATION SPECTROSCOPY OF HeH^+ MOLECULAR ION

HSUAN-CHEN CHEN, *Institue of Phtonics Technologies, National Tsing Hua University, Hsinchu, Taiwan 30013, R.O.C*; WEI-JO TING, *Department of Physics, National Tsing Hua University, Hsinchu, Taiwan 30013, R.O.C*; JOW-TSONG SHY, *Department of Physics, National Tsing Hua University, Hsinchu, Taiwan 30013, R.O.C; Institue of Phtonics Technologies, National Tsing Hua University, Hsinchu, Taiwan 30013, R.O.C*.

TA12 **15 min 11:40**

STATE OF WATER MOLECULES AND SILANOL GROUPS IN OPAL MINERALS: A NEAR INFRARED SPECTROSCOPIC STUDY OF OPALS FROM SLOVAKIA

MIROSLAV BOBON, *Department of Physics, Faculty of Natural Sciences, Constantine the Philosopher University in Nitra, Slovakia*; ALFRED A. CHRISTY, *Department of Science, Faculty of Engineering and Science, University of Agder, Serviceboks 422, 4604 Kristiansand, Norway*; DANIEL KLUVANEC and L'UDMILA ILLASOVA, *Gemological Institute, Faculty of Natural Sciences, Constantine The Philosopher University in Nitra, Slovakia*.

TB. DYNAMICS

TUESDAY, JUNE 21, 2011 – 8:30 am

Room: 170 MATH ANNEX

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

TB01 **10 min 8:30**

FREE-INDUCTION DECAY SIGNALS USING A VOLTAGE MODULATED QUANTUM CASCADE LASER

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

TB02 **15 min 8:42**

OBSERVATION OF INFRARED FREE INDUCTION DECAY AND OPTICAL NUTATION SIGNALS FROM NITROUS OXIDE USING A VOLTAGE MODULATED QUANTUM CASCADE LASER

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

TB03 **15 min 8:59**

SUB-DOPPLER SPECTRA OF INFRARED HYPERFINE TRANSITIONS OF NITRIC OXIDE USING A PULSE MODULATED QUANTUM CASCADE LASER

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

TB04 **15 min 9:16**

KINETIC INVESTIGATION OF COLLISION INDUCED EXCITATION TRANSFER IN Kr$^*(4p^55p^1)$ + Kr $(4p^6)$ AND Kr$^*(4p^55p^1)$ + He $(1s^2)$ MIXTURES

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

TB05 **15 min 9:33**

IR/THZ DOUBLE RESONANCE SPECTROSOCPY ENERGY DYNAMICS AT ATMOSPHERIC PRESSURES

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

TB06 **10 min 9:50**

ULTRAFAST STRUCTURAL DYNAMICS OF TERTIARY AMINES UPON ELECTRONIC EXCITATION

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

TB07 **10 min 10:02**

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

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

Intermission

TB08 **15 min 10:30**

PHOTOCHEMISTRY OF BENZYLALLENE: PHOTOCHEMICAL PATHWAYS TO NAPHTHALENE

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

TB09 **15 min 10:47**

BIMOLECULAR REACTIONS OF A DIFFERENT COLOR: CH_3D + CHLORINE WITH VARIED PHOTOLYSIS WAVELENGTHS

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

TB10 **15 min 11:04**

COMPARATIVE TORSION-INVERSION DYNAMICS FOR $CH_3CH_2^{\cdot}$, $CH_3OH_2^+$ AND CH_3NH_2

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

TB11 **15 min 11:21**

STATE-TO-STATE ROTATIONAL AND VIBRATIONAL ENERGY TRANSFERS FOLLOWING VIBRATIONAL EXCITATION OF (1010^00^0) AND (0112^00^0) IN THE GROUND ELECTRONIC STATE OF ACETYLENE

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

TB12 **15 min 11:38**

VIBRATIONAL PREDISSOCIATION DYNAMICS OF THE $(H_2O)_2$ DIMER

L. C. CH'NG, B. E. ROCHER, A. K. MOLLNER, and H. REISLER, *Department of Chemistry, University of Southern California, Los Angeles, CA, 90089*.

TB13 **15 min 11:55**

DETERMINATION OF THE DISSOCIATION ENERGY OF AMMONIA DIMER: A VIBRATIONAL PREDISSOCIATION STUDY

AMANDA S. CASE, CORNELIA G. HEID, SCOTT. H. KABLE, and F. FLEMING CRIM, *Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706*.

TC. MICROWAVE

TUESDAY, JUNE 21, 2011 – 8:30 am

Room: 1000 McPHERSON LAB

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

TC01 **10 min 8:30**

EASY-GOING ON-SPECTROMETER OPTIMISATION OF PHASE MODULATED HOMONUCLEAR DECOUPLING SEQUENCES IN SOLID-STATE NMR

DENNIS L. A. G. GRIMMINCK, SURESH K. VASA, W. LEO MEERTS, AND P. M. KENTGENS, *Radboud University, Institute for Molecules and Materials, Heyendaalseweg 135, NL-6525 AJ Nijmegen, The Netherlands*.

TC02 **15 min 8:42**

QUANTUM-CHEMICAL CALCULATIONS OF SPECTROSCOPIC PARAMETERS FOR ROTATIONAL SPECTROSCOPY: THE NEED OF THE INTERPLAY BETWEEN EXPERIMENT AND THEORY

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

TC03 **15 min 8:59**

ROTATIONAL SPECTRUM OF CH_2FI FROM 5 GHZ UP TO 1 THZ: ACCURATE SPECTROSCOPIC AND HYPERFINE PARAMETERS

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

TC04 **15 min 9:16**

ANALYSIS OF THE ROTATIONAL SPECTRUM OF HDO IN ITS $v_2 = 0$ AND 1 VIBRATIONAL STATES UP TO 2.8 THz

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

TC05 **15 min 9:33**

ROTATIONAL SPECTROSCOPY OF $HD^{18}O$

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

[a]A part of this work was performed at the Jet Propulsion Laboratory, California Institute of Technology under contract with the National Aeronautics and Space Administration.

TC06 **15 min 9:50**

CHIRPED-PULSE TERAHERTZ SPECTROSCOPY FOR BROADBAND TRACE GAS SENSING

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

Intermission

TC07 **15 min 10:20**

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

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

TC08 **15 min 10:37**

THE MILLIMETER/SUBMILLIMETER SPECTRUM OF METHYLPHOSPHINE, CH_3PH_2 ($\tilde{X}^1A$)

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

TC09 **15 min 10:54**

FOURIER TRANSFORM MICROWAVE SPECTRUM OF THE FeCN RADICAL ($X^4\Delta_i$) AND CONFIRMATION OF THE GROUND ELECTRONIC STATE

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

TC10 **15 min 11:11**

THE PURE ROTATIONAL SPECTRUM OF THE ZnSH RADICAL (X^2A')

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

TC11 **15 min 11:28**

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

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

[a]Support from CHE-1011214

TC12 **15 min 11:45**

CAVITY AND CHIRPED PULSE ROTATIONAL SPECTRUM OF THE LASER ABLATION SYNTHESIZED, OPEN-SHELL MOLECULE TIN MONOCHLORIDE, SnCl.[a]

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

[a]Support from CHE-1011214

TD. ELECTRONIC

TUESDAY, JUNE 21, 2011 – 8:30 am

Room: 1015 McPHERSON LAB

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

TD01 **15 min 8:30**

SPECTROSCOPIC CHARACTERIZATION OF Be_2^+ $X^2\Sigma_u^+$ AND THE IONIZATION ENERGY OF Be_2

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

TD02 **15 min 8:47**

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

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

TD03 **15 min 9:04**

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

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

TD04 **15 min 9:21**

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

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

TD05 **15 min 9:38**

HIGH RESOLUTION LASER SPECTROSCOPY OF $SrOCH_3$

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

Intermission

TD06 **15 min 10:15**

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

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

TD07 **15 min 10:32**

THE JET-COOLED HIGH RESOLUTION $\tilde{A}^2E''$-$\tilde{X}^2A_2'$ VIBRONIC BANDS OF NO_3

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

[a]present address: Lawrence Berkeley National Laboratory, Berkeley, CA 94720

TD08 **15 min 10:49**

CAVITY RINGDOWN SPECTROSCOPY AND KINETICS OF HO_2+HCHO: DETECTION OF THE ν_1 AND Ã-X̃ BANDS OF $HOCH_2OO$

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

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

TD09 **15 min 11:06**

CAVITY RINGDOWN SPECTROSCOPY AND KINETICS OF BUTOXY ISOMERIZATION: DETECTION OF THE Ã-X̃ BAND OF HOC_4H_8OO

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

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

TD10 **15 min 11:23**

STUDY OF PHENYLACETYLENE BY CAVITY RING-DOWN SPECTROSCOPY

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

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

TD11 **15 min 11:40**

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

JOSHUA A. SEBREE, NATHAN KIDWELL, EVAN BUCHANAN, TIMOTHY S. ZWIER, *Department of Chemistry, Purdue University, West Lafayette, IN 47907*; MAREK ZGIERSKI, *National Research Council Canada, Ottawa, ON*.

TE. ATMOSPHERIC SPECIES

TUESDAY, JUNE 21, 2011 – 8:30 am

Room: 2015 McPHERSON LAB

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

TE01 **15 min 8:30**

LINE PARAMETERS OF CARBON DIOXIDE IN THE 4850 CM^{-1} REGION

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

TE02 **15 min 8:47**

TOWARDS AN ACCURATE INFRARED LINELIST FOR CO_2 AND ISOTOPOLOGUES

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

TE03 **15 min 9:04**

SELF- AND AIR-BROADENING OF $^{12}C^{16}O$, $^{13}C^{16}O$ AND $^{12}C^{18}O$ AT 2.3 μm

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

TE04 **15 min 9:21**

MEASUREMENTS OF LINE POSITIONS AND INTENSITIES OF $^{14}NH_3$ IN THE 1.5 μm REGION

KEEYOON SUNG, LINDA R. BROWN, *Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr.,Pasadena, CA 91109, U.S.A.*; XINCHUAN HUANG, *SETI Institute, Mountain View, CA 94043, U.S.A.*; DAVID W. SCHWENKE, TIMOTHY J. LEE, *NASA Ames Research Center, Moffett Field, CA, 94035, U.S.A.*.

TE05 **15 min 9:38**

THE 5-0 OVERTONE BAND OF HCl BY INTRACAVITY LASER ABSORPTION SPECTROSCOPY

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

Intermission

TE06 **15 min 10:10**

FREQUENCY COMB-REFERENCED MEASUREMENTS OF SELF- AND NITROGEN-PERTURBED LINE SHAPES IN THE ν_1 + ν_3 BAND OF ACETYLENE

MATTHEW J. CICH, GARY V. LOPEZ, TREVOR J. SEARS[a], *Department of Chemistry, Stony Brook University, Stony Brook, New York 11794*; C. P. MCRAVEN, *Department of Chemistry, Brookhaven National Laboratory, Upton, New York 11973*; A. W. MANTZ, *Department of Physics, Astronomy, and Astrophysics, Connecticut College, New London, CT 06320*; and DANIEL HURTMANS, *Service de Chimie Quantique et de Photophysique(Atoms, Molecules et Atmospheres), Universite Libre de Bruxelles, Bruxelles, Belgium B-10050*.

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

TE07 **15 min 10:27**

TEMPERATURE DEPENDENCE OF SELF- and NITROGEN-GAS LINE SHAPE PERTURBATIONS IN THE ν_1 + ν_3 BAND OF ACETYLENE

MATTHEW J. CICH, GARY V. LOPEZ, TREVOR J. SEARS [a], *Department of Chemistry, Stony Brook University, Stony Brook, New York 11794*; C. P. MCRAVEN, *Department of Chemistry, Brookhaven National Laboratory, Upton, New York 11973*; A. W. MANTZ, *Department of Physics, Astronomy, and Astrophysics, Connecticut College, New London, CT 06320*; and DANIEL HURTMANS, *Service de Chimie Quantique et de Photophysique(Atoms, Molecules et Atmospheres), Universite Libre de Bruxelles, Bruxelles, Belgium B-10050*.

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

TE08 **15 min 10:44**

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

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

TE09 **15 min 11:01**

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

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

TE10 **15 min 11:18**

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

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

TE11 **15 min 11:35**

NEW HIGH RESOLUTION OZONE ABSORPTION CROSS SECTIONS

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

TE12 **15 min 11:52**

LINE MIXING IN ATMOSPHERIC OZONE

COREY CASTO AND FRANK C. DE LUCIA, *Department of Physics, The Ohio State University, Columbus, OH 43210-1106*.

TF. ASTRONOMICAL SPECIES AND PROCESSES

TUESDAY, JUNE 21, 2011 – 1:30 pm

Room: 160 MATH ANNEX

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

TF01 **15 min 1:30**

GISBERT WINNEWISSER: AN APPRECIATION

ERIC HERBST, *Departments of Physics, Chemistry, and Astronomy, The Ohio State University, Columbus OH*.

TF02 **15 min 1:47**

SCRUTINY OF THE CORE OF THE GALACTIC CENTER BY H_3^+ AND CO: GCIRS 3 AND GCIRS 1W

M. GOTO, *Max-Planck-Institute for Astronomy, Heidelberg, D-69117, Germany*; T. USUDA, *Subaru Telescope, Hilo, HI 96720*; T. R. GEBALLE, *Gemini Observatory, Hilo, HI 96720*; N. INDRIOLO, B. J. MCCALL, *Department of Astronomy and Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801*; T. OKA, *Department of Astronomy and Astrophysics and Department of Chemistry, University of Chicago, Chicago, IL 60637*.

TF03 **15 min 2:04**

INVESTIGATING THE COSMIC-RAY IONIZATION RATE IN THE GALACTIC ISM WITH H_3^+ OBSERVATIONS

NICK INDRIOLO, *Department of Astronomy, University of Illinois at Urbana-Champaign, Urbana, IL 61801*; THOMAS R. GEBALLE, *Gemini Observatory, Hilo, HI 96720*; TAKESHI OKA, *Department of Astronomy & Astrophysics and Department of Chemistry, University of Chicago, Chicago, IL 60637*; BENJAMIN J. McCALL, *Departments of Astronomy and Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801*.

TF04 **10 min 2:21**

CAVITY RING DOWN SPECTROSCOPY OF MOLECULAR IONS IN THE 3 μm REGION

JOSEPH S. GUSS, HARALD VERBRAAK and HAROLD LINNARTZ, *Leiden Observatory, University of Leiden, 2300 RA Leiden, The Netherlands*.

TF05 **15 min 2:33**

SUBMILLIMETER-WAVE ROTATIONAL SPECTROSCOPY OF H_2F^+

R. FUJIMORI, K. KAWAGUCHI, *Department of Chemistry, Faculty of Science, Okayama University, 3-1-1, Tsushima-Naka, Okayama 700-8530, Japan*; T. AMANO, *Department of Chemistry and Department of Physics and Astronomy, University of Waterloo, 200 University Avenue West, Waterloo, ON N2L 3G1, Canada*.

TF06 **15 min 2:50**

DETECTION OF FeCN ($X^4\Delta_i$) IN THE CIRCUMSTELLAR ENVELOPE OF IRC+10216

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

TF07 **15 min 3:07**

THE QUEST FOR COMPLEX MOLECULES IN SPACE. SEARCHES FOR CYANIDES RELATED TO n-PROPYL CYANIDE IN SGR B2(N)

HOLGER S. P. MÜLLER, S. SCHLEMMER, *I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany*; A. BELLOCHE, K. M. MENTEN, *MPIfR, 53121 Bonn, Germany*; A. COUTENS, A. WALTERS, *Université de Toulouse and CNRS, 31028 Toulouse, France*; J.-U. GRABOW, *Institut für Physikalische Chemie und Elektrochemie, Lehrgebiet A, Universität Hannover, 30167 Hannover, Germany*.

Intermission

TF08 **10 min 3:40**

WHAT MOLECULAR LINES CAN TELL ABOUT EARLY STAGES OF MASSIVE STARS

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

TF09 **15 min 3:52**

NUCLEAR SPIN OF H_3^+ IN DIFFUSE MOLECULAR CLOUDS

KYLE N. CRABTREE, NICK INDRIOLO, HOLGER KRECKEL, BRIAN A. TOM,[a] BENJAMIN J. McCALL, *Department of Chemistry, University of Illinois, Urbana, IL 61801, USA*.

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

TF10 **15 min 4:09**

MOLECULAR ABUNDANCES IN THE DISK OF AN ACTIVE GALACTIC NUCLEUS

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

TF11 **15 min 4:26**

A STUDY OF HCO^+ AND CS IN PLANETARY NEBULAE

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

TF12 **15 min 4:43**

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

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

TF13 **15 min 5:00**

WATER COLLISIONS WITH NORMAL AND PARAHYDROGEN

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

TF14 **15 min 5:17**

LOW TEMPERATURE LINESHAPE OF HYDROGEN DEUTERIDE

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

TF15 **15 min 5:34**

A QUANTUM CHEMICAL INVESTIGATION OF THE STABILITY AND CHEMISTRY OF THE ANIONS OF CO AND H_2CO IN ASTROPHYSICAL ICES

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

TF16 **15 min 5:51**

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

T. OKA, C. P. MORONG, *Department of Astronomy and Astrophysics and Department of Chemistry, University of Chicago, Chicago, IL 60637*; T. R. GEBALLE, *Gemini Observatory, Hilo, HI 96720*; N. INDRIOLO, B. J. MCCALL, *Department of Astronomy and Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801*; M. GOTO, *Max-Planck-Institute for Astronomy, Heidelberg, D-69117, Germany*; T. USUDA, *Subaru Telescope, Hilo, HI 96720*.

TG. ELECTRONIC

TUESDAY, JUNE 21, 2011 – 1:30 pm

Room: 170 MATH ANNEX

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

TG01 **15 min 1:30**

FREQUENCY AND TIME DOMAIN STUDIES OF TOLUENE

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

TG02 **15 min 1:47**

HYDROGEN-BOUND COMPLEXES OF TROPOLONE: GATEWAYS FOR THE INTERROGATION OF MULTIPLE PROTON-TRANSFER EVENTS

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

TG03 **15 min 2:04**

ROTATION-TUNNELING ANALYSIS OF EXCITED-STATE PROTON TRANSFER IN DEUTERATED TROPOLONE

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

TG04 **15 min 2:21**

LASER SPECTROSCOPIC STUDY ON STRUCTURES OF 3*n*-CROWN-*n* (*n* = 4, 5, 6) COMPLEXES WITH PHENOL

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

TG05 **15 min 2:38**

HIGH RESOLUTION STARK SPECTROSCOPY OF MODEL DONOR-ACCEPTOR AMINOBENZONITRILES IN THE GAS PHASE.[a]

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

[a]Work supported by the NSF (CHE-0911117).

TG06 **15 min 2:55**

ROTATIONALLY RESOLVED ELECTRONIC SPECTROSCOPY OF BIOMOLECULES IN THE GAS PHASE. MELATONIN.

JOHN T. YI, and DAVID W. PRATT, *University of Pittsburgh, Department of Chemistry, Pittsburgh, PA 15260, USA*; CHRISTIAN BRAND, MIRIAM WOLLENHAUPT, and MICHAEL SCHMITT, *Heinrich-Heine-Universität, Institut für Physikalische Chemie I, 40225 Düsseldorf, Germany*; W. LEO MEERTS, *Radboud University Nijmegen, Institute for Molecules and Materials, Heyendaalseweg 135, NL-6525 AJ Nijmegen, The Netherlands*.

TG07 **15 min 3:12**

VIBRONIC SPECTROSCOPY OF JET-COOLED 1,4-PHENYLENE DIISOCYANIDE

DEEPALI N. MEHTA, ANNA K. GUTBERLET, and TIMOTHY S. ZWIER, *Department of Chemistry, Purdue University, West Lafayette, IN 47907*.

Intermission

TG08 **15 min 3:45**

EXCITED STATE DYNAMICS OF 7-AZAINDOLE HOMODIMER IN FROZEN NITROGEN MATRIX

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

TG09 **15 min 4:02**

EXCITED STATE PERTURBATIONS OF 7-AZAINDOLE MEDIATED THROUGH MICRO-SOLVATION.[a]

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

[a] Work supported by NSF(CHE-0911117)

TG10 **15 min 4:19**

CHIROPTICAL SPECTROSCOPY IN THE VAPOR PHASE

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

TG11 **15 min 4:36**

SINGLE MOLECULE SPECTROSCOPIC STUDY OF TWO ORGANIC RECTIFIERS

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

TG12 **15 min 4:53**

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

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

TG13 **15 min 5:10**

ULTRAFAST DYNAMICS IN NITRO- AND (ORGANOPHOSPHINE)GOLD(I)-POLYCYCLIC AROMATIC HYDROCARBONS

R. AARON VOGT, CHRISTIAN REICHARDT, CARLOS E. CRESPO-HERNÁNDEZ, THOMAS G. GRAY, *Department of Chemistry and Center for Chemical Dynamics, Case Western Reserve University, Cleveland, Ohio 44106, USA*.

TG14 **15 min 5:27**

EXCITED STATE DYNAMICS IN 2-AMINOPURINE RIBONUCLEOSIDE: FROM FEMTOSECOND TO MICROSECOND TIME SCALE

CHENGWEI WEN, CHRISTIAN REICHARDT, CARLOS E. CRESPO-HERNÁNDEZ, *Department of Chemistry and Center for Chemical Dynamics, Case Western Reserve University, 10900 Euclid Ave., Cleveland, Ohio 44106*.

TH. MINI-SYMPOSIUM: SPECTROSCOPIC PERTURBATIONS

TUESDAY, JUNE 21, 2011 – 1:30 pm

Room: 1000 McPHERSON LAB

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

TH01 ***Journal of Molecular Spectroscopy Review Lecture*** **30 min 1:30**

PERTURBATIONS I HAVE KNOWN AND LOVED

ROBERT W. FIELD, *Department of Chemistry, MIT, Cambridge, MA*.

TH02 **15 min 2:05**

VIBRONIC PERTURBATIONS IN THE ELECTRONIC SPECTRUM OF BeC

BEAU J. BARKER, IVAN O. ANTONOV, MICHAEL C. HEAVEN, *Department of Chemistry, Emory University, Atlanta, GA 30322*; RICHARD DAWES, *Department of Chemistry, Missouri University of Science and Technology, Rolla, MO 65409*.

TH03 **15 min 2:22**

PERTURBATIONS IN THE SPECTRA OF HIGH RYDBERG STATES: CHANNEL INTERACTIONS, STARK AND ZEEMAN EFFECTS

CHRISTA HAASE, MARTIN SCHÄFER, STEPHEN D. HOGAN and FRÉDÉRIC MERKT, *Laboratorium für Physikalische Chemie, ETH-Zürich, 8093 Zürich, Switzerland*.

TH04 **15 min 2:39**

DATA AND ANALYSIS OF SPIN-ORBIT COUPLED $A^1\Sigma_u^+$ AND $b^3\Pi_u$ STATES OF Cs_2

ANDREY V. STOLYAROV[a], *Department of Chemistry, Moscow State University, GSP-2 Leninskie gory 1/3, Moscow 119992, Russia*; THOMAS H. BERGEMAN, *Department of Physics and Astronomy, State University of New York, Stony Brook, New York 11794-3800*.

[a]Support by RFBR is gratefully acknowledged

TH05 **15 min 2:56**

SPECTROSCOPIC SIGNATURES OF ISOMERIZATION IN THE S_1 STATE OF C_2H_2

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

TH06 **15 min 3:13**

EVIDENCE OF PERTURBATIONS ON THE S_1 SURFACE OF ACETYLENE FROM PATTERNS IN STIMULATED EMISSION PUMPING SPECTRA

G. BARRATT PARK, JOSHUA H. BARABAN, ADAM H. STEEVES, and ROBERT W. FIELD, *Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139*.

Intermission

TH07 **15 min 3:45**

THE GERADE RYDBERG STATES OF MOLECULAR HYDROGEN

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

TH08 **15 min 4:02**

ROTATIONALLY RESOLVED SPECTROSCOPY OF THE ELECTRONICALLY EXCITED C AND D STATES OF ArXe AND KrXe

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

TH09 **15 min 4:19**

ANALYSIS OF STRONGLY PERTURBED $1\,^1\Pi - 2\,^3\Sigma^+ - b\,^3\Pi$ STATES OF THE KRb MOLECULE

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

TH10 **15 min 4:36**

OBSERVATION OF THE SYSTEM $(1)^1\Sigma_u^+$-$(1)^3\Pi_u$ of SR_2 BY FOURIER TRANSFORM SPECTROSCOPY AND ITS ANALYSIS

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

TH11 **15 min 4:53**

A NEW ANALYSIS OF A VERY OLD SPECTRUM: THE HIGHLY PERTURBED $A^2\Pi_i$ - $X^2\Pi_i$ BAND SYSTEM OF THE CHLORINE CATION (Cl_2^+)

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

TH12 **15 min 5:10**

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

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

TH13 **15 min 5:27**

LASER-INDUCED FLUORESCENCE SPECTROSCOPY ON ROTATIONAL DISTRIBUTION OF HfF PHOTOIONS

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

TH14 **15 min 5:44**

PERTURBATIONS IN THE GROUND ELECTRONIC STATE ROTATIONAL SPECTRUM OF TRANSITION-METAL CONTAINING MOLECULES

D. T. HALFEN, *Department of Chemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, AZ 85721*; R. W. FIELD, *Department of Chemistry, MIT, Cambridge, MA 02139*; and L. M. ZIURYS, *Department of Chemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, AZ 85721*.

TI. INFRARED/RAMAN

TUESDAY, JUNE 21, 2011 – 1:30 pm

Room: 1015 McPHERSON LAB

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

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

INFRARED SPECTRA OF COMPLEXES CONTAINING ACETYLENE-d2

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

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

HIGH RESOLUTION OVERTONE SPECTROSCOPY OF ACETYLENE VAN DER WAALS COMPLEXES

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

TI03 **10 min** **2:04**

HIGH RESOLUTION OVERTONE SPECTROSCOPY OF THE ACETYLENE VAN DER WAALS DIMER, $^{12}(C_2H_2)_2$

K. DIDRICHE, C. LAUZIN, T. FOLDES, D. GOLEBIOWSKI, M. HERMAN, *Service de Chimie quantique et Photophysique CP160/09, Faculté des Sciences, Université Libre de Bruxelles (U.L.B.), Av. Roosevelt, 50, B-1050, Bruxelles, Belgium*; C. LEFORESTIER, *ACTMM-CC 15.01, Institut Charles Gerhardt, 34095 Montpellier, France*.

TI04 **15 min** **2:16**

THE WEAKLY–BOUND CO_2–ACETYLENE COMPLEX: FUNDAMENTAL AND TORSIONAL COMBINATION BAND IN THE CO_2 ν_3 REGION

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

TI05 **15 min** **2:33**

HIGH RESOLUTION INFRARED AND MICROWAVE SPECTRA OF NH_3-HCCH AND NH_3-OCS COMPLEXES: STUDIES OF WEAK C-H$\cdots$N HYDROGEN BOND AND ELECTRIC MULTIPOLE INTERACTIONS

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

TI06 **15 min** **2:50**

INFRARED SPECTRA OF WATER BENDING BANDS OF PROPYLENE OXIDE-WATER COMPLEXES: SEQUENTIAL SOLVATION OF A CHIRAL MOLECULE IN WATER

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

Intermission

TI07 **15 min 3:20**

FIRST INFRARED SPECTRA OF CN-RARE GAS AND CN-H_2/D_2 COMPLEXES VIA IR-UV FLUORESCENCE DEPLETION SPECTROSCOPY[a]

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

[a]Research is supported by the Chemistry Division of the National Science Foundation

TI08 **15 min 3:37**

CARBON DIOXIDE CLUSTERS: $(CO_2)_6$ TO $(CO_2)_{13}$

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

TI09 **15 min 3:54**

THEORETICAL AND EXPERIMENTAL STUDY OF THE ROVIBRATIONAL SPECTRA OF CO_2-(*para*-H_2)-He TRIMERS

HUI LI, *Institute of Theoretical Chemistry, State Key Lab. of Theoretical & Computational Chemistry, Jilin Univ., 2519 Jiefang Rd, Changchun 130023, P.R.China; Chemistry Dept., Univ. of Waterloo, Waterloo, Ontario N2L 3G1, Canada*; ROBERT J. LE ROY, PIERRE-NICHOLAS ROY, *Chemistry Dept., Univ. of Waterloo, Waterloo, Ontario N2L 3G1, Canada*; A. R. W. McKELLAR, *Steacie Institute for Molecular Sciences, NRCC, Ottawa, Ontario K1A OR6, Canada*.

TI10 **15 min 4:11**

SPECTROSCOPIC OBSERVATION OF CS_2 DIMER

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

TI11 **15 min 4:28**

INFRARED SPECTRA OF CS_2 TRIMER: OBSERVATION OF AN ISOMER WITH D_3 SYMMETRY

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

TI12 **15 min 4:45**

INFRARED SPECTRA OF He–CS_2, Ne–CS_2, AND Ar–CS_2

F. MIVEHVAR, J. NOROOZ OLIAEE, N. MOAZZEN-AHMADI, *Department of Physics and Astronomy, University of Calgary, Calgary, AB T2N 1N4, Canada*.

TJ. THEORY

TUESDAY, JUNE 21, 2011 – 1:30 pm

Room: 2015 McPHERSON LAB

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

TJ01 **15 min** **1:30**

A SEMICLASSICAL DIRECT POTENTIAL FITTING SCHEME FOR DIATOMICS

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

TJ02 **15 min** **1:47**

UNEXPECTED PROPERTIES OF THE MORSE OSCILLATOR

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

TJ03 **15 min** **2:04**

IMPROVED DIABATIC MODEL FOR VIBRONIC COUPLING IN THE GROUND ELECTRONIC STATE OF NO_3

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

TJ04 **15 min** **2:21**

EFFECT OF JAHN-TELLER AND SPIN-ORBIT COUPLING ON $\tilde{X}^2E$ INFRARED SPECTRUM OF CH_3O

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

TJ05 **15 min** **2:38**

VIBRATIONAL DYNAMICS AROUND THE CONICAL INTERSECTION RESULTING FROM THE $\tilde{A} \rightarrow \tilde{X}$ LASER INDUCED FLUORESCENCE OF THE METHOXY (CH_3O) RADICAL

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

TJ06 **15 min** **2:55**

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

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

TJ07 **15 min** **3:12**

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

D. LARESE, *Department of Chemistry, Yale University, New Haven CT 06520-8107, USA*; F. IACHELLO, *Center for Theoretical Physics, Yale University, New Haven CT 06520-8120, USA*.

TJ08 **15 min 3:29**

VIBRATIONALLY AVERAGED LONG-RANGE MOLECULE-MOLECULE DISPERSION COEFFICIENTS FROM COUPLED-CLUSTER CALCULATIONS

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

Intermission

TJ09 **15 min 4:00**

EXOMOL: MOLECULAR LINE LISTS FOR EXOPLANET AND OTHER ATMOSPHERES

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

TJ10 **15 min 4:17**

USING DIFFUSION MONTE CARLO TO PROBE THE ROTATIONALLY EXCITED STATES OF H_3^+ AND ITS ISOTOPOLOGUES

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

TJ11 **10 min 4:34**

COMPUTATIONAL HIGH-FREQUENCY OVERTONE SPECTRA OF THE WATER AMMONIA COMPLEX

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

TJ12 **10 min 4:46**

A COMPUTATIONAL STUDY OF THE VIBRATIONAL O–H STRETCHING AND H–O–H BENDING SPECTRUM OF THE WATER TRIMER

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

TJ13 **15 min 4:58**

COLLISION INDUCED VELOCITY CHANGES FROM MOLECULAR DYNAMIC SIMULATIONS. APPLICATION TO THE SPECTRAL SHAPE OF THE Q(1) RAMAN LINES OF H_2/H_2

H.TRAN and J.M. HARTMANN, *Laboratoire Interuniversitaire des Systemes Atmospheriques, Universite paris Est Creteil et Universite paris Diderot, 94010 Creteil Cedex, France*.

TJ14 **15 min 5:15**

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

JING YANG and PIERRE-NICHOLAS ROY, *Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada*.

TJ15 **15 min** **5:32**

SIMULATION STUDIES OF THE VIBRATIONAL DYNAMICS OF $para$-HYDROGEN CLUSTERS

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

TJ16 **15 min** **5:49**

MIXED CLUSTERS OF H_2 AND H_2O: INSIGHTS FROM THEORY AND SIMULATIONS

TAO ZENG, HUI LI, ROBERT J. LE ROY, PIERRE-NICHOLAS ROY, *Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada*.

WA. PLENARY

WEDNESDAY, JUNE 22, 2011 – 8:30 am

Room: AUDITORIUM, INDEPENDENCE HALL

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

WA01 **40 min 8:30**

THE ATMOSPHERIC CHEMISTRY EXPERIMENT, ACE: LATEST RESULTS

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

WA02 **40 min 9:15**

CHASING NONEXISTENT COMPOUNDS WITH LASERS: ELECTRONIC SPECTROSCOPY OF MAIN GROUP TRANSIENT MOLECULES, FREE RADICALS, AND IONS

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

Intermission

WA03 **40 min 10:20**

WATCHING CONFORMATIONS OF BIOMOLECULES: A MICROWAVE SPECTROSCOPY APPROACH

J. C. LÓPEZ, *Grupo de Espectroscopía Molecular (GEM). Edificio Quifima. Laboratorios de Espectroscopía y Bioespectroscopía. Parque Científico. Universidad de Valladolid, 47011 Valladolid. (Spain).*

WA04 **40 min 11:05**

POLAR MOLECULES IN THE QUANTUM REGIME

DEBORAH S. JIN, JUN YE, *JILA, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY AND UNIVERSITY OF COLORADO, BOULDER, CO 80309-0440, USA*.

WF. ASTRONOMICAL SPECIES AND PROCESSES

WEDNESDAY, JUNE 22, 2011 – 1:30 pm

Room: 160 MATH ANNEX

Chair: MARYVONNE GERIN, Ecole Normale Superieure, Paris, France

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

INTERSTELLAR NITRILE CHEMISTRY AS REVEALED BY CHIRPED-PULSE FTMW SPECTROSCOPY

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

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

3-D SUBMILLIMETER SPECTROSCOPY OF ASTROPHYSICAL 'WEEDS' – CONTINUED ANALYSIS

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

WF03 **10 min** **2:04**

PERFORMANCE OF THE NEW 0.4 mm RECEIVER (602-720 GHz) AT THE SUB-MILLIMETER TELESCOPE OF THE ARIZONA RADIO OBSERVATORY

JESSICA L. DODD, L. M. ZIURYS, R. W. FREUND, E. F. LAURIA, *Department of Chemistry, Department of Astronomy, Arizona Radio Observatory, The University of Arizona, Tucson, AZ 85721*.

WF04 **15 min** **2:16**

HIGHLY ACCURATE QUARTIC FORCE FIELDS, VIBRATIONAL FREQUENCIES, AND SPECTROSCOPIC CONSTANTS FOR CYCLIC AND LINEAR $C_3H_3^+$ INCLUDING ^{13}C AND DEUTERIUM ISOTOPOLOGUES

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

WF05 **15 min** **2:33**

A SEARCH FOR HYDROXYLAMINE (NH_2OH) TOWARDS IRC+10216, ORION-S, ORION(KL), SGRB2(N), SGRB2(OH), W51M AND W3(IRS5)

ROBIN L. PULLIAM, ANTHONY J. REMIJAN, *National Radio Astronomy Observatory, Charlottesville, VA 22903*; JOANNA CORBY, *Dept. of Astronomy, Dept. of Chemistry, University of Virginia and National Radio Astronomy Observatory, Charlottesville, VA 22903*.

WF06 **10 min 2:50**

A SEARCH FOR INTERSTELLAR CARBON-CHAIN ALCOHOL HC_4OH IN THE STAR FORMING REGION L1527

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

WF07 **5 min 3:02**

LABORATORY SUBMILLIMETER SPECTROSCOPY AS A PROBE OF METHANOL PHOTODISSOCIATION

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

WF08 **10 min 3:09**

NEW ACETYLENE $^{12}C_2H_2$ MEASUREMENTS USING SOLEIL SYNCHROTRON

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

WF09 **15 min 3:21**

THE MILLIMETERWAVE SPECTRUM OF n-BUTYL CYANIDE

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

WF10 **15 min 3:38**

ROTATIONALLY RESOLVED SPECTRA OF THE $B^2\Pi$ - $X^2\Pi$ $0_0{}^0$ AND $\mu^2\Sigma$ - $\mu^2\Sigma$ $11_1{}^1$ TRANSITIONS OF C_6H AND C_6D

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

Intermission

WF11 **10 min 4:15**

PROSPECTIVE WORK FOR ALMA: THE MILLIMETERWAVE AND SUBMILLIMETERWAVE SPECTRUM OF DEUTERATED GLYCOLALDEHYDE

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

[a]Permanent address: IRAP, Université de Toulouse, UPS-OMP, CNRS; 9 Av. colonel Roche, BP 44346, 31028 Toulouse cedex 4, France

WF12 **15 min 4:27**

THE MICROWAVE SPECTRUM OF PARTIALLY DEUTERATED SPECIES OF DIMETHYL ETHER[a]

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

[a]This work is supported by ANR-08-BLAN-0054, ANR-08-BLAN-0225, and by the PCMI French program.

WF13 **15 min 4:44**

PROSPECTIVE WORK FOR ALMA: THE MILLIMETERWAVE AND SUBMILLIMETERWAVE SPECTRUM OF ^{13}C-GLYCOLALDEHYDE

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

WF14 **15 min 5:01**

EXPERIMENTAL ELECTRONIC SPECTROSCOPY OF TWO PAHs: NAPHTHALENE AND 2-METHYL NAPHTHALENE

H. FRIHA, *ISMO, CNRS, Université Paris- Sud, Orsay, 91400, France*; G. FERAUD, *ISMO, CNRS, Université Paris- Sud, Orsay, 91400, France*; T. PINO, *ISMO, CNRS, Université Paris- Sud, Orsay, 91400, France*; PH. BRECHIGNAC, *ISMO, CNRS, Université Paris- Sud, Orsay, 91400, France*; P. PARNEIX, *ISMO, CNRS, Université Paris- Sud, Orsay, 91400, France*; Z. DHAOUDI, *LSAMA, Faculté des Sciences de Tunis, Campus Universitaire 2092, Manar II, Tunisie*; N. JAIDANE, *LSAMA, Faculté des Sciences de Tunis, Campus Universitaire 2092, Manar II, Tunisie*; H.GALILA, *LSAMA, Faculté des Sciences de Tunis, Campus Universitaire 2092, Manar II, Tunisie*; T. TROY, *School of Chemistry, The University of Sydney, NSW 2006, Australia*; T. SCHMIDT, *School of Chemistry, The University of Sydney, NSW 2006, Australia*.

WF15 **15 min 5:18**

HIGH RESOLUTION SPECTROSCOPY AND GLOBAL ANALYSIS OF THE TETRADECAD REGION OF METHANE $^{12}CH_4$

A. NIKITIN, *Institute of Atmospheric Optics, 634055 Tomsk, Russia and Laboratoire GSMA, UMR 6089 CNRS-Université de Reims Champagne Ardenne, Moulin de la Housse BP 1039, Cases 16-17, F-51687 Reims Cedex 2, France*; V. BOUDON, C. WENGER, *Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR 5209 CNRS-Université de Bourgogne, 9. Av. A. Savary, BP 47870, F-21078 Dijon Cedex, France*; L. R. BROWN, *Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Drive, Pasadena, California 91109, USA*; S. BAUERECKER, *Physical Chemistry, ETH Zürich, CH-8093 Zürich, Switzerland and Institut für Physikalische und Theoretische Chemie, Technische Universität Braunschweig, D-38106, Germany*; S. ALBERT, M. QUACK, *Physical Chemistry, ETH Zürich, CH-8093 Zürich, Switzerland*.

WF16 **5 min 5:35**

LONG PATH- HIGH RESOLUTION SPECTRUM OF METHANE. TOWARDS TITAN'S ATMOSPHERE

LUDOVIC DAUMONT, VLADIMIR TYUTEREV, LAURENCE REGALIA, XAVIER THOMAS, PIERRE VON DER HEYDEN, *Groupe de Spectrométrie Moléculaire et Atmosphérique,UMR CNRS 6089, Université de Reims Champagne-Ardenne, U.F.R. Sciences, B.P. 1039, 51687 Reims Cedex 2, France*; ANDREI NIKITIN, *Laboratory of Theoretical Spectroscopy, Institute of Atmospheric Optics, Russian Academy of Sciences, 1, Akademichesky Avenue, 634055 Tomsk, Russian Federation*; LINDA BROWN, *Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Drive, Pasadena, CA 91109, USA*.

WF17 **15 min 5:42**

THE $4\nu_3$ SPECTRAL REGION OF METHANE

D. CHRIS BENNER, V. MALATHY DEVI, JENNIFER HAYS, *Department of Physics, College of William and Mary, Williamsburg, VA 23187-8795*; J. J. O'BRIEN, S. SHAJI, *Department of Chemistry and Biochemistry, University of Missouri - St. Louis, St. Louis, MO 63121-4400*; P. T. SPICKLER, C. P. HOUCK, J. A. COAKLEY, KASIE J. HAGA, JUSTIN D. DOLPH, *Department of Physics, Bridgewater College, Bridgewater, VA 22812*.

WG. ELECTRONIC

WEDNESDAY, JUNE 22, 2011 – 1:30 pm

Room: 170 MATH ANNEX

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

WG01 **15 min 1:30**

APPROXIMATE THEORETICAL MODEL FOR THE FIVE ELECTRONIC STATES (Ω = 5/2, 3/2, 3/2, 1/2, 1/2) ARISING FROM THE GROUND $3d^9$ CONFIGURATION IN NICKEL HALIDE MOLECULES AND FOR ROTATIONAL LEVELS OF THE TWO Ω = 1/2 STATES IN THAT MANIFOLD

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

WG02 **15 min 1:47**

OBSERVATION OF $\Omega = 1/2$ STATES IN NiH THROUGH COLLISIONALLY INDUCED FLUORESCENCE

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

[a]Current address : Harvard-Smithsonian Center for Astrophysics, Atomic and Molecular Physics Division, Cambridge MA 02138, USA

WG03 **15 min 2:04**

NEW BANDS OF NICKEL FLUORIDE IN THE NEAR INFRARED BY INTRACAVITY LASER ABSORPTION SPECTROSCOPY

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

WG04 **10 min 2:21**

INTRACAVITY LASER ABSORPTION SPECTROSCOPY OF PLATINUM FLUORIDE IN THE NEAR INFRARED

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

WG05 **15 min 2:33**

THE ELECTRONIC SPECTRUM AND MOLECULAR STRUCTURE OF HAsO, THE ARSENIC ANALOG OF HNO

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

WG06 **15 min 2:50**

THE PFI-ZEKE SPECTROSCOPY STUDY OF HfS^+ AND THE IONIZATION ENERGY OF HfS

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

Intermission

WG07 **15 min 3:30**

THEORETICAL STUDIES OF ELECTRONIC SPECTRA AND BONDING OF AlCl/AlF($X^1\Sigma^+$, $a^3\Pi$, $A^1\Pi$) WITH EXCITED STATES EXHIBITING RECOUPLED PAIR BONDING

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

WG08 **15 min 3:47**

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

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

WG09 **10 min 4:04**

ELECTRONIC TRANSITIONS AND SPIN-ORBIT SPLITTING OF LANTHANUM DIMER

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

WG10 **15 min 4:16**

LASER INDUCED FLUORESCENCE SPECTROSCOPY OF COBALT MONOBORIDE

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

WG11 **15 min 4:33**

HIGH RESOLUTION LASER SPECTROSCOPY OF RHODIUM MONOBROMIDE.

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

WG12 **15 min 4:50**

THE VISIBLE SPECTRUM OF IRIDIUM MONOHYDRIDE AND MONODEUTERIDE.

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

WG13 **15 min 5:07**

THE VISIBLE SPECTRUM OF ZIRCONIUM DIOXIDE, ZrO_2

ANH LE AND TIMOTHY C. STEIMLE, *Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287*; VARUN GUPTA AND JOHN P. MAIER , *Department of Chemistry, University of Basel, Basel, Switzerland*.

WG14 **15 min 5:24**

SEQUENTIAL OXIDATION OF TRANSITION METAL SUBOXIDE CLUSTER ANIONS

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

WH. MICROWAVE

WEDNESDAY, JUNE 22, 2011 – 1:30 pm

Room: 1000 McPHERSON LAB

Chair: DeWAYNE T. HALFEN, University of Arizona, Tucson, Arizona

WH01 **15 min 1:30**

REASSIGNMENT OF MILLIMETERWAVE SPECTRUM OF THE HCN INTERNAL ROTATION BANDS OF H_2-HCN

KENSUKE HARADA, RISA YAMANAKA, and KEIICHI TANAKA, *Department of Chemistry, Faculty of Sciences, Kyushu University, Fukuoka, 812-8581 JAPAN*.

WH02 **15 min 1:47**

MILLIMETERWAVE SPECTROSCOPY OF THE INTERNAL ROTATION BANDS OF Ne-DCN

NAOKO OYAMADA, KENSUKE HARADA, and KEIICHI TANAKA, *Department of Chemistry, Faculty of Science, Kyushu University, Hakozaki, Higashiku, Fukuoka, 812-8581 JAPAN*.

WH03 **15 min 2:04**

STUDY OF He_N-HCN CLUSTERS USING ROTATIONAL SPECTROSCOPY

STEVE DEMPSTER, OLEKSANDR SUKHORUKOV, QI-YI LEI, and WOLFGANG JÄGER, *Department of Chemistry, University of Alberta, Edmonton, Canada T6G 2G2*.

WH04 **15 min 2:21**

MICROWAVE SPECTRA AND STRUCTURES OF $H_2O\cdots AgF$

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

WH05 **15 min 2:38**

INTERNAL ROTATION IN $CF_3I\cdots NH_3$ AND $CF_3I\cdots N(CH_3)_3$ PROBED BY CP-FTMW SPECTROSCOPY

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

WH06 **15 min 2:55**

INTERNAL MOTION EFFECTS IN THE MICROWAVE SPECTRUM OF ARGON-*CIS*-1,2-DIFLUOROETHYLENE

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

WH07 **15 min 3:12**

THE MICROWAVE SPECTRUM OF ARGON-VINYL CHLORIDE

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

Intermission

WH08 **10 min 3:45**

HALOGEN BOND AND INTERNAL DYNAMICS IN $CClF_3$-H2O

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

WH09 **15 min 3:57**

WEAK C–H···O INTERACTIONS AND H_2O INTERNAL ROTATION IN THE $HCClF_2$–H_2O AND $HCBrF_2$–H_2O DIMERS

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

WH10 **15 min 4:14**

CHIRPED-PULSE, FTMW SPECTROSCOPY OF THE LACTIC ACID-H_2O SYSTEM

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

WH11 **15 min 4:31**

STRUCTURE STUDY OF THE CHIRAL LACTIDE MOLECULES BY CHIRPED-PULSE FTMW SPECTROSCOPY

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

WH12 **15 min 4:48**

THE CHIRPED-PULSE AND CAVITY BASED FTMW SPECTROSCOPY OF THE METHYL LACTATE-WATER AND METHYL LACTATE-DEUTERIUM OXIDE DIMERS

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

WH13 **15 min 5:05**

THE PURE ROTATIONAL SPECTRUM OF PERFLUOROOCTANONITRILE, $C_7F_{15}CN$, STUDIED USING CAVITY- AND CHIRPED-PULSED FOURIER TRANSFORM MICROWAVE SPECTROSCOPIES

C. T. DEWBERRY, G. S. GRUBBS II, S. A. COOKE, *Department of Chemistry, The University of North Texas, 1155 Union Circle, # 305070 Denton, TX 76203-5017, USA*; W. C. BAILEY, *Chemistry-Physics Department, Kean University, 1000 Morris Avenue, Union, NJ 07080, USA*.

WH14 **15 min 5:22**

EVIDENCE FOR A NON-PLANAR C=(CCC) STRUCTURE IN HEXAFLUOROISOBUTENE AND HEXAFLUOROACETONE IMINE: A PURE ROTATIONAL SPECTROSCOPIC STUDY

G. S. GRUBBS II, C. T. DEWBERRY, B. E. LONG, S. A. COOKE, *Department of Chemistry, The University of North Texas, 1155 Union Circle, # 305070 Denton, TX 76203-5017, USA*; W. C. PRINGLE, *Department of Chemistry, Wesleyan University, Hall-Atwater Laboratories, 52 Lawn Ave, Middletown, CT 06459-0180*.

WI. MINI-SYMPOSIUM: SPECTROSCOPIC PERTURBATIONS

WEDNESDAY, JUNE 22, 2011 – 1:30 pm

Room: 1015 McPHERSON LAB

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

WI01 ***INVITED TALK*** **30 min 1:30**

INVISIBLE ELECTRONIC STATES AND THEIR DYNAMICS REVEALED BY PERTURBATIONS

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

WI02 **15 min 2:05**

INTERNAL AND EXTERNAL PERTURBATIONS IN ELECTRONIC SPECTROSCOPY. THE STARK SPECTRUM OF INDOLE-NH_3.[a]

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

[a]Work supported by NSF (CHE-0911117).

WI03 **15 min 2:22**

NOVEL PATTERNS OF TORSION - INVERSION TUNNELING AND TORSION - ROTATION COUPLING IN THE ν_{11} CH - STRETCH REGION OF CH_3NH_2

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

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

WI04 **15 min 2:39**

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

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

WI05 **15 min 2:56**

THE VISIBLE SPECTRUM OF Si_3

XIUJUAN ZHUANG, TIMOTHY C. STEIMLE, *Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287*; N. REILLY, D. KOKKIN and M. C. McCARTHY, *Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts 02138, USA*; J. F. STANTON , *Chemistry Department and Biochemistry, U. of Texas, Austin, TX 78712, USA*; T. D. CRAWFORD and B. FORTENBERRY, *Chemistry Department, Virgina Tech, Blackbury VA 24061, USA*; J. P. MAIER , *Department of Chemistry, University of Basel, Basel, Switzerland*.

WI06 **15 min 3:13**

EXPERIMENTAL CHARACTERIZATION OF THE WEAKLY ANISOTROPIC CN $X^2\Sigma^+$ + Ne POTENTIAL FROM IR-UV DOUBLE RESONANACE STUDIES OF THE CN-Ne COMPLEX[a]

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

[a]Research is supported by the Chemistry Division of the NSF

Intermission

WI07 **15 min 3:45**

TERAHERTZ SPECTROSCOPY OF HIGH K METHANOL TRANSITIONS

JOHN C. PEARSON[a], SHANSHAN YU, HARSHAL GUPTA and BRIAN J DROUIN, *Jet Propulsion Laboratory, California Institute of Technology, 4800 0ak Grove Dr., Pasadena CA 91109*.

[a]A part of this work was performed at the Jet Propulsion Laboratory, California Institute of Technology under contract with the National Aeronautics and Space Administration.

WI08 **15 min 4:02**

SYMMETRY DEPENDENCE OF THE RO-VIBRONIC DISTRIBUTIONS OF THE ND_2 A^2A_1 FRAGMENTS FROM THE PHOTODISSOCIATION OF THE A STATES OF ND_3 AND ND_2H AT 193.3 NM

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

WI09 **15 min 4:19**

VIBRATIONAL COUPLING PATHWAYS IN THE CH STRETCH REGION OF CH_3OH AND CH_3OD AS REVEALED BY IR AND FTMW-IR SPECTROSCOPIES

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

WI10 **15 min 4:36**

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

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

WI11 **15 min 4:53**

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

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

WI12 **15 min 5:10**

OPTICAL PUMPING AND ELECTRON SPIN RESONANCE OF SINGLE ^{87}Rb ATOMS ON HELIUM NANODROPLETS

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

WI13 **15 min 5:27**

HIGHLY EXCITED STATES OF Cs ATOMS ON HELIUM NANODROPLETS

F. LACKNER, M. THEISEN, M. KOCH, and W.E. ERNST, *Institute of Experimental Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria*.

WJ. RADICALS AND IONS

WEDNESDAY, JUNE 22, 2011 – 1:30 pm

Room: 2015 McPHERSON LAB

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

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

RECONCILING EXPERIMENT AND THEORY: THE INTERESTING AND UNUSUAL CASE OF THE HOOO RADICAL

VALERIO LATTANZI, M.C. McCARTHY, *Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, and School of Engineering and Applied Science, Harvard University, Cambridge, MA 02138*; and JOHN F. STANTON, *Institute for Theoretical Chemistry, Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, TX 78712, United States*.

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

FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF THE HOSO RADICAL

VALERIO LATTANZI, M.C. McCARTHY, *Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, and School of Engineering and Applied Science, Harvard University, Cambridge, MA 02138*; and FILIPPO TAMASSIA, *Dipartimento di Chimica Fisica e Inorganica, Università di Bologna, V.le Risorgimento 4, I-40136 Bologna, Italy*.

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

HIGH RESOLUTION INFRARED SPECTROSCOPY OF THE PO_2 RADICAL

MICHAEL A. LAWSON, KRISTIAN J. HOFFMAN and PAUL B. DAVIES, *Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge, CB2 1EW, U.K.*.

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

SUBMILLIMETER-WAVE ROTATIONAL SPECTRA OF DNC

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

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

HIGH RESOLUTION FOURIER TRANSFORM SPECTROSCOPY OF TRANSIENT SPECIES ON THE FAR INFRARED "AILES" BEAMLINE OF SOLEIL SYNCHROTRON.

M. A. MARTIN-DRUMEL[a], O. PIRALI[a], D. BALCON[a], P. BRECHIGNAC, *Institut des Sciences Moléculaires d'Orsay (ISMO), CNRS, Université Paris XI, Orsay, France*; M. VERVLOET, P. ROY, *SOLEIL Synchrotron, AILES beamline, Saint-Aubin, France*.

[a] ALSO AT: SOLEIL SYNCHROTRON, AILES BEAMLINE, SAINT-AUBIN, FRANCE.

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

CALCULATION OF THE TRANSITION DIPOLE MOMENT OF THE $\tilde{A} \leftarrow \tilde{X}$ ELECTRONIC TRANSITION OF THE $C_2H_5O_2$ FROM THE PEAK ABSORPTION CROSS-SECTION

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

WJ07 **15 min 3:12**

ELECTRONIC SPECTROSCOPY OF COBALT-NEON CATION

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

Intermission

WJ08 **15 min 3:45**

ROVIBRATIONAL SPECTROSCOPY OF ALUMINUM CARBONYL CLUSTERS IN HELIUM NANODROPLETS

T. LIANG, A. M. MORRISON, S. D. FLYNN, and G. E. DOUBERLY, *DEPARTMENT OF CHEMISTRY, UNIVERSITY OF GEORGIA, ATHENS, GEORGIA 30602-2556*.

WJ09 **15 min 4:02**

PYROLYSIS OF ACETALDEHYDE: A FLEETING GLIMPSE OF VINYLIDENE

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

WJ10 **15 min 4:19**

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

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

[a]present address: Lawrence Berkeley National Laboratory, Berkeley, CA 94720

WJ11 **15 min 4:36**

OBSERVATION OF THE $\widetilde{A}$ - $\widetilde{X}$ ELECTRONIC TRANSITION OF THE 2-HYDROXYPROPYL PEROXY RADICAL VIA CAVITY RINGDOWN SEPCTROSCOPY

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

WJ12 **15 min 4:53**

VIBRATIONAL SPECTRUM OF THE THIOMETHOXY (CH_3S) RADICAL INVESTIGATED WITH INFRARED-VACUUM ULTRAVIOLET PHOTOIONIZATION

HUI-LING HAN, LUNG FU, *Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu 30010, Taiwan.*; YUAN-PERN LEE, *Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu 30010, Taiwan and Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan.*.

WJ13 **15 min 5:10**

CAVITY RING-DOWN SPECTROSCOPY OF THE $1^2B_1 - \tilde{X}^2A_1$ TRANSITION OF THE PHENYL RADICAL

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

RA. MINI-SYMPOSIUM: FUNDAMENTAL PHYSICS

THURSDAY, JUNE 23, 2011 – 8:30 am

Room: 160 MATH ANNEX

Chair: NEIL SHAFER-RAY, University of Oklahoma, Norman, Oklahoma

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

TESTS OF PARITY AND TIME-REVERSAL VIOLATION USING DIATOMIC MOLECULES

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

[a]This work supported by NSF

RA02 **15 min 9:05**

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

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

RA03 **15 min 9:22**

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

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

RA04 **10 min 9:39**

PERMANENT ELECTRON ELECTRIC DIPOLE MOMENT SEARCH IN THE $X^3\Delta_1$ GROUND STATE OF TUNGSTEN CARBIDE MOLECULES

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

RA05 **10 min 9:51**

THEORETICAL STUDY OF THE PbF AND PbO MOLECULES[a]

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

[a]This work supported by RFBR Grants No. 09–03–01034

RA06 **15 min 10:03**

THE EFFECTIVE HAMILTONIAN FOR THE GROUND STATE OF $^{207}Pb^{19}F$ AND NEW MEASUREMENTS OF THE FINE STRUCTURE SPECTRUM NEAR 1.2 μm.

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

[a]Current Address: Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973

Intermission

RA07 **15 min 10:40**

A PbF PROBE FOR THE ELECTRON ELECTRIC DIPOLE MOMENT

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

RA08 **10 min 10:57**

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

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

[a]Current Address: Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973

RA09 **15 min 11:09**

STARK SPECTROSCOPY OF PBF MOLECULE

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

RA10 **15 min 11:26**

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

BEAU J. BARKER, IVAN O. ANTONOV, VLADIMIR E. BONDYBEY, and MICHAEL C. HEAVEN, *Department of Chemistry, Emory University, Atlanta, GA 30322*.

RB. ATMOSPHERIC SPECIES

THURSDAY, JUNE 23, 2011 – 8:30 am

Room: 170 MATH ANNEX

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

RB01 **15 min 8:30**

NITROGEN-BROADENED $^{13}CH_4$ AT 80 TO 296 K

M. A. H. SMITH, *Science Directorate, NASA Langley Research Center, Hampton, VA 23681*; K. SUNG, L. R. BROWN, T. J. CRAWFORD, *Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr.,Pasadena, CA 91109*; A. W. MANTZ, *Dept. of Physics, Astronomy and Geophysics, Connecticut College, New London, CT 06320*; V. MALATHY DEVI and D. CHRIS BENNER, *The College of William and Mary, Williamsburg, VA 23187*.

RB02 **15 min 8:47**

MEASUREMENT OF CH_3D ABSORPTION CROSS SECTIONS, PRESSURE BROADENING, AND SHFT COEFFICIENTS IN THE 1.65 μm SPECTRAL REGION BY USING CONTINUOUS AVE CAVITY RING-DOWN SPECTROSCOPY

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

RB03 **15 min 9:04**

HIGH-RESOLUTION SPECTROSCOPY AND PRELIMINARY GLOBAL ANALYSIS OF C–H STRETCHING VIBRATIONS OF C_2H_4 IN THE 3000 AND 6000 CM^{-1} REGIONS

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

RB04 **15 min 9:21**

THE THZ ABSORPTION OF METHYL BROMIDE (CH_3BR)

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

RB05 **15 min 9:38**

IMPACT OF ATMOSPHERIC CLUTTER ON DOPPLER-LIMITED GAS SENSORS IN THE SUBMILLIMETER/TERAHERTZ

IVAN R. MEDVEDEV, *Department of Physics, Wright State University, 3640 Colonel Glenn Highway, Dayton, OH 45435, USA*; CHRISTOPHER F. NEESE, FRANK C. DE LUCIA, *Department of Physics, Ohio State University, 191 West Woodruff Ave., Columbus, OH 43210, USA*; GRANT M. PLUMMER, *Enthalpy Analytical, Inc., 2202 Ellis Road, Durham, North Carolina 27703, USA*.

RB06 **15 min 9:55**

HIGH RESOLUTION SPECTROSCOPY USING A TUNABLE THZ SYNTHESIZER BASED ON PHOTOMIXING

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

Intermission

RB07 **15 min 10:30**

SENSORS ACROSS THE SPECTRUM

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

RB08 **15 min 10:47**

NEW CHIRPED-PULSE THZ FOURIER TRANSFORM TECHNIQIES FOR DETERMINATION OF LINESHAPE PARAMETERS FOR ATMOSPHERIC SPIECIES

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

RB09 **15 min 11:04**

INFRARED ABSORPTION OF CH_3SONO DETECTED WITH TIME-RESOLVED FOURIER-TRANSFORM SPECTROSCOPY

YUAN-PERN LEE, *Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu 30010, Taiwan and Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan*; JIN-DAH CHEN, *Department of Applied Chemistry, National Chiao Tung University, Hsinchu 30010, Taiwan*.

RB10 **10 min 11:21**

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

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

RB11 **15 min 11:33**

RULES APPLICABLE FOR SPECTROSCOPIC PARAMETERS OF H_2O TRANSITIONS INVOLVING HIGH J STATES

Q. MA, *NASA/Goddard Institute for Space Studies and Department of Applied Physics and Applied Mathematics, Columbia University, 2880 Broadway, New York, NY 10025*; R. H. TIPPING, *Department of Physics and Astronomy, University of Alabama, Tuscaloosa, AL 35487*.

RC. MICROWAVE

THURSDAY, JUNE 23, 2011 – 8:30 am

Room: 1000 McPHERSON LAB

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

RC01 **15 min** **8:30**

FOURIER TRANSFORM MICROWAVE SPECTRUM OF THE YC_2 (X^2A_1) RADICAL

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

RC02 **15 min** **8:47**

OBSERVATION OF LOW J TRANSITIONS OF LASER ABLATED ALKALI HALIDES

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

RC03 **15 min** **9:04**

ROTATIONAL SPECTROSCOPY OF ZnCCH ($X^2\Sigma^+$)AT MICROWAVE AND MILLIMETER WAVELENGTHES

J. MIN, D. T. HALFEN, M. SUN, B. T. HARRIS, L. M. ZIURYS, *University of Arizona, Deptment of Chemistry and Biochemitry and Steward Observatory, Tucson, AZ-85721*.

RC04 **15 min** **9:21**

FOURIER TRANSFORM MICROWAVE SPECTRUM OF MgCCH ($X^2\Sigma^+$)

J. MIN, D. T. HALFEN, M. SUN, B. T. HARISS, L. M. ZIURYS, *University of Arizona, Deptment of Chemistry and Biochemitry and Steward Observatory, Tucson, AZ-85721*; D. J. CLOUTHIER, *University of Kentucky, Deptment of Chemistry, Lexington, KY-40506*.

RC05 **15 min** **9:38**

A CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE SPECTROMETER COMBINED WITH A LASER ABLATION SOURCE

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

RC06 **15 min** **9:55**

TECHNIQUES FOR HIGH-BANDWIDTH ($\geq$30 GHz) CHIRPED-PULSE MILLIMETER/SUBMILLIMETER-WAVE SPECTROSCOPY

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

Intermission

RC07 **15 min 10:30**

PROBING VITAMINE C, ASPIRIN AND PARACETAMOL IN THE GAS PHASE: HIGH RESOLUTION ROTATIONAL STUDIES

S. MATA, C. CABEZAS, M. VARELA, I. PENA, A. NINO, 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)*; J.-U. GRABOW, *Gottfried-Wilhelm-Leibniz-Universität, Institut für Physikalische Chemie & Elektrochemie, Callinstraße 3A, 30167 Hannover, Germany*.

RC08 **15 min 10:47**

JET COOLED ROTATIONAL STUDIES OF DIPEPTIDES

C. CABEZAS, M. VARELA 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)*.

RC09 **15 min 11:04**

CHIRPED-PULSED FTMW SPECTRUM OF VALERIC ACID AND 5-AMINOVALERIC ACID. A STUDY OF AMINO ACID MIMICS IN THE GAS PHASE[a]

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

[a]Work supported by NSF (CHE-0618740 and -0911117).

RC10 **15 min 11:21**

STRUCTURE STUDY OF FORMIC ACID CLUSTERS BY CHIRPED-PULSE FTMW SPECTROSCOPY

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

RC11 **15 min 11:38**

A CHIRPED PULSE FTMW STUDY OF THE STRUCTURE OF PHENOL DIMER

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

RC12 **15 min 11:55**

OBSERVATION OF C$-$H$\cdots\pi$ INTERACTIONS: MICROWAVE SPECTRA AND STRUCTURES OF THE $CH_2FX\cdots HCCH$ (X=F,Cl) WEAKLY BOUND COMPLEXES

LENA F. ELMUTI, DANIEL A. OBENCHAIN, DON L. JURKOWSKI, AMELIA J. SANDERS, REBECCA A. PEEBLES, SEAN A. PEEBLES, *Department of Chemistry, Eastern Illinois University, 600 Lincoln Avenue, Charleston, IL 61920*; AMANDA L. STEBER, JUSTIN L. NEILL, BROOKS H. PATE, *Department of Chemistry, University of Virginia, McCormick Rd., PO Box 400319, Charlottesville, VA 22904*.

RD. MINI-SYMPOSIUM: SPECTROSCOPIC PERTURBATIONS

THURSDAY, JUNE 23, 2011 – 8:30 am

Room: 1015 McPHERSON LAB

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

RD01 *INVITED TALK* **30 min 8:30**

SPECTROSCOPIC SIGNATURES OF BOND BREAKING INTERNAL ROTATION IN HCP

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

RD02 **15 min 9:05**

PERTURBATION FACILITATED DISPERSED FLUORESCENCE AND STIMULATED EMISSION PUMPING SPECTROSCOPIES OF HCP

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

RD03 **15 min 9:22**

COLLISIONAL ORIENTATION TRANSFER FACILIATED POLAROZATION SPECTROSCOPY[a]

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

[a]Funded by NSF PHY 0555608 and PHY 0855502

RD04 **10 min 9:39**

THE $X^1\Sigma^+$ AND $B^1\Pi$ STATES OF LiRb AND PROSPECTS FOR CREATING ULTRACOLD GROUND STATE LiRb MOLECULES

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

RD05 **15 min 9:51**

OPTICAL STARK SPECTROSCOPY OF CHLORO-METHYLENE, HCCl

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

Intermission

RD06 **15 min 10:20**

PHASE SPACE EXPLORATION OF ACETYLENE AT ENERGIES UP TO 13,000 cm^{-1}

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

RD07 **15 min 10:37**

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

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

RD08 **15 min 10:54**

THE HIGH RESOLUTION SPECTRUM OF THE $Ar-C_2H_2$ COMPLEX

C. LAUZIN, K. DIDRICHE, M. HERMAN, *Service de Chimie quantique et Photophysique CP160/09, Faculté des Sciences, Université Libre de Bruxelles (U.L.B.), Av. Roosevelt, 50, B-1050, Bruxelles, Belgium*; AND L. H. COUDERT, *LISA, CNRS/Universités Paris Est et Paris Diderot, 61 Avenue du Général de Gaulle, 94010 Créteil, France*.

RD09 **15 min 11:11**

IR EMISSION SPECTROSCOPY OF AMMONIA: LINELISTS AND ASSIGNMENTS

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

RD10 **15 min 11:28**

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

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

RD11 **15 min 11:45**

AUTOIONIZATION BRANCHING RATIOS FOR METAL HALIDE MOLECULES

JEFFREY J. KAY, *Lawrence Livermore National Laboratory, Livermore, CA 94550*; ROBERT W. FIELD, *Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139*.

RE. DYNAMICS

THURSDAY, JUNE 23, 2011 – 8:30 am

Room: 2015 McPHERSON LAB

Chair: MARILYNN JACOX, NIST, Gaithersburg, Maryland

RE01 **15 min** **8:30**

INTER-RING AND HEXYL CHAIN TORSIONAL POTENTIALS IN POLY (3-HEXYLTHIOPHENE) OLIGOMERS: SCALING WITH THE LENGTH OF THE CONJUGTED POLYMER BACKBONE

RAM S. BHATTA, DAVID S. PERRY, *Department of Chemistry, The University of Akron, OH 44325-3601*; YENENEH YIMER AND MESFIN TSIGE, *Department of Polymer Science, The University of Akron, OH 44325-3909*.

RE02 **15 min** **8:47**

VIBRATIONAL STATE DEPENDENT LARGE AMPLITUDE TUNNELING DYNAMICS IN MALONALDEHYDE

GRANT BUCKINGHAM AND DAVID J. NESBITT, *JILA, National Institute of Standards and Technology and University of Colorado, and Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO 80309*.

RE03 **15 min** **9:04**

VIBRATIONAL RELAXATION AND CONTROL OF SALICYLIDENE ANILINE

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

RE04 **15 min** **9:21**

DEVELOPMENT OF FEMTOSECOND STIMULATED RAMAN SPECTROSCOPY AS A PROBE OF VIBRATIONAL DYNAMICS

RYAN D. KIEDA, KRISTIN A. BRINEY, ADAM D. DUNKELBERGER, and F. FLEMING CRIM, *Department of Chemistry, Universtiy of Wisconsin-Madison, Madison, WI 53706*.

RE05 **15 min** **9:38**

VIBRATIONAL DYNAMICS OF TRICYANOMETHANIDE

DANIEL WEIDINGER, CASSIDY HOUCHINS, and JEFFREY C. OWRUTSKY, *Code 6111, Naval Research Laboratory, 4555 Overlook Ave SW, Washington, D.C. 20375*.

Intermission

RE06 **15 min** **10:10**

PHOTOCHEMISTRY OF HALOGENATED TRANSITION METAL DIANIONS

ALEXANDER N. TARNOVSKY, IGOR L. ZHELDAKOV, EVGENIIA V. BUTAEVA, and ANDREY S. MERESHCHENKO, *Department of Chemistry, Bowling Green State University, Bowling Green, OH, 43402*.

RE07 **15 min 10:27**

PHOTOCHEMISTRY OF BROMOFORM AND TRIBROMIDES OF OTHER ELEMENTS IN SOLUTION

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

RE08 **15 min 10:44**

ISOMERIZATION BETWEEN CH_2ClI AND CH_2Cl-I IN CRYOGENIC MATRICES STUDIED ON ULTRAFAST TIMESCALE

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

RE09 **15 min 11:01**

ISOMERIZATION OF CH_2Cl-I TO CH_2ClI IN CRYOGENIC MATRICES: A STUDY ON ULTRAFAST TIMESCALE

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

RE10 **15 min 11:18**

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

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

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

RE11 **15 min 11:35**

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

CAO GUO, CHRISTIAN REICHARDT AND CARLOS E. CRESPO-HERNÁNDEZ, *Department of Chemistry and the Center for Chemical Dynamics, Case Western Reserve University, 10900 Euclid Avenue, Cleveland, Ohio 44106*.

RF. MINI-SYMPOSIUM: THE THz COSMOS

THURSDAY, JUNE 23, 2011 – 1:30 pm

Room: 160 MATH ANNEX

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

RF01 *INVITED TALK* **30 min 1:30**

INTERSTELLAR HYDRIDE SPECTROSCOPY WITH HERSCHEL

MARYVONNE GERIN, *LERMA, CNRS UMR8112, OBSEVATOIRE DE PARIS & ECOLE NORMALE SUPERIEURE, 24 RUE LHOMOND, 75231 PARIS CEDEX 05, FRANCE*; and THE PRISMAS CONSORTIUM,.

RF02 **15 min 2:05**

CHEMICAL HERSCHEL SURVEYS OF STAR FORMING REGIONS (CHESS)

MARTIN EMPRECHTINGER, *California Institute of Technology, Pasadena CA 91125 (email: emprecht@caltech.edu)*.

RF03 **15 min 2:22**

OBSERVATIONS OF INTERSTELLAR HYDROGEN FLUORINE AND HYDROGEN CHLORIDE IN THE GALAXY

RAQUEL R. MONJE, DAREK C. LIS, THOMAS G. PHILLIPS, PAUL F. GOLDSMITH, MARTIN EMPRECHTINGER, *California Institute of Technology, 1200 E. California Blvd., Pasadena, CA 91125-4700, USA* ; DAVID A. NEUFELD, *Johns Hopkins University, USA*.

RF04 **15 min 2:39**

THE STRATOSPHERIC OBSERVATORY FOR INFRARED ASTRONOMY (SOFIA)

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

RF05 **15 min 2:56**

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

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

RF06 **15 min 3:13**

ROTATIONAL SPECTROSCOPY FOR ASTROPHYSICAL APPLICATIONS: THE THZ FREQUENCY REGION

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

Intermission

RF07 **15 min 3:45**

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

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

RF08 **15 min 4:02**

PROGRESS TOWARDS THE ROTATIONAL SPECTRUM OF H_5^+ AND ITS ISOTOPOLOGUES

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

RF09 **15 min 4:19**

ANALYSIS OF NEW DATA SETS PERTAINING TO THE WATER MOLECULE

S. YU, J. C. PEARSON, B. J. DROUIN, *Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109, USA*; H. S. P. MÜLLER, S. BRÜNKEN, *I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany*; M. A. MARTIN-DRUMEL, O. PIRALI, D. BALCON, M. VERVLOET, *Ligne AILES – Synchrotron SOLEIL, L'Orme des Merisiers, Saint Aubin, 91192 Gif-sur-Yvette, France*; AND L. H. COUDERT, *LISA, CNRS/Universités Paris Est et Paris Diderot, 61 Avenue du Général de Gaulle, 94010 Créteil, France*.

RF10 **15 min 4:36**

VIBRATIONALLY HOT HCN IN THE LABORATORY AND IRC+10216

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

[a] A part of this work was performed at the Jet Propulsion Laboratory, California Institute of Technology under contract with the National Aeronautics and Space Administration.

RF11 **15 min 4:53**

SHOCK-INDUCED MOLECULAR ASTROCHEMISTRY IN DENSE CLOUDS

JEONGHEE RHO, *SOFIA Mission Operations, USRA, NASA Ames Research Center*; JOHN HEWITT, *NASA/Goddard Space Flight Center*; WILLIAM REACH, *SOFIA Mission Operations, USRA, NASA Ames Research Center*; MORTEN ANDERSEN, *ESA, ESTEC, Netherlands*; JEAN-PHILIPPE BERNARD, *CNRS, Toulouse, France*.

RF12 **15 min 5:10**

THE LABORATORY AND OBSERVATIONAL STUDY OF 2-BUTANONE AS A TEST FOR ORGANIC CHEMICAL COMPLEXITY IN VARIOUS INTERSTELLAR PHYSICAL ENVIRONMENTS

JAY A. KROLL, and SUSANNA L. WIDICUS WEAVER, *Department of Chemistry, Emory University, Atlanta, GA 30322*; STEVEN T. SHIPMAN, *Division of Natural Sciences, New College of Florida, Sarasota, FL 34243*.

RF13 **15 min 5:27**

HIGH RESOLUTION FAR INFRARED FOURIER TRANSFORM SPECTROSCOPY OF THE NH_2 RADICAL.

M. A. MARTIN-DRUMEL, O. PIRALI, D. BALCON, *SOLEIL Synchrotron, AILES beamline, Saint-Aubin, France and Institut des Sciences Moleculaires d'Orsay, ISMO, CNRS, Universite Paris XI, Orsay, France*; M. VERVLOET, *SOLEIL Synchrotron, AILES beamline, Saint-Aubin, France*.

RF14 **15 min 5:44**

THE PURE ROTATIONAL SPECTRA OF ACETALDEHYDE AND GLYCOLALDEHYDE ISOTOPOLOGUES MEASURED IN NATURAL ABUNDANCE BY CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE SPECTROSCOPY

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

RF15 **15 min 6:01**

THE THZ SPECTRUM OF GLYCOLALDEHYDE

MANUEL GOUBET, THERESE R. HUET, IMANE HAYKAL, LAURENT MARGULES, *Laboratoire PhLAM, UMR8523 CNRS-Universite Lille 1, F-59655 Villeneuve d'Ascq Cedex, France*; OLIVIER PIRALI, PASCALE ROY, *Ligne AILES - Synchrotron SOLEIL, L'Orme des Merisiers Saint Aubin, F-91192 Gif-sur-Yvette, France*.

RG. INFRARED/RAMAN

THURSDAY, JUNE 23, 2011 – 1:30 pm

Room: 170 MATH ANNEX

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

RG01 **15 min 1:30**

VIBRATIONAL SPECTRA OF CRYOGENIC PEPTIDE IONS USING H_2 PREDISSOCIATION SPECTROSCOPY

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

RG02 **15 min 1:47**

VIBRATIONAL CHARACTERIZATION OF SIMPLE PEPTIDES USING CRYOGENIC INFRARED PHOTODISSOCIATION OF H_2-TAGGED, MASS-SELECTED IONS

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

RG03 **15 min 2:04**

USING AN ORGANIC SCAFFOLD TO MODULATE THE QUANTUM STRUCTURE OF AN INTRAMOLECULAR PROTON BOND: CRYOGENIC VIBRATIONAL PREDISSOCIATION SPECTROSCOPY OF H_2 ON PROTONATED 8-NAPHTHALENE-1-AMINE

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

RG04 **15 min 2:21**

APPLICATION OF INFRARED MULTIPHOTON DISSOCIATION SPECTROSCOPY FOR THE STUDY OF CHIRAL RECOGNITION IN THE PROTONATED SERINE CLUSTERS: PART II

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

RG05 **15 min 2:38**

ROTATION-VIBRATION SPECTRA OF MALONALDEHYDE OBTAINED WITH FAR-INFRARED SYNCHROTRON RADIATION

D. W. TOKARYK, S. C. ROSS, D. FORTHOMME, J. E. PRESCOTT, *Department of Physics and Centre for Laser, Atomic and Molecular Sciences, University of New Brunswick, Fredericton, NB, Canada E3B 5A3*; K. M. T. YAMADA, F. ITO, *EMTech, AIST, Tsukuba-West, Tsukuba, Ibaraki, Japan*.

RG06 **15 min 2:55**

IR SPECTROSCOPIC AND THEORETICAL STUDY OF NEW PHOTOCHROMIC SYSTEMS BASED ON CYMANTRENE DERIVATIVES.

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

Intermission

RG07 **10 min 3:30**

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

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

RG08 **15 min 3:42**

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

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

RG09 **15 min 3:59**

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

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

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

RG10 **15 min 4:16**

INFRARED ION-GAIN SPECTROSCOPY AND FRACTIONAL ABUNDANCE MEASUREMENTS OF CONFORMER POPULATIONS

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

RG11 **15 min 4:33**

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

JACOB C. DEAN, EVAN G. BUCHANAN, ANNA GUTBERLET, WILLIAM H. JAMES III, BIDYUT BISWAS, P. V. RAMACHANDRAN, and TIMOTHY S. ZWIER, *Department of Chemistry, Purdue University, West Lafayette, IN 47907*.

RG12 **15 min 4:50**

THE TORSIONAL FUNDAMENTAL BAND OF METHYLFORMATE

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

RG13 **15 min 5:07**

A FAR INFRARED SYNCHROTRON-BASED INVESTIGATION OF 3-OXETANONE

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

RG14 **15 min 5:24**

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

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

[a]Current address: Inorganic Chemistry Laboratory, South Parks Road, University of Oxford, UK OX1 3QR

RH. MICROWAVE

THURSDAY, JUNE 23, 2011 – 1:30 pm

Room: 1000 McPHERSON LAB

Chair: NICHOLAS WALKER, University of Bristol, Bristol, United Kingdom

RH01 **15 min 1:30**

WAVEGUIDE CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE (CP-FTMW) SPECTRUM OF ALLYL CHLORIDE

ERIN B. KENT, MORGAN N. McCABE, MARIA A. PHILLIPS, BRITTANY P. GORDON and STEVEN T. SHIPMAN, *Division of Natural Sciences, New College of Florida, Sarasota, FL 34243*.

RH02 **15 min 1:47**

WAVEGUIDE CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE (CP-FTMW) SPECTRUM OF ORTHO-FLUOROTOLUENE

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

RH03 **15 min 2:04**

A LOOK AT A SERIES OF ALKYL AND PERFLUOROALKYL BROMIDES AND CHLORIDES

BRITTANY E. LONG, STEPHEN A. COOKE, *Department of Chemistry, The University of North Texas, 1155 Union Circle, #305070, Denton, TX 76203-5017, U.S.A.*; GARRY S. GRUBBS II, *Department of Chemistry, Wesleyan University, Hall-Atwater Laboratories, 52 Lawn Ave., Middletown, CT 06459-0180, U.S.A.*

RH04 **15 min 2:21**

METHYL GROUP INTERNAL ROTATION IN THE PURE ROTATIONAL SPECTRUM OF 1,1-DIFLUOROACETONE

G. S. GRUBBS II, S. A. COOKE, *Department of Chemistry, The University of North Texas, 1155 Union Circle, # 305070 Denton, TX 76203-5017, USA*; P. GRONER, *Department of Chemistry, University of Missouri-Kansas City, 5100 Rockhill Road, Kansas City, MO 64110*.

RH05 **15 min 2:38**

FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF ALKALI METAL ACETYLIDES

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

RH06 **15 min 2:55**

ANALYSIS OF ROTATIONAL STRUCTURE IN THE HIGH-RESOLUTION INFRARED SPECTRA OF THE *TRANS*-HEXATRIENE-1,1-D_2 AND -*CIS*-1-D_1 SPECIES

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

RH07 **15 min 3:12**

ANALYSIS OF THE ROTATIONAL STRUCTURE IN THE HIGH-RESOLUTION INFRARED SPECTRUM OF *TRANS*-HEXATRIENE-1-$^{13}C_1$

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

Intermission

RH08 **15 min 3:45**

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

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

RH09 **15 min 4:02**

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

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

RH10 **15 min 4:19**

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

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

RH11 **15 min 4:36**

THE MICROWAVE SPECTRUM OF METHYL VINYL KETONE REVISITED

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

RH12 **10 min 4:53**

HIGH RESOLUTION ROTATIONAL SPECTROSCOPY OF A FLEXIBLE CYCLIC ETHER

F. GÁMEZ AND B. MARTÍNEZ-HAYA, *Departamento de Sistemas Físicos, Químicos y Naturales, Universidad Pablo de Olavide, 41013 Seville, Spain*; S. BLANCO, 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)*.

RH13 **15 min 5:05**

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

B. E. LONG, G. S. GRUBBS II, S. A. COOKE, *Department of Chemistry, The University of North Texas, 1155 Union Circle, # 305070 Denton, TX 76203-5017, USA*.

RI. THEORY

THURSDAY, JUNE 23, 2011 – 1:30 pm

Room: 1015 McPHERSON LAB

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

RI01 *INVITED TALK* **30 min 1:30**

COMPOSITE APPROACHES FOR AB INITIO SPECTROSCOPY: THE CCN, CCSb, AND HNNO RADICALS

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

RI02 **15 min 2:05**

EMPLOYING DIFFUSION MONTE CARLO IN THE CALCULATION OF MINIMIZED ENERGY PATHS OF THE $CH_3^+ + H_2 \leftrightarrow CH_5^+ \leftrightarrow CH_3^+ + H_2$ REACTION AND ITS ISOTOPIC VARIANTS

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

RI03 **15 min 2:22**

POTENTIAL ENERGY SURFACES OF M+NG, M = K, RB, CS AND NG = HE, NE, AR

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

RI04 **15 min 2:39**

A QUANTUM CHEMICAL STUDY OF XH AND XH_2 (X=Be,C,N,O): $2s^2$ RECOUPLED PAIR BONDING

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

RI05 **15 min 2:56**

COMPUTATIONAL AND SPECTROSCOPIC STUDY OF THE B-N DATIVE BOND IN AMMONIA BORANE

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

RI06 **15 min 3:13**

EXCITED STATES IN SOLUTION AT EOM-CCSD LEVEL WITH THE POLARIZABLE CONTINUUM MODEL OF SOLVATION

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

Intermission

RI07 **15 min 3:45**

EXPLORING TRANSITION METAL CATALYZED REACTIONS VIA AB INITIO REACTION PATHWAYS

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

RI08 **15 min 4:02**

NON-PRODUCT SMOLYAK GRIDS FOR COMPUTING SPECTRA: HOW AND WHY?

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

RI09 **15 min 4:19**

USING A NON-PRODUCT QUADRATURE GRID TO COMPUTE THE VIBRATIONAL SPECTRUM OF C_2H_4

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

RI10 **15 min 4:36**

PROGRESS TOWARDS THE ACCURATE CALCULATION OF ANHARMONIC VIBRATIONAL STATES OF FLUXIONAL MOLECULES AND CLUSTERS WITHOUT A POTENTIAL ENERGY SURFACE

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

RI11 **15 min 4:53**

HOW LIGAND PROPERTIES AFFECT THE FORMATION AND CHARACTERISTICS OF RECOUPLED PAIR BONDS

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

RI12 **15 min 5:10**

A QUANTUM CHEMICAL STUDY OF THE STRUCTURE AND CHEMISTRY OF $HZnCH_3$, A TRANSITION METAL COMPOUND WITH $4s^2$ RECOUPLED PAIR BONDING

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

RI13 **15 min 5:27**

THE SEARCH FOR AN OBSERVABLE HELIUM COMPLEX

ADRIAN M. GARDNER, TIMOTHY G. WRIGHT, *School of Chemistry, University of Nottingahm, University Park, Nottingham, NG7 2RD, United Kingdom*; and COREY J. EVANS, *Department of Chemistry, University of Leicester, University Road, Leicester, LE1 7RH, United Kingdom*.

RJ. RADICALS AND IONS

THURSDAY, JUNE 23, 2011 – 1:30 pm

Room: 2015 McPHERSON LAB

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

RJ01 **15 min 1:30**

DEHYROGENATION OF ETHYLENE: SPECTROSCOPY AND STRUCTURES OF La(C_2H_2) AND La(C_4H_6) COMPLEXES

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

RJ02 **15 min 1:47**

DEHYDROGENATION AND C-H BOND INSERTION OF PROPENE: La(η^2-C_3H_4) AND HLa(η^3-C_3H_5)

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

RJ03 **15 min 2:04**

OBSERVATION OF TWO La(C_3H_2) ISOMERS FORMED BY DEHYDROGENATION OF PROPYNE

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

RJ04 **15 min 2:21**

VIBRONIC SPECTROSCOPY OF THE PHENYLCYANOMETHYL RADICAL

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

RJ05 **15 min 2:38**

SPECTROSCOPIC IDENTIFICATION OF ISOMERIC TRIMETHYLBENZYL RADICALS GENERATED IN CORONA DISCHARGE OF TETRAMETHYLBENZENE

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

RJ06 **15 min 2:55**

INFRARED SPECTRA OF PRODUCTS OF THE ULTRAVIOLET AND VACUUM ULTRAVIOLET IRRADIATION OF BENZENE TRAPPED IN SOLID NEON

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

Intermission

RJ07 **15 min 3:30**

INFRARED SPECTROSCOPY OF PROTONATED MIXED BENZENE-WATER CLUSTERS

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

RJ08 **15 min 3:47**

MASS-ANALYZED THRESHOLD IONIZATION AND STRUCTURES OF M_3C_2(M=Sc, La)

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

RJ09 **15 min 4:04**

VIBRATIONAL AND GEOMETRIC STRUCTURES OF La_3C_2O AND $La_3C_2O^+$ FROM MASSE-ANALYZED THRESHOLD IONIZATION

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

RJ10 **15 min 4:21**

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

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

RJ11 **15 min 4:38**

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

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

RJ12 **15 min 4:55**

VIBRATIONALLY MEDIATED ELECTRON CAPTURE IN THE $CO_2(H_2O)_6$ ANION

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

RJ13 **15 min 5:12**

INFRARED PREDISSOCIATION SPECTROSCOPY OF H_2-TAGGED DICARBOXYLIC ACID ANIONS

ARRON B. WOLK, *Chemistry Laboratory, Yale University, P.O. Box 208107, New Haven, CT 06520*; MICHAEL Z. KAMRATH, *Chemistry Laboratory, Yale University, P.O. Box 208107, New Haven, CT 06520*; CHRISTOPHER M. LEAVITT, *Chemistry Laboratory, Yale University, P.O. Box 208107, New Haven, CT 06520*; and MARK A. JOHNSON, *Chemistry Laboratory, Yale University, P.O. Box 208107, New Haven, CT 06520*.

FA. MINI-SYMPOSIUM: THE THz COSMOS

FRIDAY, JUNE 24, 2011 – 8:30 am

Room: 160 MATH ANNEX

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

FA01 *INVITED TALK* **30 min 8:30**

EXPLORING NEW SPECTRAL WINDOWS WITH THE HERSCHEL SPACE OBSERVATORY

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

FA02 **15 min 9:05**

HERSCHEL OBSERVATIONS OF EXTRA-ORDINARY SOURCES (HEXOS): ANALYSIS OF THE HIFI 1.2 THZ WIDE SPECTRAL SURVEY TOWARD ORION KL

N. R. CROCKETT, E. A. BERGIN, S. WANG, *Department of Astronomy, University of Michigan, 500 Church Street, Ann Arbor, MI 48109, USA*; G. BLAKE, M. EMPRECHTINGER, D. LIS, *California Institute of Technology, Cahill Center for Astronomy and Astrophysics 301-17, Pasadena, CA 91125 USA*; H. GUPTA, J. PEARSON, S. YU, *Jet Propulsion Laboratory, Caltech, Pasadena, CA 91109, USA*; T. BELL, J. CERNICHARO, *Centro de Astrobiología (CSIC/INTA), Laboratiorio de Astrofísica Molecular, Ctra. de Torrejón a Ajalvir, km 4 28850, Torrejón de Ardoz, Madrid, Spain*; S. LORD, *Infrared Processing and Analysis Center, California Institute of Technology, MS 100-22, Pasadena, CA 91125*; R. PLUME, *Department of Physics and Astronomy, University of Calgary, 2500 University Drive NW, Calgary, AB T2N 1N4, Canada*; P. SCHILKE, *Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany*; and F. VAN DER TAK, *SRON Netherlands Institute for Space Research, PO Box 800, 9700 AV, Groningen, The Netherlands*.

FA03 **15 min 9:22**

DETECTION OF OH^+ AND H_2O^+ TOWARD ORION KL

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

[a]A part of this work was performed at the Jet Propulsion Laboratory, California Institute of Technology under contract with the National Aeronautics and Space Administration.

FA04 **15 min 9:39**

IS WATER ICE THE PRECURSOR TO OH^+ AND H_2O^+ IN ORION KL?

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

Intermission

FA05 **15 min 10:10**

REACHING THE LINE CONFUSION LIMIT: ANALYSIS OF THE λ=1.3 mm SPECTRUM OF ORION-KL

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

FA06 **15 min 10:27**

^{15}N/^{14}N RATIO DETERMINATION IN THE ISM WITH HERSCHEL WITH HIGH RESOLUTION SPECTROSCOPY OF NITROGEN RADICALS

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

FA07 **15 min 10:44**

THZ SPECTROSCOPY OF ^{13}C ISOTOPIC SPECIES OF A "WEED": ACETALDEHYDE

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

FA08 **15 min 11:01**

THE ROTATIONAL SPECTRUM OF $^{13}CH_3NH_2$ UP TO 1 THz

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

FA09 **10 min 11:18**

THE EXTENDED SPECTROSCOPIC DATABASE ON FORMAMIDE: PARENT, ^{13}C AND DEUTERATED SPECIES UP TO 1 THz

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

FA10 ***Post-deadline Abstract*** **10 min 11:30**

MONTE CARLO MODELING OF GAS-GRAIN CHEMISTRY IN STAR-FORMING REGIONS

A.I. VASYUNIN, E. HERBST, *The Ohio State University*.

FB. THEORY

FRIDAY, JUNE 24, 2011 – 8:30 am

Room: 170 MATH ANNEX

Chair: JOHN HERBERT, The Ohio State University, Columbus, Ohio

FB01 **15 min 8:30**

AUGER ELECTRONS VIA K_α X-RAY LINES OF PLATINUM COMPOUNDS FOR NANOTECHNOLOGICAL APPLICATIONS

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

FB02 **15 min 8:47**

A QUANTUM CHEMICAL EXPLORATION OF THE SF_nO SERIES ($n = 1 - 5$): AN ATOM-BY-ATOM APPROACH

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

FB03 **10 min 9:04**

A COMPUTATIONAL INVESTIGATION OF c-C_3H_2...HX(X = F, Cl, Br) H-BONDED COMPLEXES

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

FB04 **15 min 9:16**

ELECTRONIC STRUCTURE OF ETHYNYL SUBSTITUTED CYCLOBUTADIENES

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

FB05 **15 min 9:33**

AB INITIO INVERSTAGATION OF THE EXCITED STATES OF NUCLEOBASES AND NUCLEOSIDES

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

FB06 **15 min 9:50**

APPLICATIONS OF PATH INTEGRAL LANGEVIN DYNAMICS TO WEAKLY BOUND CLUSTERS AND BIOLOGICAL MOLECULES

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

Intermission

FB07 **15 min** **10:30**

INTERPRETATION OF THE IR/UV SPECTRA OF Ac-Trp-Tyr-NH_2 and Ac-Trp-Tyr-Ser-NH_2 USING MOLECULAR DYNAMICS AND AB INITIO METHODS.[a]

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

[a]Work supported in part by NSF CHE-0911117

FB08 **15 min** **10:47**

APPLICATION OF EFFECTIVE FRAGMENT POTENTIAL METHOS TO THE REDOX POTENTIAL OF GREEN FLUORESCENT PROTEIN

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

FB09 **15 min** **11:04**

VIBRONIC COUPLING IN ASYMMETRIC DIMERS: GENERALIZATION OF THE FULTON-GOUTERMAN APPROACH

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

FB10 ***Post-deadline Abstract*** **15 min** **11:21**

PREDICTION OF FUNDAMENTAL VIBRATIONAL FREQUENCIES AND INFRARED INTENSITIES: A BENCHMARK STUDY

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

FB11 ***Post-deadline Abstract*** **10 min** **11:38**

VIBRATIONAL CORRECTIONS TO MOLECULAR PROPERTIES: SECOND-ORDER VIBRATIONAL PERTURBATION THEORY VS VARIATIONAL COMPUTATIONS

MICHAEL E. HARDING, JUANA VÁZQUEZ, JOHN F. STANTON, *Institute for Theoretical Chemistry, Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, TX 78712 , USA*; GREGOR DIEZEMANN, and JÜRGEN GAUSS, *Institut für Physikalische Chemie, Universität Mainz, Jakob-Welder-Weg 11, D-55128 Mainz, Germany*.

FC. INFRARED/RAMAN

FRIDAY, JUNE 24, 2011 – 8:30 am

Room: 1000 McPHERSON LAB

Chair: MANFRED WINNEWISSER, The Ohio State University, Columbus, OH

FC01 **15 min 8:30**

NEW METHOD OF FITTING EXPERIMENTAL RO-VIBRATIONAL INTENSITIES TO THE DIPOLE MOMENT FUNCTION: APPLICATION TO HCl

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

FC02 **15 min 8:47**

EXTENSIVE AND HIGHLY ACCURATE LINE LISTS FOR HYDROGEN HALIDES

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

FC03 **15 min 9:04**

NEAR-INFRARED OVERTONE SPECTROSCOPY OF TRITIATED WATER

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

FC04 **15 min 9:21**

ANALYSIS OF THE VIBRATIONAL SPECTRA OF $P_3N_3(OCH_2CF_3)_6$ AND $P_4N_4(OCH_2CF_3)_8$

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

FC05 **15 min 9:38**

GAS PHASE THZ SPECTROSCOPY OF ORGANOSULFIDE AND ORGANOPHOSPHOROUS COMPOUNDS USING A SYNCHROTRON SOURCE

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

Intermission

FC06 **15 min 10:15**

HIGH RESOLUTION INFRARED SPECTRA OF SPIROPENTANE, (C_5H_8)

J. E. PRICE AND K. COULTERPAK, *DEPARTMENT OF CHEMISTRY, OREGON STATE UNIVERSITY, CORVALLIS, OR 97332-4003, U.S.A.*; T. MASIELLO, *DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY, CALIFORNIA STATE UNIVERSITY, EAST BAY, HAYWARD, CA 94542 U.S.A.*; J. W. NIBLER, *DEPARTMENT OF CHEMISTRY, OREGON STATE UNIVERSITY, CORVALLIS, OR 97332-4003 U.S.A.*; A. WEBER, *OPTICAL TECHNOLOGY DIVISION, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY, GAITHERSBURG, MD 20899, U.S.A.*; A. MAKI, *15012 24th AVE., S.E. MILL CREEK, WA 98012 U.S.A.*; AND T. A. BLAKE, *PACIFIC NORTHWEST NATIONAL LABORATORY, P.O. BOX 999, MAIL STOP K8-88, RICHLAND, WA 99355 U.S.A*.

FC07 **5 min 10:32**

C-H STRETCH OVERTONE SPECTRA OF FLUORINATED ETHERS

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

FC08 ***Post-deadline Abstract*** **15 min 10:39**

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

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

FC09 ***Post-deadline Abstract*** **15 min 10:56**

ROTATIONALLY-RESOLVED INFRARED SPECTROSCOPY OF THE POLYCYCLIC AROMATIC HYDROCARBON PYRENE ($C_{16}H_{10}$) IN THE MID-INFRARED USING A QUANTUM CASCADE LASER-BASED CAVITY RINGDOWN SPECTROMETER

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

FC10 **10 min 11:13**

VIBRATIONAL SPECTROSCOPIC STUDY ON SOME HOFMANN TYPE CLATHRATES: M(2-(1-CYCLOHEXENYL)ETHYLAMINE)$_2$ Ni(CN)$_4$.2BENZENE (M =Ni AND Cd)

TEKİN İZG; *DEPARTMENT OF PHYSICS, ARTS AND SCIENCE FACULTY, İNÖNÜ UNIVERSITY, MALATYA, 44069, TURKEY*; CEMAL PARLAK, *DEPARTMENT OF PHYSICS, ARTS AND SCIENCE FACULTY, DUMLUPINAR UNIVERSITY, KÜTAHYA, 43100, TURKEY*; MUSTAFA SENYEL, *DEPARTMENT OF PHYSICS, SCIENCE FACULTY, ANADOLU UNIVERSITY, ESKİŞEHİR, 26470, TURKEY*.

FD. MINI-SYMPOSIUM: FUNDAMENTAL PHYSICS

FRIDAY, JUNE 24, 2011 – 8:30 am

Room: 1015 McPHERSON LAB

Chair: TREVOR SEARS, Brookhaven National Laboratory, Upton, New York

FD01 *INVITED TALK* **30 min 8:30**

TIME-DOMAIN MW SPECTROSCOPY: FUNDAMENTAL PHYSICS FROM MOLECULAR ROTATION

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

FD02 **15 min 9:05**

HIGH PRECISION UV MEASUREMENTS IN CO, TOWARDS A LABORATORY TEST OF THE TIME-INVARIANCE OF μ.

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

FD03 **15 min 9:22**

PROSPECTS FOR RAPID DECELERATION OF DIATOMIC MOLECULES WITH OPTICAL BICHROMATIC FORCES

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

FD04 **15 min 9:39**

DECELERATION AND TRAPPING OF HEAVY DIATOMIC MOLECULES FOR PRECISION MEASUREMENTS

J. E. VAN DEN BERG, S. N. HOEKMAN TURKESTEEN, E. B. PRINSEN, S. HOEKSTRA, *Zernikelaan 25, 9747 AA, Groningen, The Netherlands*.

FD05 **15 min 9:56**

INVESTIGATION OF THE USE OF HE – DIATOMIC VAN DER WAALS COMPLEXES AS A PROBE OF TIME-REVERSAL VIOLATION

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

Intermission

FD06 **15 min 10:30**

FREQUENCY COMB VELOCITY MODULATION SPECTROSCOPY

KEVIN C. COSSEL, LAURA C. SINCLAIR, TYLER COFFEY, ERIC CORNELL, and JUN YE, *JILA, National Institute of Standards and Technology and University of Colorado Department of Physics, University of Colorado, Boulder, Colorado 80309-0440, USA*.

FD07 **15 min 10:47**

OPTICAL PULSE-SHAPING FOR INTERNAL COOLING OF MOLECULAR IONS

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

FD08 ***Post-deadline Abstract*** **15 min 11:04**

RELATIVISTIC COMBINED PSEUDOPOTENTIAL−RESTORATION METHOD FOR STUDYING MULTITUDE OF PROPERTIES IN HEAVY-ATOM SYSTEMS[a]

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

[a]This work is supported by the RFBR Grant No. 09–03–01034

FD09 ***Post-deadline Abstract*** **15 min 11:21**

SPECTROSCOPIC CHARATERIZATION OF ThF AND THE LOW-LYING STATES OF ThF^+

BEAU J. BARKER, IVAN O. ANTONOV, and MICHAEL C. HEAVEN, *Department of Chemistry, Emory University, Atlanta, GA 30322*.

FE. MATRIX/CONDENSEDPHASE

FRIDAY, JUNE 24, 2011 – 8:30 am

Room: 2015 McPHERSON LAB

Chair: JAY C. AMICANGELO, Penn State Erie, The Behrend College, Erie, Pennsylvania

FE01 **15 min 8:30**

TOWARD A CONTINUOUS-WAVE SOLID HYDROGEN RAMAN LASER FOR MOLECULAR SPECTROSCOPY APPLICATIONS

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

FE02 **15 min 8:47**

PHOTODISSOCIATION OF FORMIC ACID ISOLATED IN SOLID PARAHYDROGEN

DAVID T. ANDERSON, LEIF O. PAULSON, *Department of Chemistry, University of Wyoming, Laramie, WY 82071-3838*.

FE03 **15 min 9:04**

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

F. LACKNER, M. THEISEN, and W.E. ERNST, *Institute of Experimental Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria*.

FE04 **15 min 9:21**

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

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

FE05 **15 min 9:38**

LASER SPECTROSCOPY OF HYDROGEN PEROXIDE EMBEDDED IN HELIUM NANODROPLETS

CHRISSY J. KNAPP, PAUL L. RASTON, and WOLFGANG JÄGER, *Department of Chemistry, University of Alberta, Edmonton, AB, Canada T6G 2G2*.

Intermission

FE06 ***Post-deadline Abstract*** **10 min 10:15**

PYRIDINE AGGREGATION IN HELIUM NANODROPLETS

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

FE07 ***Post-deadline Abstract*** **15 min 10:27**

IR SPECTROSCOPY STUDY ON THE $(HCl)_n(H_2O)_m$ AGGREGATION IN HELIUM NANODROPLETS

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

FE08 ***Post-deadline Abstract*** **10 min 10:44**

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

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

FE09 ***Post-deadline Abstract*** **15 min 10:56**

INELASTIC SCATTERING OF RADICALS FROM A LIQUID SURFACE

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

AUTHOR INDEX

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